



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 12:07 am BST

PDB ID : 3KOX  
Title : Crystal Structure of ornithine 4,5 aminomutase in complex with 2,4-diaminobutyrate (Anaerobic)  
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.  
Deposited on : 2009-11-14  
Resolution : 2.40 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

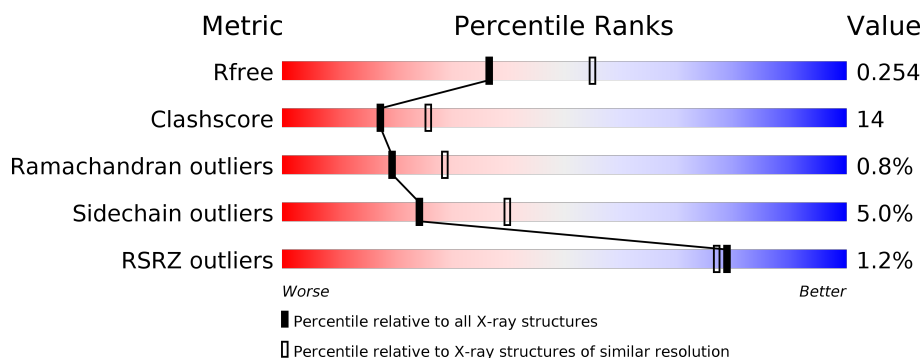
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>3%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• 5%</div> </div> </div>
1	B	763	<div> <div></div> <div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	C	763	<div> <div></div> <div> <div>72%</div> <div>21%</div> <div>• 5%</div> </div> </div>
1	D	763	<div> <div>•</div> <div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div> </div>
2	E	121	<div> <div>•</div> <div> <div>69%</div> <div>18%</div> <div>• 10%</div> </div> </div>
2	F	121	<div> <div>•</div> <div> <div>69%</div> <div>21%</div> <div>• 10%</div> </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	-	-	-
3	B12	B	1801	X	-	-	-
3	B12	C	1801	X	-	-	-
4	5AD	A	1500	X	-	-	-
4	5AD	D	1500	X	-	-	-
5	Z98	A	767	-	-	X	-
5	Z98	B	767	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27379 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
			5651	3561	981	1075	34			
1	B	728	Total	C	N	O	S	0	0	0
			5672	3579	984	1075	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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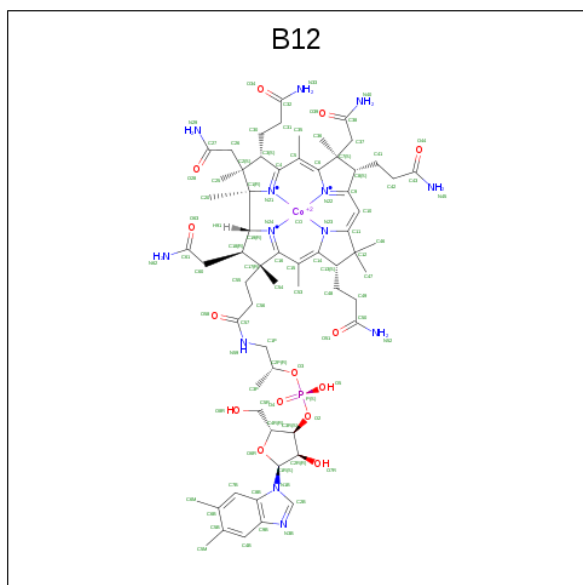
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	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.

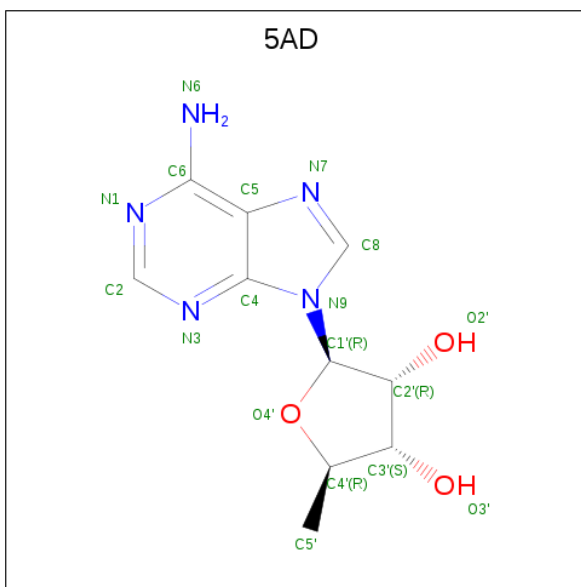
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	F	109	Total	C	N	O	S	0	0	0
			858	539	152	163	4			
2	G	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	H	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			

