



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 02:37 am BST

PDB ID : 3KOY  
Title : Crystal Structure of ornithine 4,5 aminomutase in complex with ornithine (Aerobic)  
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.  
Deposited on : 2009-11-14  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

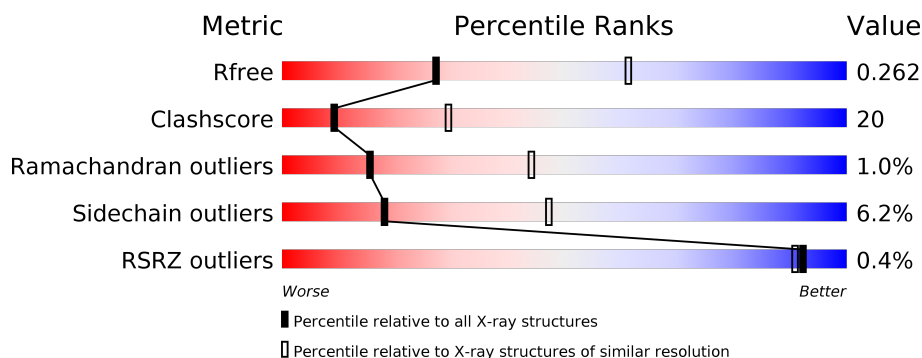
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	763	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>61%</span> <span>32%</span> <span>• 5%</span> </div> </div>
1	B	763	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>58%</span> <span>34%</span> <span>• 5%</span> </div> </div>
1	C	763	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>59%</span> <span>33%</span> <span>• 5%</span> </div> </div>
1	D	763	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>62%</span> <span>31%</span> <span>• 5%</span> </div> </div>
2	E	121	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>54%</span> <span>36%</span> <span>• 9%</span> </div> </div>
2	F	121	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>61%</span> <span>26%</span> <span>• 9%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	121	
2	H	121	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	B12	A	1801	X	-	X	-
3	B12	B	1801	X	-	X	-
3	B12	C	1801	X	-	X	-
3	B12	D	1801	X	-	X	-
5	5AD	A	1500	X	-	-	-
5	5AD	B	1500	X	-	-	-
5	5AD	C	1500	X	-	-	-
5	5AD	D	1500	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26592 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 D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5634	3550	976	1075	33			
1	B	728	Total	C	N	O	S	0	0	0
			5665	3574	983	1074	34			
1	C	728	Total	C	N	O	S	0	0	0
			5654	3570	981	1069	34			
1	D	728	Total	C	N	O	S	0	0	0
			5664	3575	984	1071	34			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
A	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
A	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
A	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
A	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
A	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
A	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
A	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
A	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
A	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
A	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
A	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
A	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
A	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
B	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
B	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
B	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
B	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
B	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
B	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
B	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
B	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
B	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
B	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
B	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
B	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
B	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
C	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
C	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
C	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
C	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5

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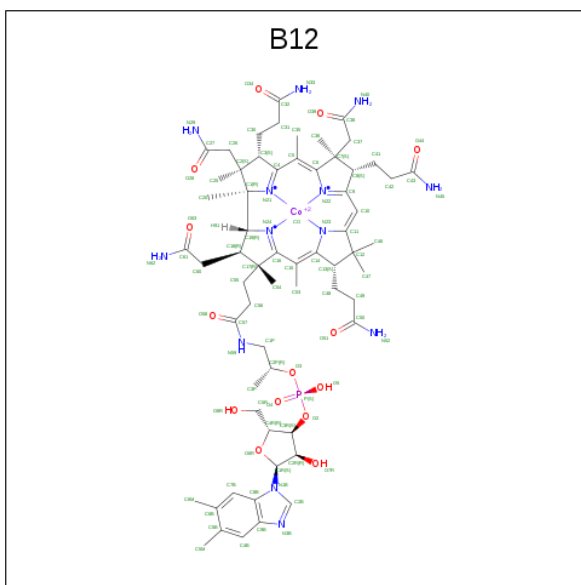
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
C	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
C	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
C	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
C	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
C	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
C	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
D	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
D	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
D	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
D	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
D	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
D	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
D	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
D	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
D	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
D	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
D	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
D	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
D	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

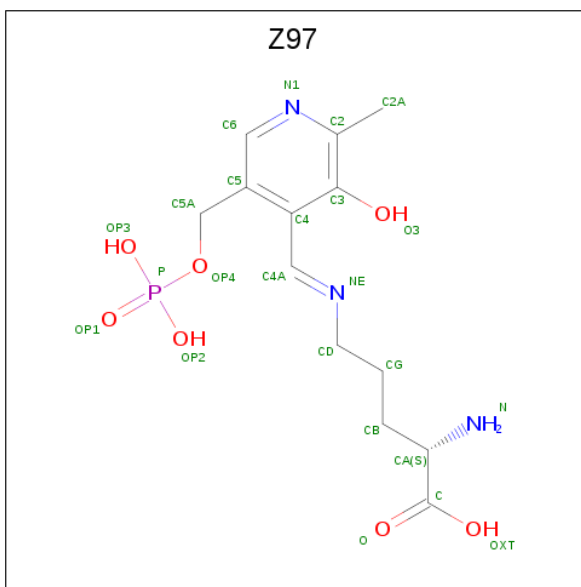
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			
2	F	110	Total	C	N	O	S	0	0	0
			863	542	153	164	4			
2	G	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			
2	H	110	Total	C	N	O	S	0	0	0
			860	541	153	162	4			

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



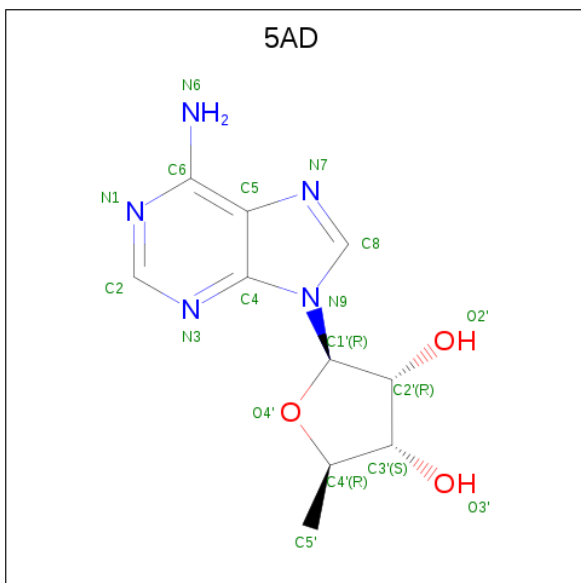
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 4 is (E)-N 5 -({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl} methylidene)-L-ornithine (three-letter code: Z97) (formula:  $C_{13}H_{20}N_3O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	B	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	C	1	Total	C	N	O	P	0	0
			24	13	3	7	1		
4	D	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).





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







I113
Q114
ILE
PHE
LYS
GLY
GLY
VAL
LYS

• Molecule 2: D-ornithine aminomutase S component



MET	LYS	ARG	ALA	D5	D6	F7	Q8	Q9	R10	L14	S18	D19	E20	E21	R25	R29	V34	I38	D39	L40	T46	P47	S52	V53	L54	L55	R56	M57	G58	F59	K65	K70	R74	G75	L76	M77	G78	K79	G82	H83	I84	Y85	Y86	K87	I88	E91
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S95	Y96	R97	E98	A99	G100	L101	A102	L103	Q114	ILE	PHE	LYS	GLY	VAL	LYS
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• Molecule 2: D-ornithine aminomutase S component



MET	LYS	ARG	ALA	D5	D6	F7	Q8	Q9	R10	R11	L17	E21	R25	F26	R27	E28	M29	V34	D35	P36	D39	L40	G41	P47	R51	S52	V53	M57	G58	F59	K65	D69	L76	M77	G78	K79	G82	H83	Y86	E98	A99	G100	L101	A102	L103
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K107	Y108	W109	D110	D111	Q114	ILE	PHE	LYS	GLY	GLY	VAL	LYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.52Å 233.22Å 124.14Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	60.37 – 2.80 64.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (60.37-2.80) 93.8 (64.70-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.183 , 0.263 0.183 , 0.262	Depositor DCC
$R_{free}$ test set	4265 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26592	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 13.10% 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: Z97, 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	0.43	0/5739	0.61	0/7776
1	B	0.44	0/5770	0.61	0/7809
1	C	0.43	0/5759	0.60	0/7796
1	D	0.44	0/5769	0.61	0/7808
2	E	0.44	0/872	0.59	0/1170
2	F	0.44	0/875	0.63	0/1174
2	G	0.42	0/872	0.58	0/1170
2	H	0.46	0/872	0.57	0/1170
All	All	0.43	0/26528	0.61	0/35873

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	5634	0	5544	217	0
1	B	5665	0	5629	238	0
1	C	5654	0	5621	223	0
1	D	5664	0	5636	231	0
2	E	860	0	865	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	863	0	867	30	0
2	G	860	0	865	42	0
2	H	860	0	865	34	0
3	A	91	0	87	24	0
3	B	91	0	87	22	0
3	C	91	0	87	26	0
3	D	91	0	87	33	0
4	A	24	0	18	0	0
4	B	24	0	18	4	0
4	C	24	0	18	2	0
4	D	24	0	18	3	0
5	A	18	0	8	3	0
5	B	18	0	8	4	0
5	C	18	0	9	2	0
5	D	18	0	8	2	0
All	All	26592	0	26345	1054	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 20.