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



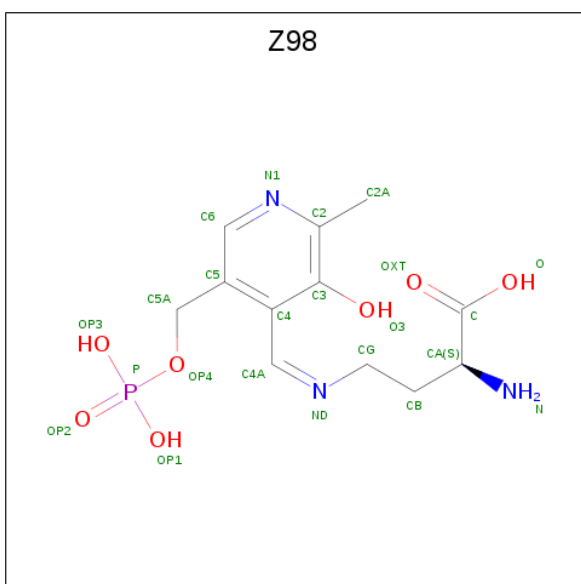
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
3	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 4 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



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 (2S)-2-amino-4-[(1Z)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}butanoic acid (three-letter code: Z98) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>3</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 23	C 12	N 3	O 7	P 1	0	0
5	B	1	Total 23	C 12	N 3	O 7	P 1	0	0
5	C	1	Total 23	C 12	N 3	O 7	P 1	0	0
5	D	1	Total 23	C 12	N 3	O 7	P 1	0	0

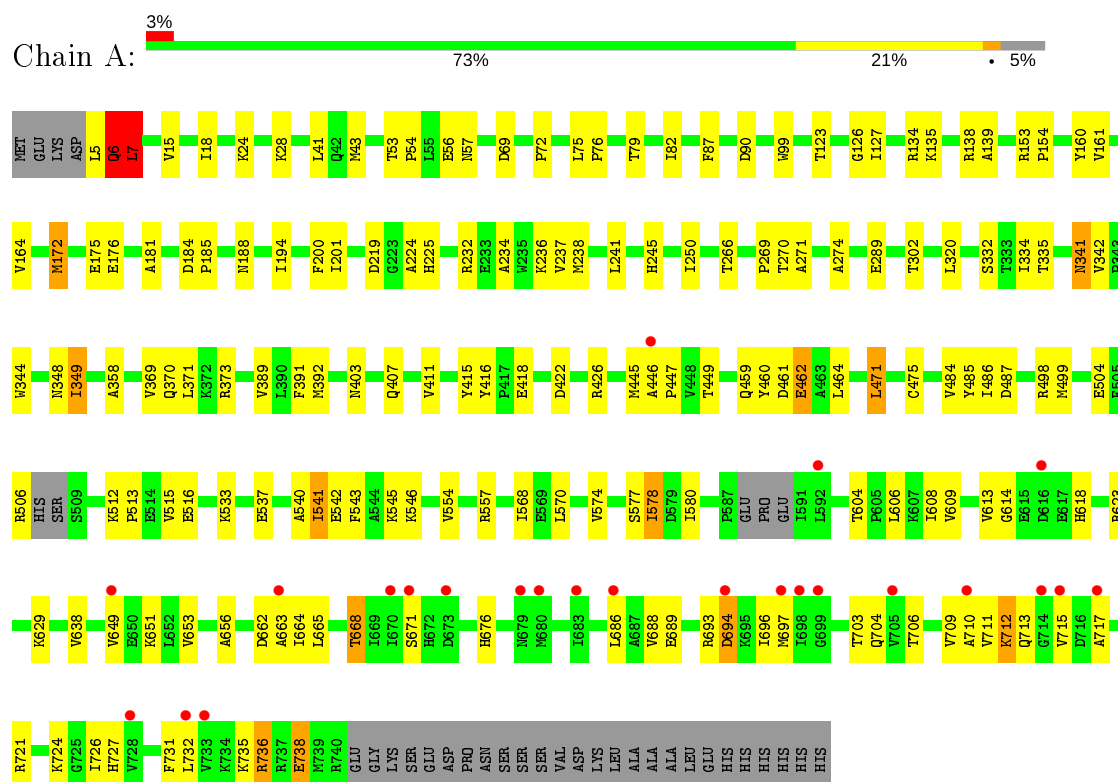
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total 144	O 144	0	0
6	E	15	Total 15	O 15	0	0
6	B	199	Total 199	O 199	0	0
6	F	33	Total 33	O 33	0	0
6	C	145	Total 145	O 145	0	0
6	G	17	Total 17	O 17	0	0
6	D	217	Total 217	O 217	0	0
6	H	17	Total 17	O 17	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: D-ornithine aminomutase E component