The worst 5 of 1054 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)
2:E:5:ASP:HA	2:E:7:PHE:N	1.53	1.22
2:F:5:ASP:HA	2:F:7:PHE:N	1.61	1.13
1:A:43:MET:HE1	1:A:72:PRO:HA	1.30	1.09
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.36	1.07
1:A:306:GLU:HG3	1:A:307:ALA:H	0.87	1.03

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	722/763 (95%)	651 (90%)	61 (8%)	10 (1%)	11	34
1	B	722/763 (95%)	659 (91%)	56 (8%)	7 (1%)	15	44
1	C	722/763 (95%)	658 (91%)	58 (8%)	6 (1%)	19	49
1	D	722/763 (95%)	670 (93%)	49 (7%)	3 (0%)	34	66
2	E	108/121 (89%)	102 (94%)	5 (5%)	1 (1%)	17	46
2	F	108/121 (89%)	100 (93%)	6 (6%)	2 (2%)	8	26
2	G	108/121 (89%)	98 (91%)	8 (7%)	2 (2%)	8	26
2	H	108/121 (89%)	95 (88%)	12 (11%)	1 (1%)	17	46
All	All	3320/3536 (94%)	3033 (91%)	255 (8%)	32 (1%)	15	44

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	E	6	ASP
1	C	6	GLN
1	C	461	ASP
2	G	6	ASP

### 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	594/644 (92%)	574 (97%)	20 (3%)	37	71
1	B	602/644 (94%)	560 (93%)	42 (7%)	15	40
1	C	600/644 (93%)	558 (93%)	42 (7%)	15	40
1	D	602/644 (94%)	558 (93%)	44 (7%)	14	38
2	E	89/100 (89%)	83 (93%)	6 (7%)	16	43
2	F	90/100 (90%)	84 (93%)	6 (7%)	16	43
2	G	89/100 (89%)	83 (93%)	6 (7%)	16	43
2	H	89/100 (89%)	83 (93%)	6 (7%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2755/2976 (93%)	2583 (94%)	172 (6%)	18	47

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	VAL
1	C	497	VAL
1	D	668	THR
1	C	39	GLU
1	C	206	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	245	HIS
1	D	248	ASN
1	D	115	HIS
1	B	630	HIS
1	D	245	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	5AD	A	1500	3	17,20,20	2.09	4 (23%)	15,30,30	4.04	7 (46%)
3	B12	A	1801	1,5	80,101,101	1.09	4 (5%)	101,166,166	2.02	23 (22%)
3	B12	D	1801	1,5	80,101,101	1.12	6 (7%)	101,166,166	1.97	18 (17%)
5	5AD	B	1500	3	17,20,20	2.31	5 (29%)	15,30,30	4.57	7 (46%)
5	5AD	D	1500	3	17,20,20	2.28	6 (35%)	15,30,30	4.13	8 (53%)
3	B12	B	1801	1,5	80,101,101	1.10	5 (6%)	101,166,166	1.96	22 (21%)
4	Z97	C	767	-	20,24,24	2.70	6 (30%)	24,33,33	1.66	4 (16%)
4	Z97	A	767	-	20,24,24	2.72	8 (40%)	24,33,33	1.74	6 (25%)
4	Z97	B	767	-	20,24,24	2.52	6 (30%)	24,33,33	1.55	3 (12%)
5	5AD	C	1500	3	17,20,20	2.25	5 (29%)	15,30,30	4.14	8 (53%)
3	B12	C	1801	1,5	80,101,101	1.18	6 (7%)	101,166,166	2.17	19 (18%)
4	Z97	D	767	-	20,24,24	2.68	7 (35%)	24,33,33	1.95	6 (25%)

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	5AD	A	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
3	B12	A	1801	1,5	1/1/36/38	22/51/223/223	0/3/11/11
3	B12	D	1801	1,5	1/1/36/38	14/51/223/223	0/3/11/11
5	5AD	B	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
5	5AD	D	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
3	B12	B	1801	1,5	1/1/36/38	17/51/223/223	0/3/11/11
4	Z97	C	767	-	-	6/14/18/18	0/1/1/1
4	Z97	A	767	-	-	5/14/18/18	0/1/1/1
4	Z97	B	767	-	-	7/14/18/18	0/1/1/1
5	5AD	C	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
3	B12	C	1801	1,5	1/1/36/38	8/51/223/223	0/3/11/11
4	Z97	D	767	-	-	5/14/18/18	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	767	Z97	C4-C5	6.96	1.50	1.42
4	D	767	Z97	C4-C5	6.81	1.50	1.42
4	A	767	Z97	C4-C5	6.66	1.50	1.42
4	B	767	Z97	C4-C5	6.42	1.50	1.42
4	C	767	Z97	C4A-NE	5.38	1.45	1.27

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1500	5AD	C5'-C4'-C3'	12.46	128.78	115.70
5	C	1500	5AD	C5'-C4'-C3'	10.53	126.75	115.70
5	D	1500	5AD	C5'-C4'-C3'	10.12	126.33	115.70
5	A	1500	5AD	C5'-C4'-C3'	9.85	126.04	115.70
3	A	1801	B12	C1-C19-N24	9.39	116.81	106.24

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1500	5AD	C2'
5	A	1500	5AD	C3'
3	A	1801	B12	C19
3	D	1801	B12	C19
5	B	1500	5AD	C2'

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C54-C17-C55-C56
3	A	1801	B12	C18-C17-C55-C56
3	A	1801	B12	C56-C57-N59-C1P
3	A	1801	B12	C1P-C2P-O3-P

There are no ring outliers.

11 monomers are involved in 114 short contacts:

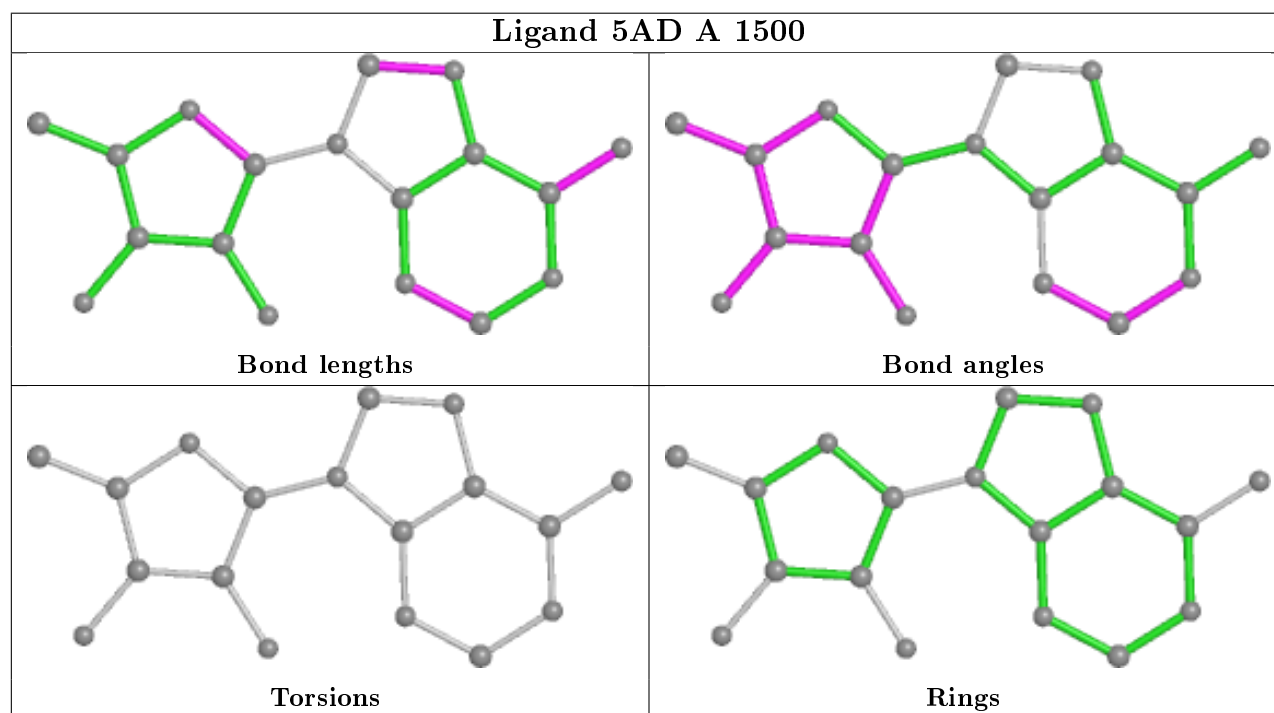
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1500	5AD	3	0
3	A	1801	B12	24	0
3	D	1801	B12	33	0
5	B	1500	5AD	4	0