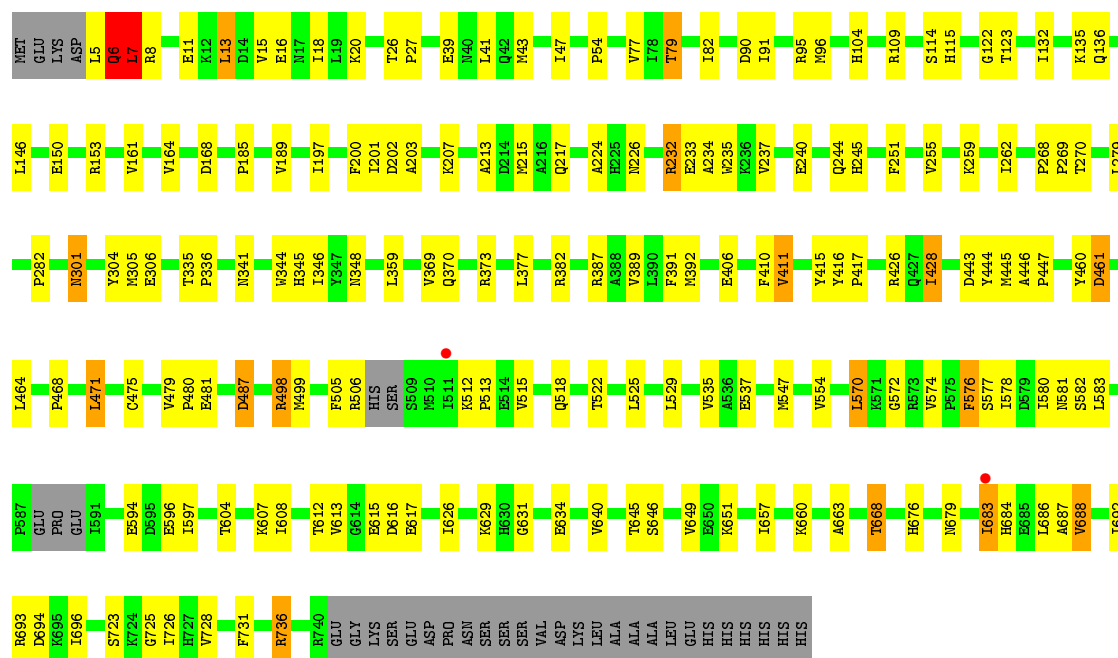
- Molecule 1: D-ornithine aminomutase E component





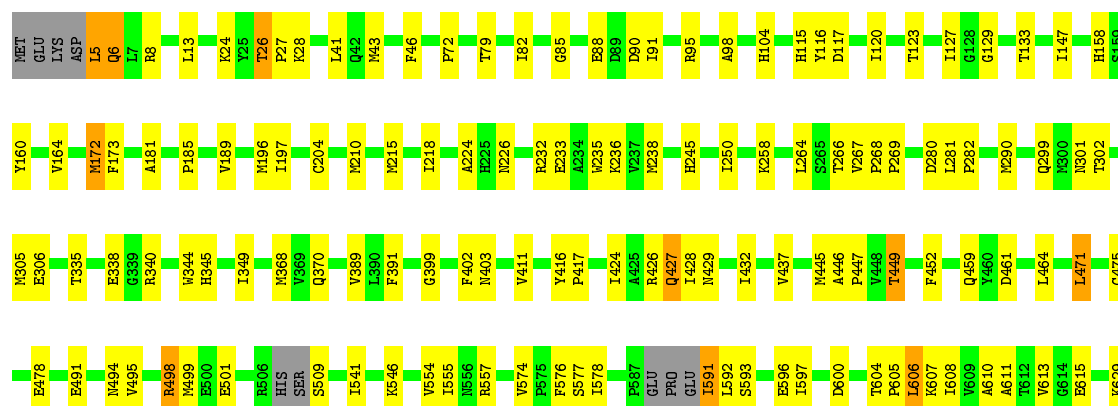
- Molecule 1: D-ornithine aminomutase E component