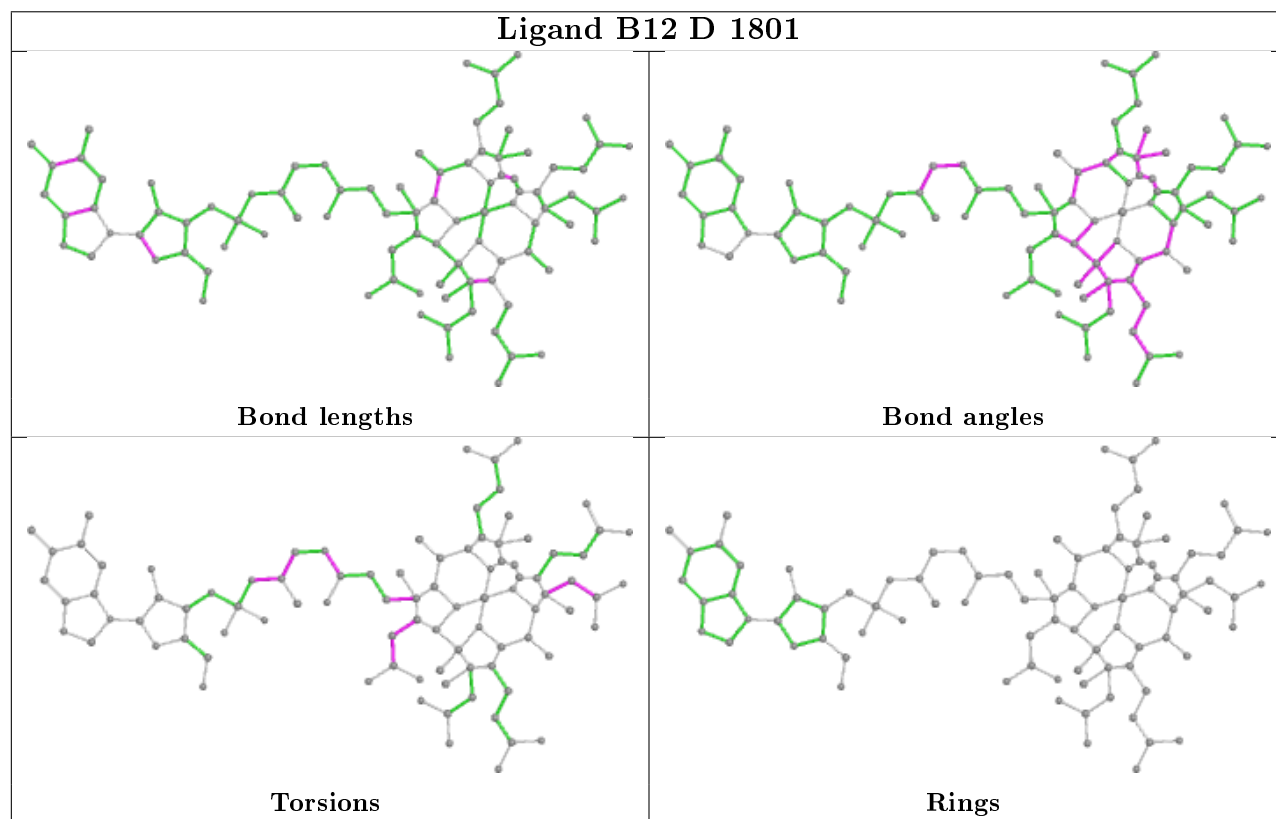
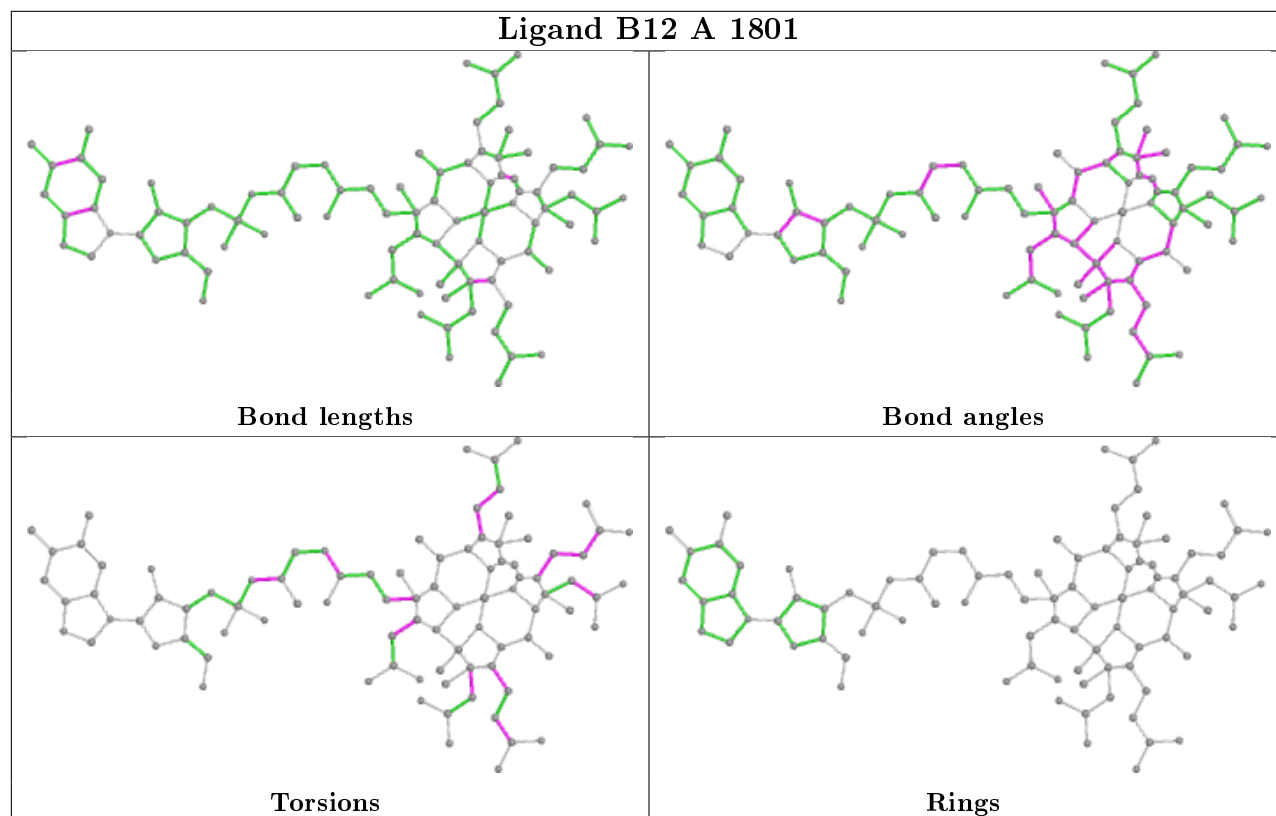
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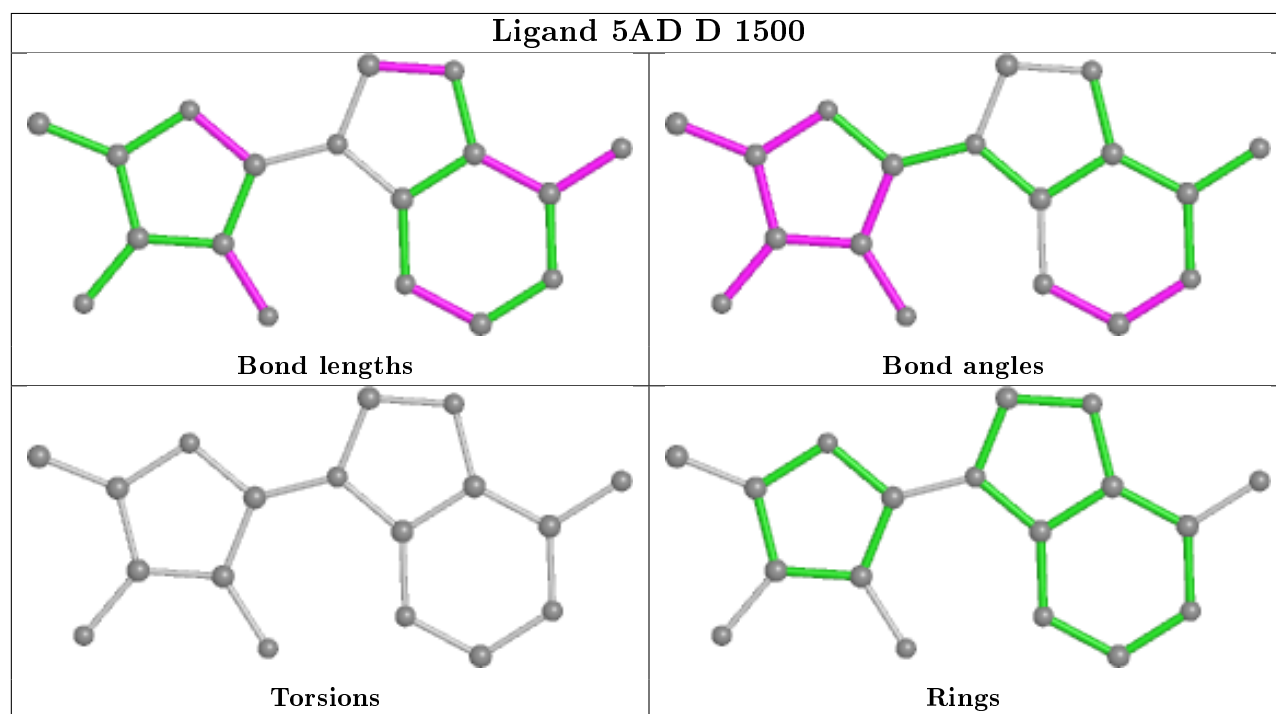
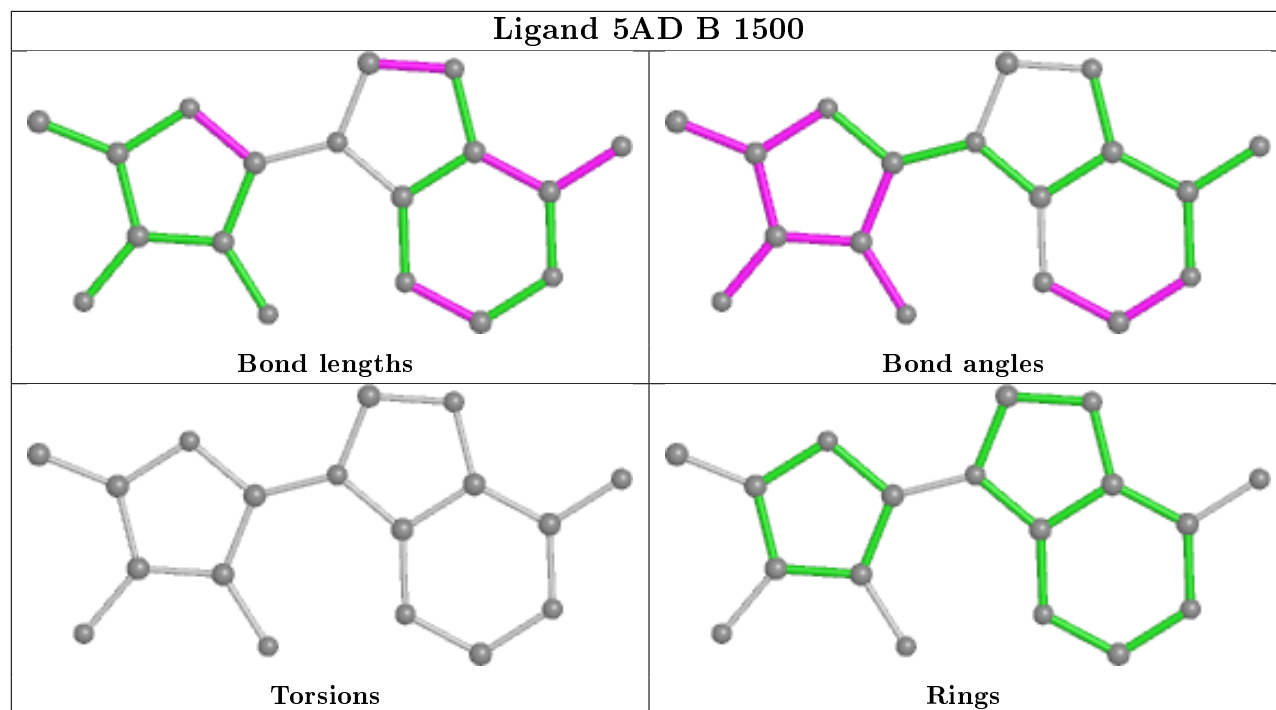
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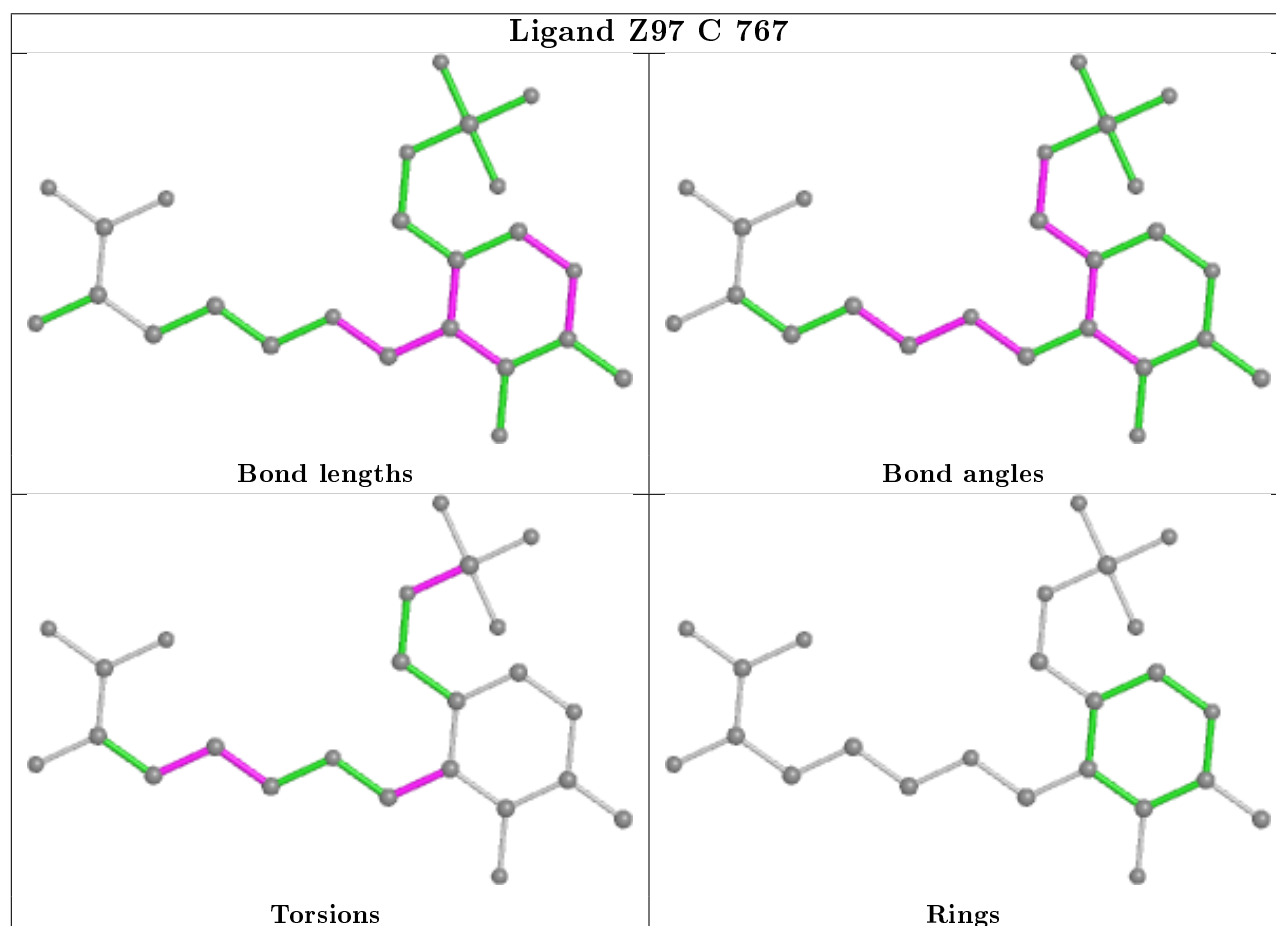
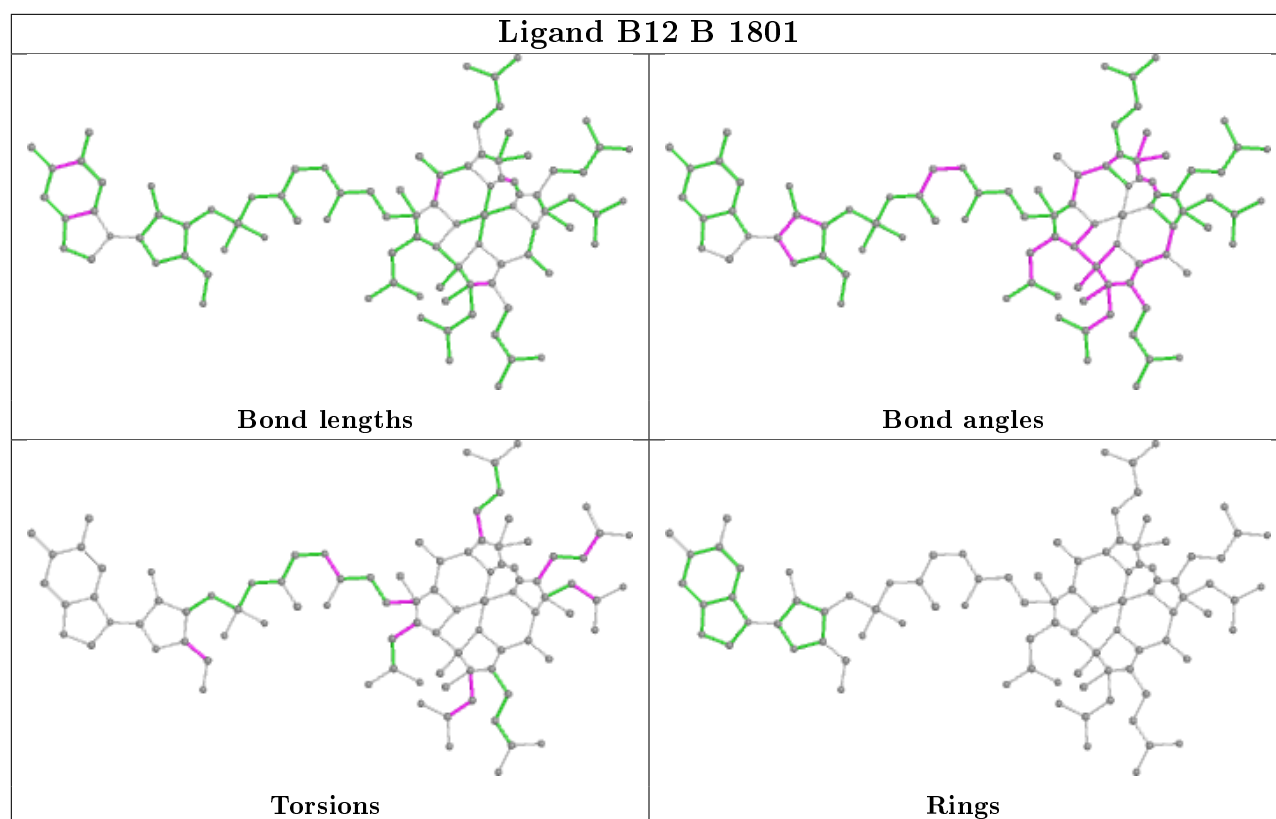
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1500	5AD	2	0
3	B	1801	B12	22	0
4	C	767	Z97	2	0
4	B	767	Z97	4	0
5	C	1500	5AD	2	0
3	C	1801	B12	26	0
4	D	767	Z97	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