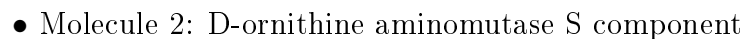
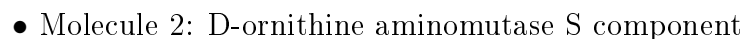
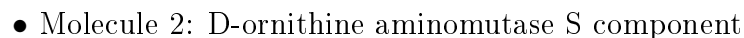
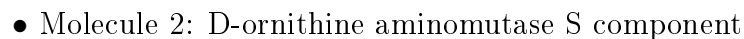
Chain C: 72% 21% 5%



- Molecule 1: D-ornithine aminomutase E component

Chain D: 74% 19% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.96 Å 231.69 Å 123.89 Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	64.23 – 2.40 64.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.23-2.40) 99.9 (64.23-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.40 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.190 , 0.257 0.191 , 0.254	Depositor DCC
$R_{free}$ test set	7055 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27379	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.36% 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: B12, 5AD, Z98

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	0.73	1/5756 (0.0%)	0.79	1/7794 (0.0%)
1	B	0.81	1/5777 (0.0%)	0.85	7/7818 (0.1%)
1	C	0.72	0/5759	0.79	4/7796 (0.1%)
1	D	0.82	0/5769	0.81	2/7808 (0.0%)
2	E	0.74	0/867	0.72	1/1163 (0.1%)
2	F	0.86	0/870	0.85	1/1167 (0.1%)
2	G	0.69	1/867 (0.1%)	0.75	0/1163
2	H	0.79	0/867	0.73	0/1163
All	All	0.77	3/26532 (0.0%)	0.80	16/35872 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CG-CD	5.84	1.60	1.51
2	G	20	GLU	CG-CD	5.45	1.60	1.51
1	B	149	GLU	CG-CD	5.39	1.60	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	D	498	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	498	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	92	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	498	ARG	NE-CZ-NH1	6.91	123.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	GLN	Peptide
1	D	6	GLN	Peptide

## 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	5651	0	5584	158	0
1	B	5672	0	5644	174	0
1	C	5654	0	5621	172	0
1	D	5664	0	5636	148	0
2	E	855	0	863	17	0
2	F	858	0	865	17	0
2	G	855	0	863	19	0
2	H	855	0	863	15	0
3	A	91	0	87	15	0
3	B	91	0	87	19	0
3	C	91	0	87	16	0
3	D	91	0	87	14	0
4	A	18	0	11	2	0
4	B	18	0	12	2	0
4	C	18	0	12	3	0
4	D	18	0	12	4	0
5	A	23	0	14	10	0
5	B	23	0	14	9	0
5	C	23	0	14	8	0
5	D	23	0	14	8	0
6	A	144	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	199	0	0	14	0
6	C	145	0	0	15	0
6	D	217	0	0	20	0
6	E	15	0	0	1	0
6	F	33	0	0	2	0
6	G	17	0	0	2	0
6	H	17	0	0	1	0
All	All	27379	0	26390	730	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 14.

The worst 5 of 730 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)
5:B:767:Z98:H4A	1:D:629:LYS:NZ	1.46	1.28
1:B:649:VAL:HG22	1:B:683:ILE:HD11	1.20	1.17
1:B:396:ILE:HD12	2:F:29:MET:HE3	1.15	1.15
1:A:629:LYS:NZ	5:C:767:Z98:H4A	1.64	1.12
1:C:41:LEU:HD23	1:C:43:MET:HE2	1.28	1.12

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%)	674 (93%)	42 (6%)	6 (1%)	19 29
1	B	722/763 (95%)	683 (95%)	32 (4%)	7 (1%)	15 23
1	C	722/763 (95%)	691 (96%)	22 (3%)	9 (1%)	13 19
1	D	722/763 (95%)	690 (96%)	30 (4%)	2 (0%)	41 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	107/121 (88%)	101 (94%)	5 (5%)	1 (1%)	17	25
2	F	107/121 (88%)	103 (96%)	3 (3%)	1 (1%)	17	25
2	G	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
2	H	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
All	All	3316/3536 (94%)	3153 (95%)	137 (4%)	26 (1%)	19	29