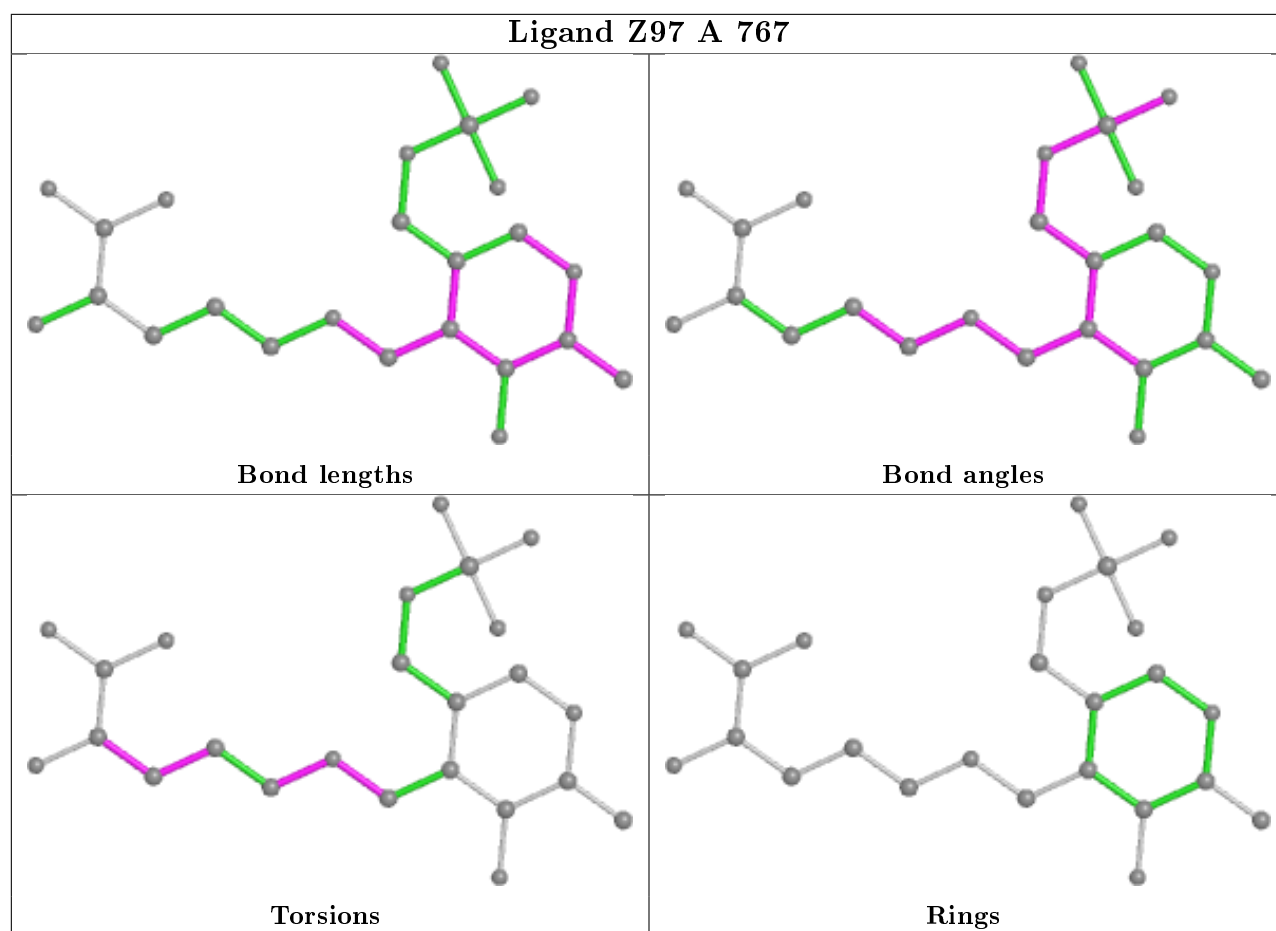




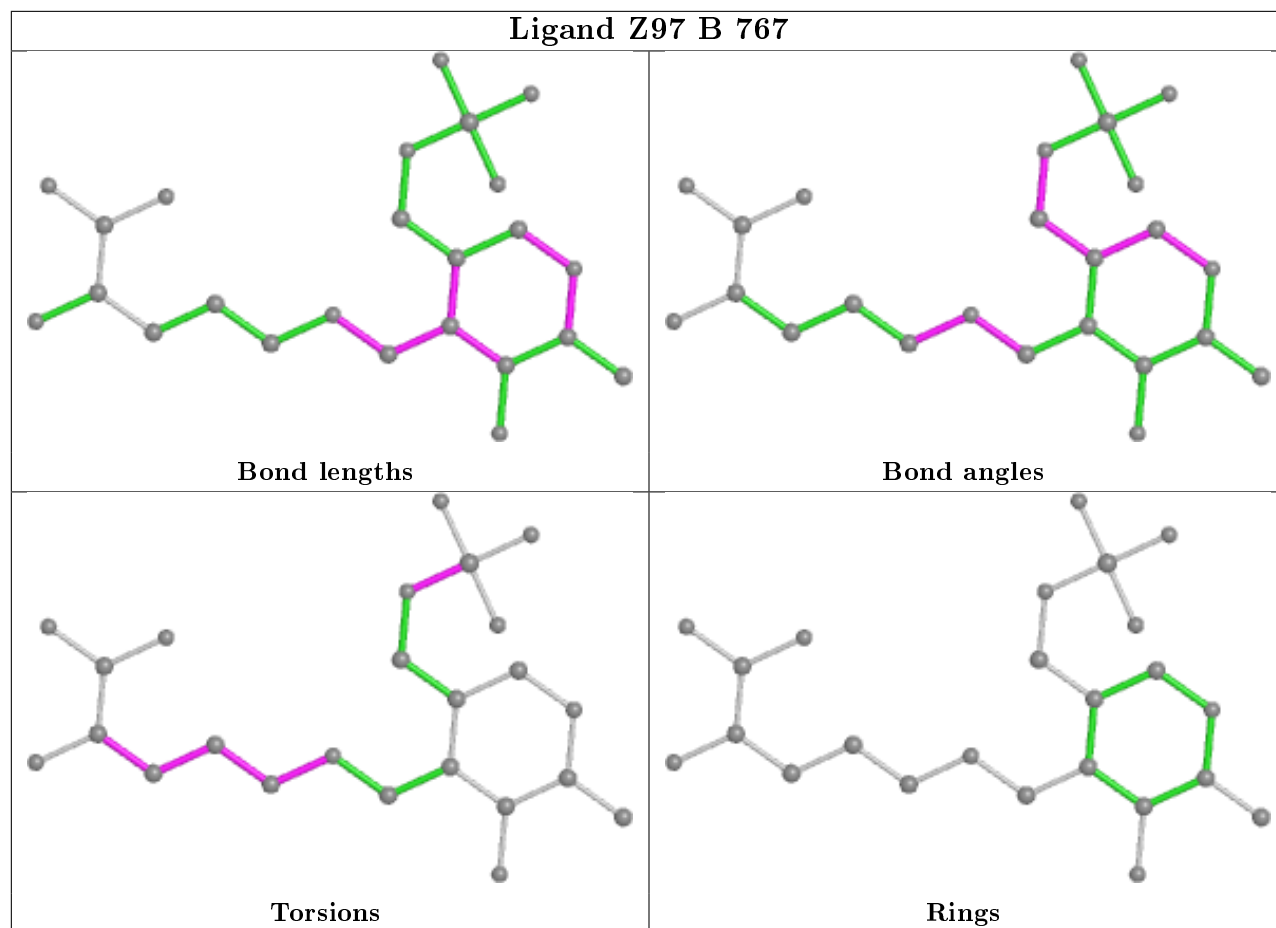




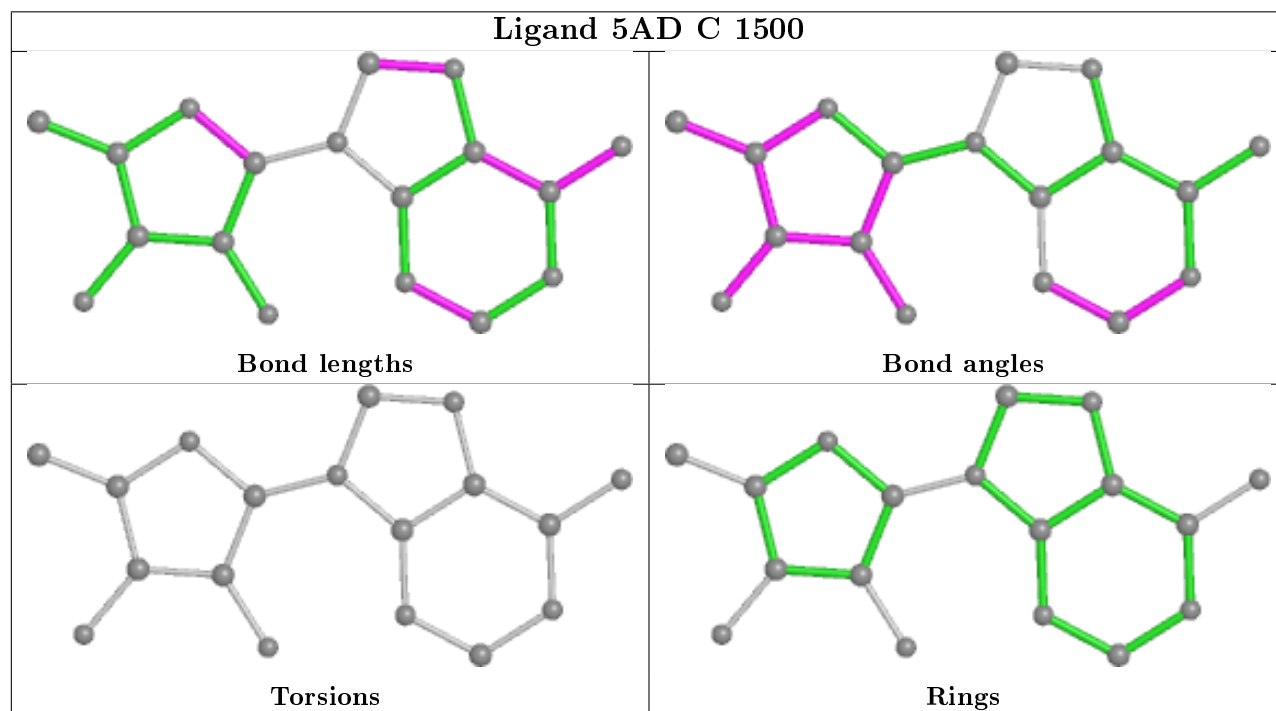


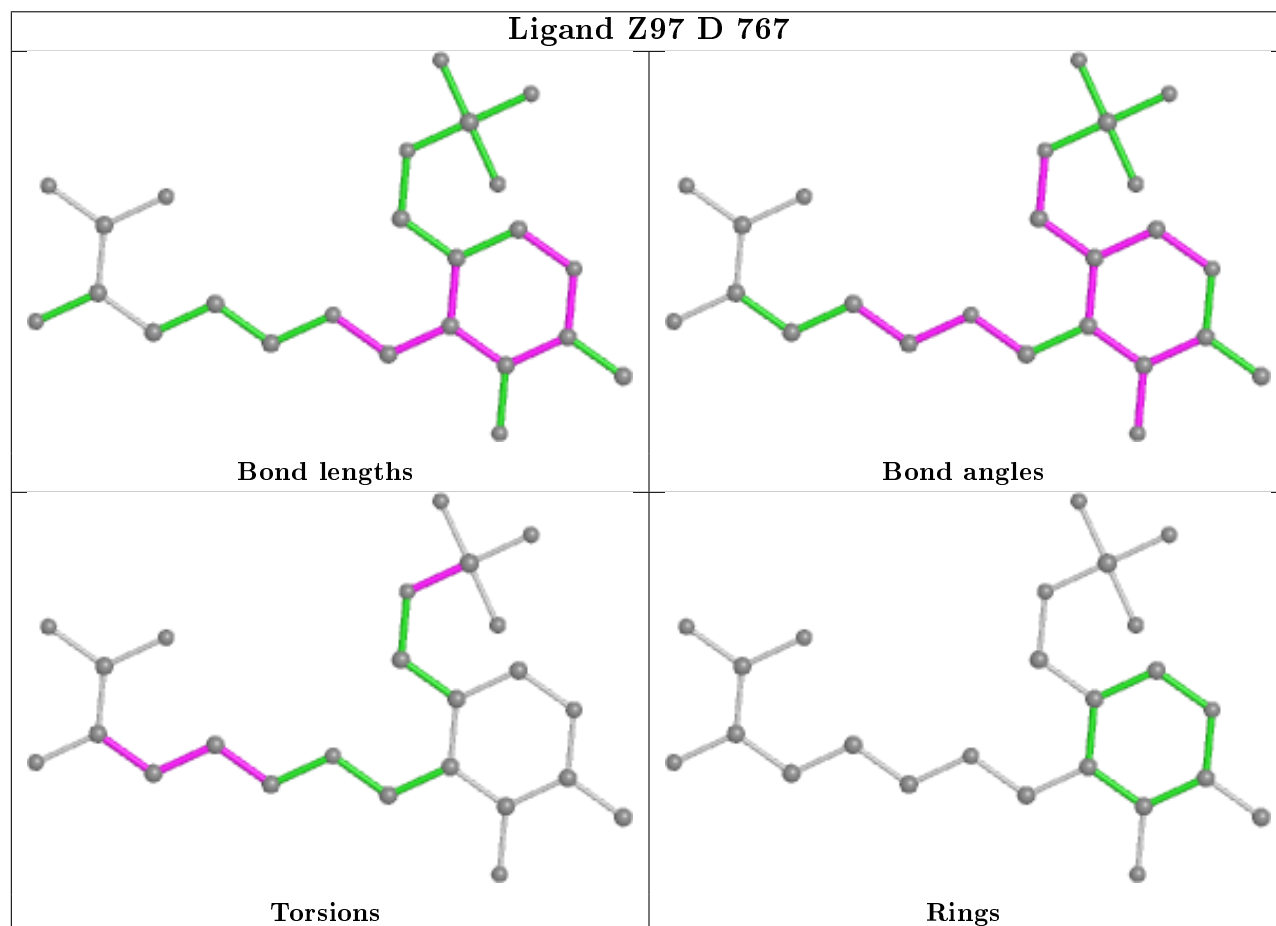
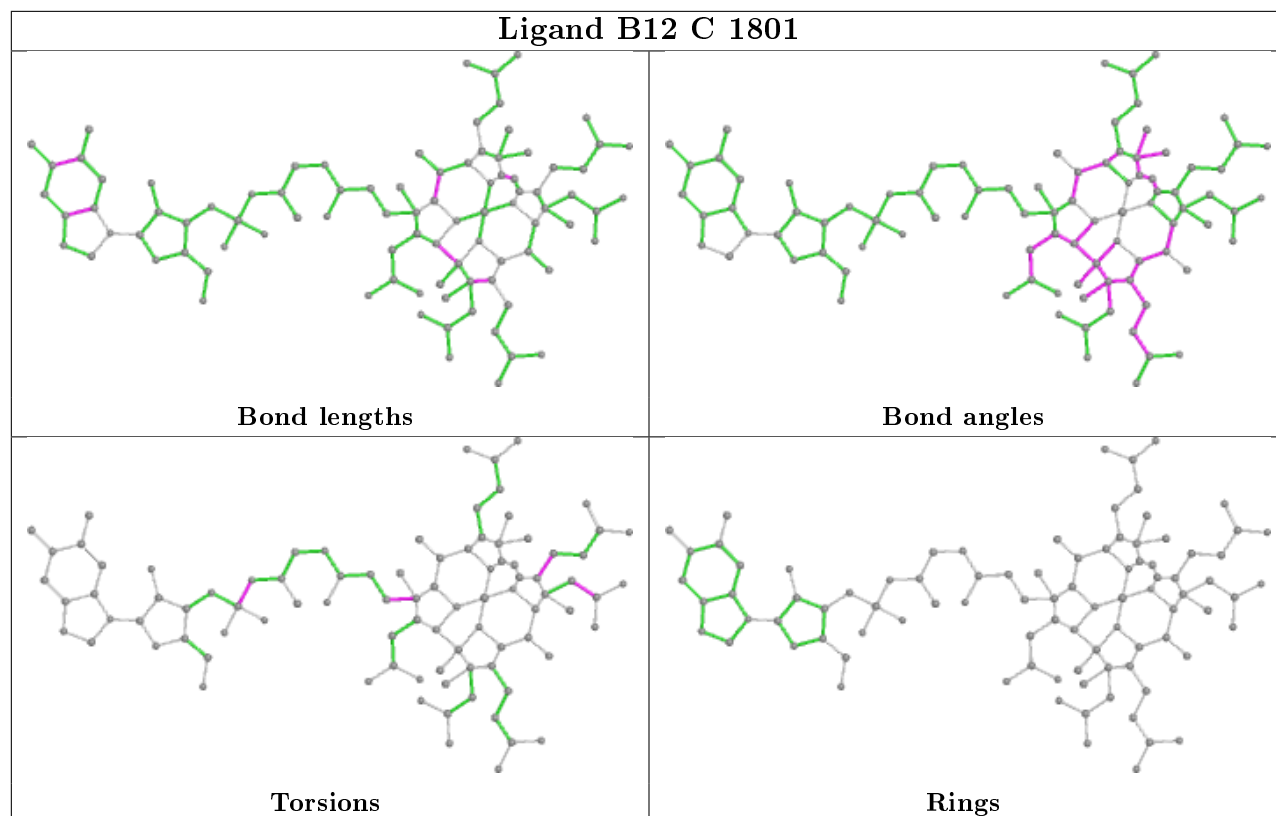


## Ligand Z97 B 767



## Ligand 5AD C 1500





## 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	728/763 (95%)	-0.41	7 (0%) 82 77	16, 34, 103, 118	0
1	B	728/763 (95%)	-0.59	0 100 100	15, 33, 66, 95	0
1	C	728/763 (95%)	-0.59	0 100 100	19, 38, 61, 83	0
1	D	728/763 (95%)	-0.46	8 (1%) 80 75	17, 32, 89, 104	0
2	E	110/121 (90%)	-0.45	0 100 100	25, 40, 62, 73	0
2	F	110/121 (90%)	-0.60	0 100 100	26, 38, 53, 72	0
2	G	110/121 (90%)	-0.46	0 100 100	32, 45, 69, 80	0
2	H	110/121 (90%)	-0.41	0 100 100	25, 38, 57, 86	0
All	All	3352/3536 (94%)	-0.51	15 (0%) 92 91	15, 36, 83, 118	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	710	ALA	3.4
1	D	647	VAL	2.9
1	D	714	GLY	2.8
1	A	717	ALA	2.6
1	A	617	GLU	2.2

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

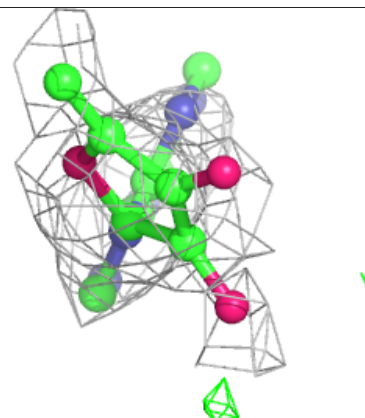
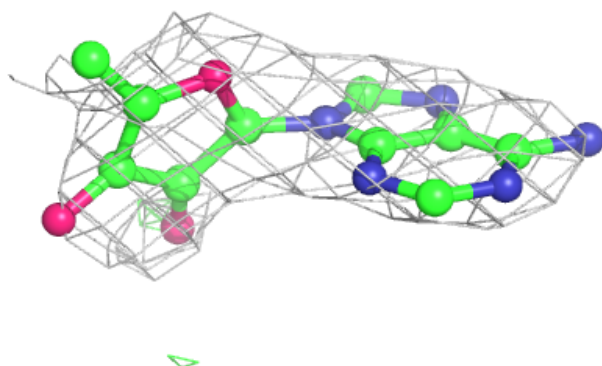
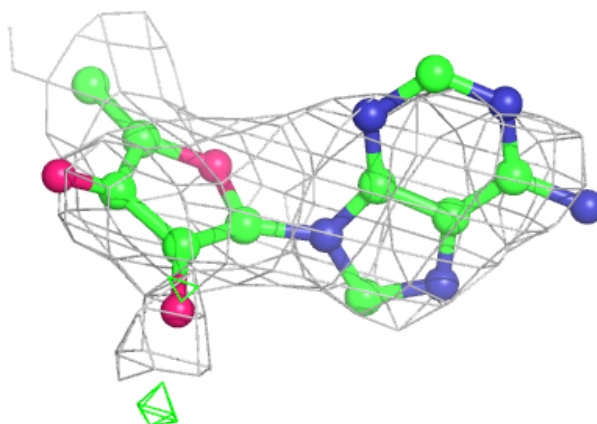
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	5AD	C	1500	18/18	0.86	0.24	78,87,94,97	0
5	5AD	B	1500	18/18	0.88	0.33	64,76,83,84	0
5	5AD	D	1500	18/18	0.92	0.22	48,60,65,66	0
3	B12	A	1801	91/91	0.93	0.27	57,87,98,99	0
5	5AD	A	1500	18/18	0.93	0.21	37,46,54,55	0
3	B12	D	1801	91/91	0.94	0.19	40,73,84,86	0
4	Z97	C	767	24/24	0.97	0.18	35,40,50,56	0
4	Z97	A	767	24/24	0.97	0.18	22,29,36,38	0
4	Z97	B	767	24/24	0.97	0.15	22,32,46,50	0
3	B12	B	1801	91/91	0.97	0.18	35,55,67,70	0
3	B12	C	1801	91/91	0.97	0.16	20,34,46,51	0
4	Z97	D	767	24/24	0.97	0.17	25,36,41,44	0