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	462	GLU
1	B	7	LEU
1	B	739	MET
1	C	6	GLN

### 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	598/644 (93%)	568 (95%)	30 (5%)	24	40
1	B	604/644 (94%)	577 (96%)	27 (4%)	27	44
1	C	600/644 (93%)	573 (96%)	27 (4%)	27	44
1	D	602/644 (94%)	566 (94%)	36 (6%)	19	31
2	E	89/100 (89%)	83 (93%)	6 (7%)	16	26
2	F	90/100 (90%)	85 (94%)	5 (6%)	21	34
2	G	89/100 (89%)	84 (94%)	5 (6%)	21	34
2	H	89/100 (89%)	86 (97%)	3 (3%)	37	56
All	All	2761/2976 (93%)	2622 (95%)	139 (5%)	24	40

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	736	ARG
1	C	301	ASN
1	D	657	ILE
2	F	31	GLU
1	C	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	518	GLN
1	C	301	ASN
1	D	459	GLN
1	C	36	GLN
1	C	331	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	Z98	B	767	-	19,23,23	1.60	5 (26%)	24,32,32	1.88	5 (20%)
3	B12	B	1801	1,4	80,101,101	1.18	5 (6%)	101,166,166	2.27	20 (19%)
5	Z98	D	767	-	19,23,23	1.60	3 (15%)	24,32,32	1.67	4 (16%)
4	5AD	B	1500	3	17,20,20	1.56	3 (17%)	15,30,30	1.70	3 (20%)
3	B12	C	1801	1,4	80,101,101	1.16	6 (7%)	101,166,166	2.23	16 (15%)
3	B12	A	1801	1,4	80,101,101	1.07	5 (6%)	101,166,166	2.22	18 (17%)
4	5AD	C	1500	3	17,20,20	1.35	3 (17%)	15,30,30	2.56	7 (46%)
4	5AD	D	1500	3	17,20,20	1.65	5 (29%)	15,30,30	3.08	6 (40%)
4	5AD	A	1500	3	17,20,20	1.74	5 (29%)	15,30,30	2.85	7 (46%)
3	B12	D	1801	1,4	80,101,101	1.10	5 (6%)	101,166,166	2.09	17 (16%)
5	Z98	C	767	-	19,23,23	1.57	3 (15%)	24,32,32	1.83	6 (25%)
5	Z98	A	767	-	19,23,23	2.04	7 (36%)	24,32,32	2.42	5 (20%)

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	Z98	B	767	-	-	5/13/17/17	0/1/1/1
3	B12	B	1801	1,4	1/1/36/38	3/51/223/223	0/3/11/11
5	Z98	D	767	-	-	5/13/17/17	0/1/1/1
3	B12	A	1801	1,4	1/1/36/38	14/51/223/223	0/3/11/11
3	B12	C	1801	1,4	1/1/36/38	6/51/223/223	0/3/11/11
4	5AD	B	1500	3	-	0/0/20/20	0/3/3/3
4	5AD	C	1500	3	-	0/0/20/20	0/3/3/3
4	5AD	D	1500	3	1/1/4/4	0/0/20/20	0/3/3/3
4	5AD	A	1500	3	1/1/4/4	0/0/20/20	0/3/3/3
3	B12	D	1801	1,4	-	2/51/223/223	0/3/11/11
5	Z98	C	767	-	-	5/13/17/17	0/1/1/1
5	Z98	A	767	-	-	8/13/17/17	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C11-C10	-6.01	1.30	1.40
3	B	1801	B12	C8B-C9B	4.56	1.49	1.40
3	B	1801	B12	C11-C10	-4.30	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1500	5AD	C2'-C1'	-4.26	1.47	1.53
4	D	1500	5AD	O4'-C1'	4.10	1.46	1.41

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	B12	C20-C1-C19	-11.58	98.19	109.36
3	A	1801	B12	C20-C1-C19	-10.08	99.64	109.36
3	C	1801	B12	C20-C1-C19	-9.37	100.33	109.36
3	A	1801	B12	C1-C19-N24	9.29	116.69	106.24
3	D	1801	B12	C1-C19-N24	8.98	116.34	106.24

All (5) chirality outliers are listed below:

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

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	767	Z98	N-CA-CB-CG
5	B	767	Z98	CA-CB-CG-ND
5	B	767	Z98	C4-C4A-ND-CG
5	D	767	Z98	CA-CB-CG-ND
5	D	767	Z98	C4-C4A-ND-CG

There are no ring outliers.