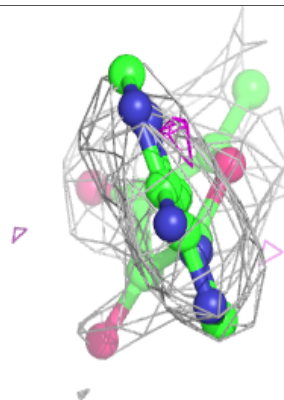
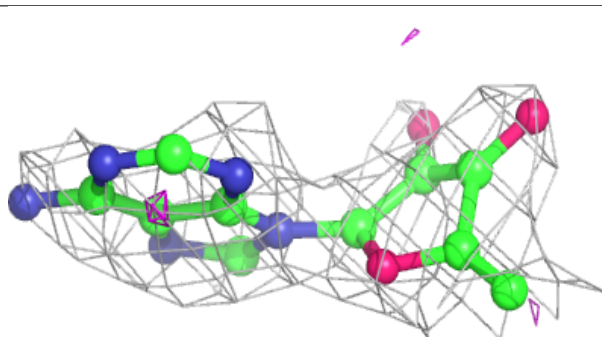
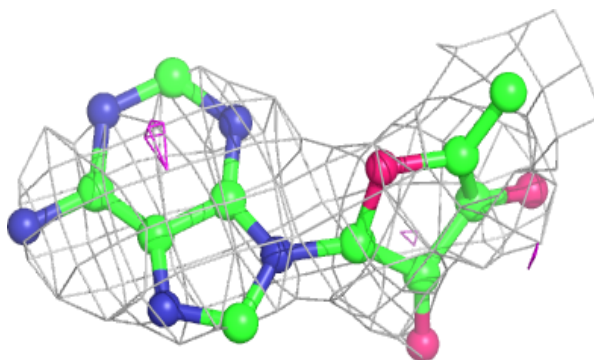
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5AD C 1500:**

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

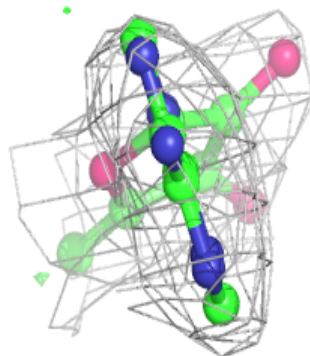
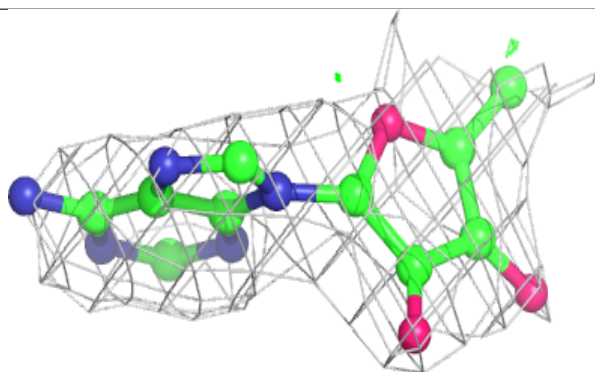
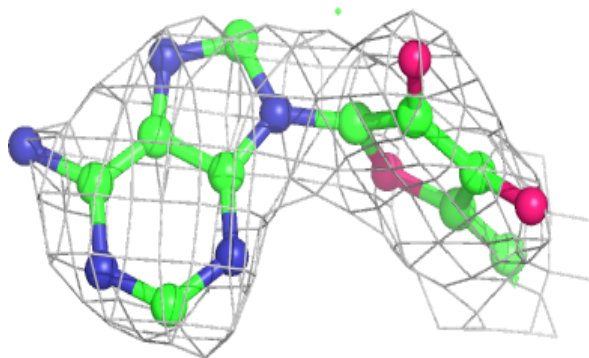
**Electron density around 5AD B 1500:**

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and green (positive)

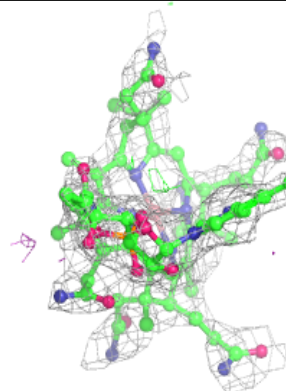
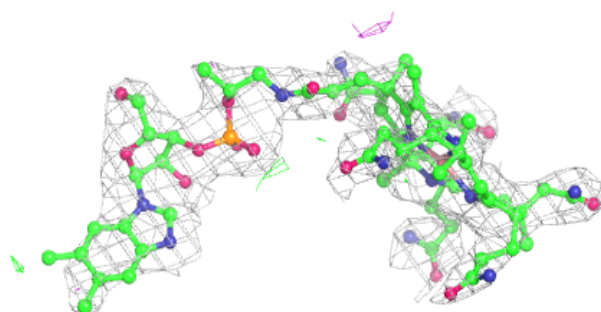
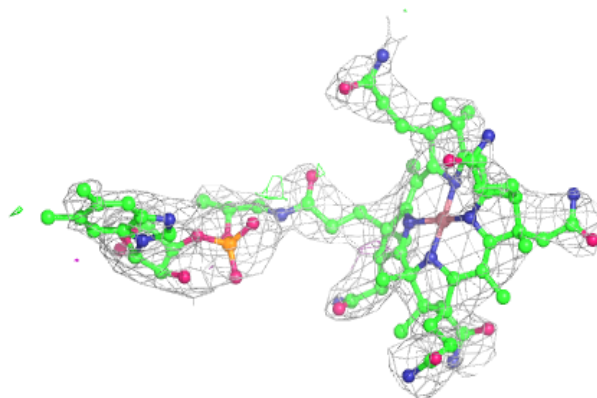


**Electron density around 5AD D 1500:**

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

**Electron density around B12 A 1801:**

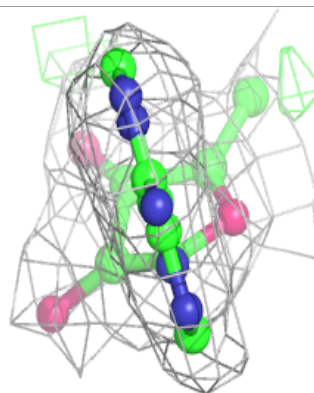
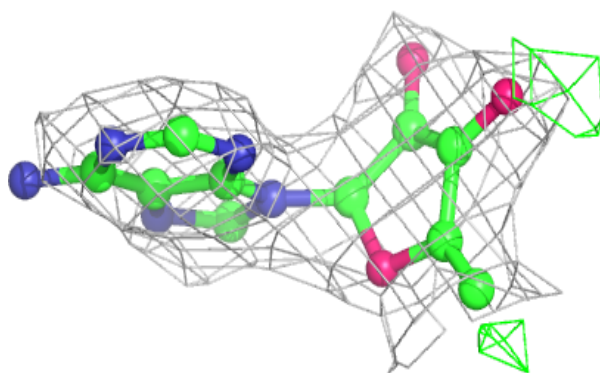
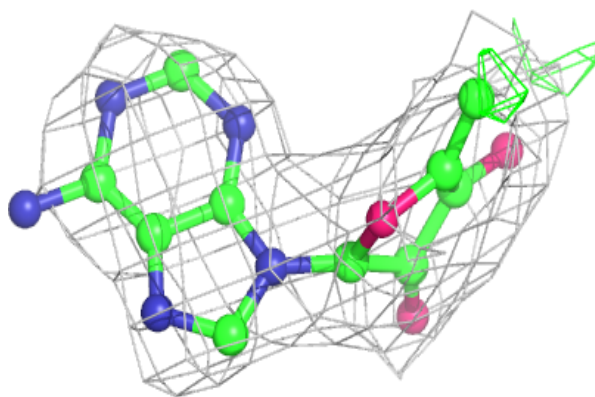
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



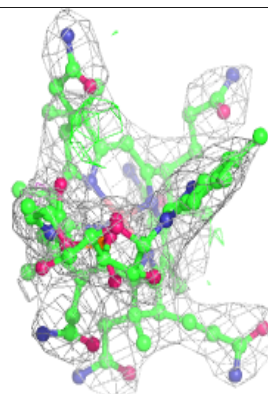
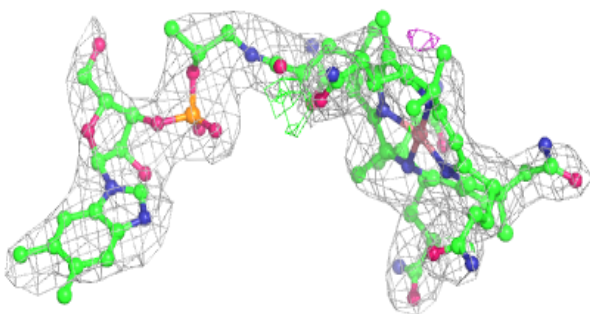
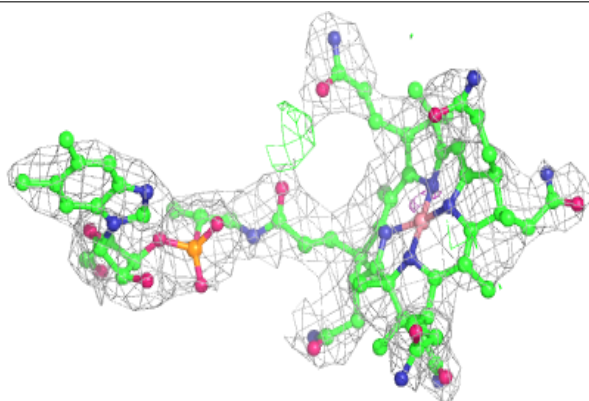


**Electron density around 5AD A 1500:**

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

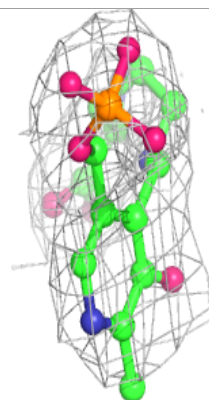
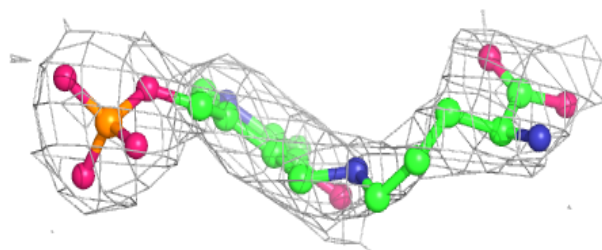
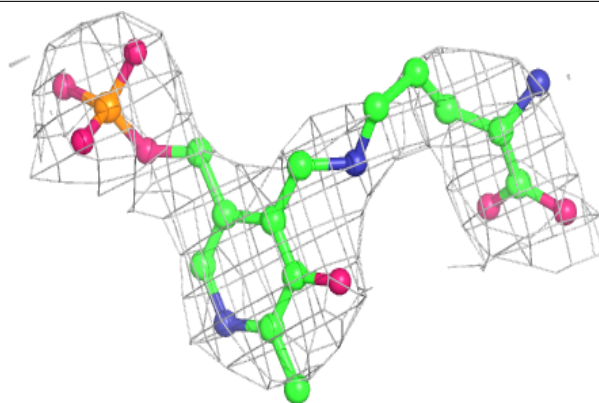
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and green (positive)

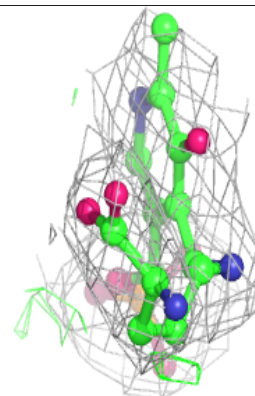
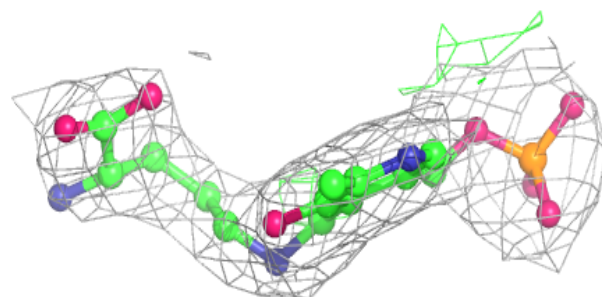
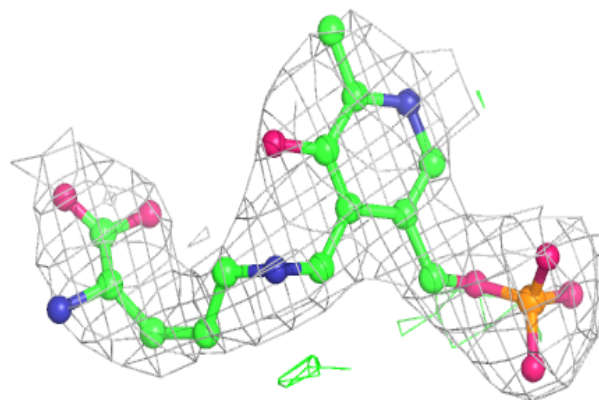


**Electron density around Z97 C 767:**

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and green (positive)

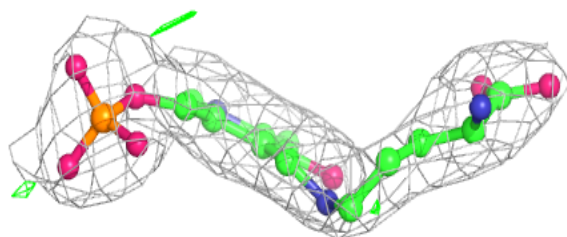
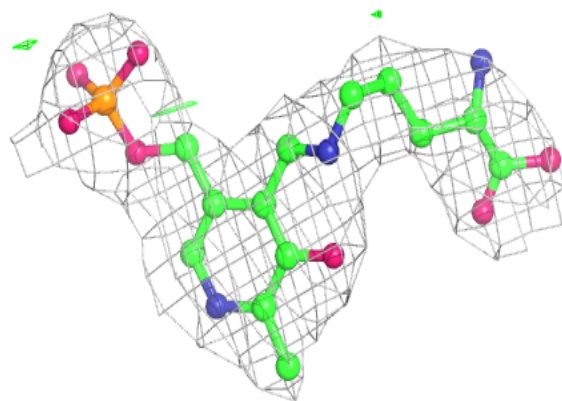
**Electron density around Z97 A 767:**

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

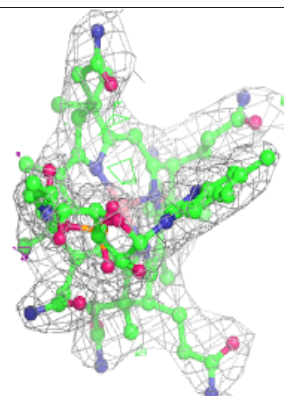
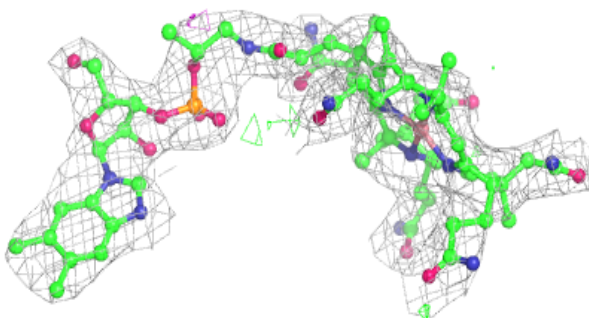
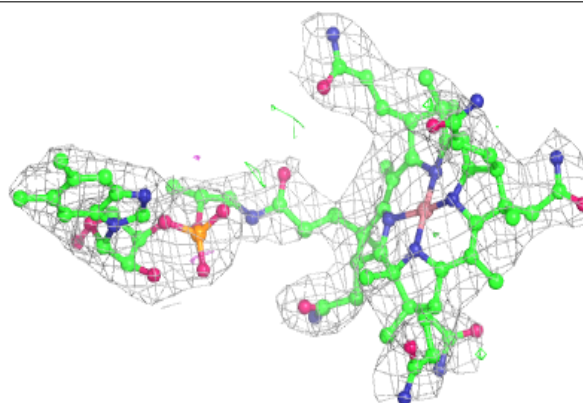


**Electron density around Z97 B 767:**

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

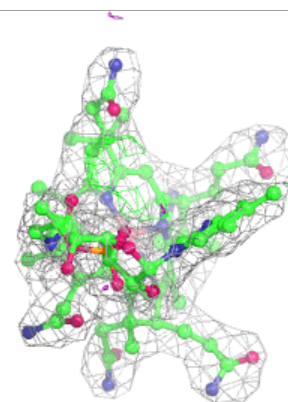
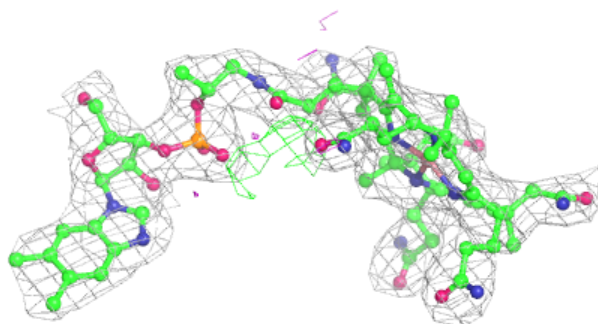
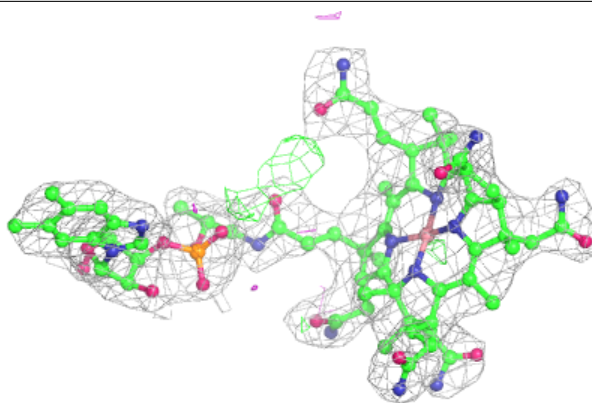
**Electron density around B12 B 1801:**

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

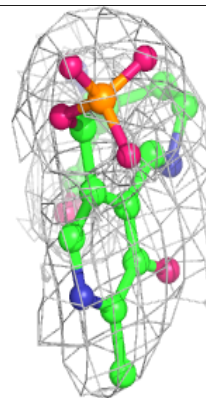
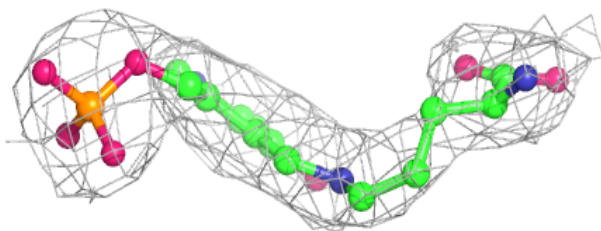
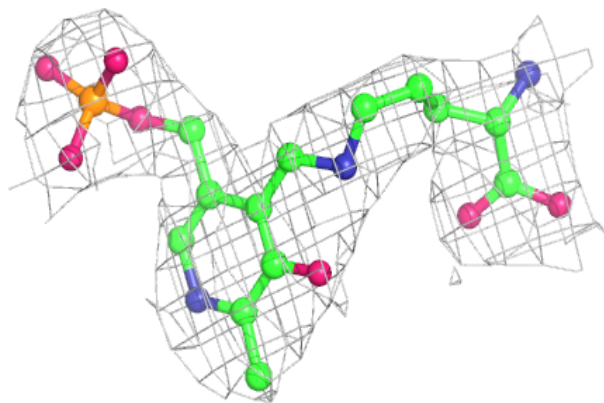


**Electron density around B12 C 1801:**

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

**Electron density around Z97 D 767:**

$2mF_o-DF_c$  (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.