12 monomers are involved in 99 short contacts:

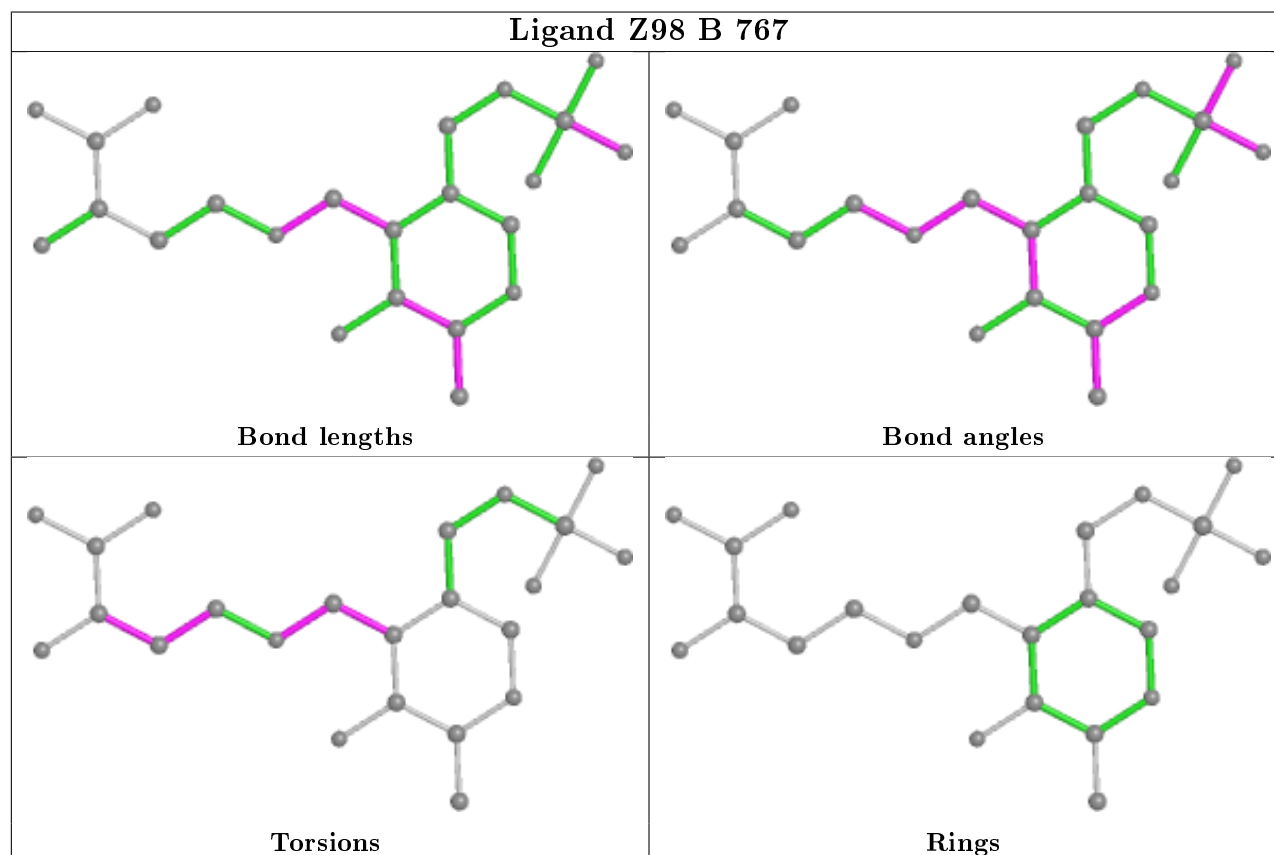
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	767	Z98	9	0
3	B	1801	B12	19	0
5	D	767	Z98	8	0
4	B	1500	5AD	2	0
3	C	1801	B12	16	0
3	A	1801	B12	15	0
4	C	1500	5AD	3	0

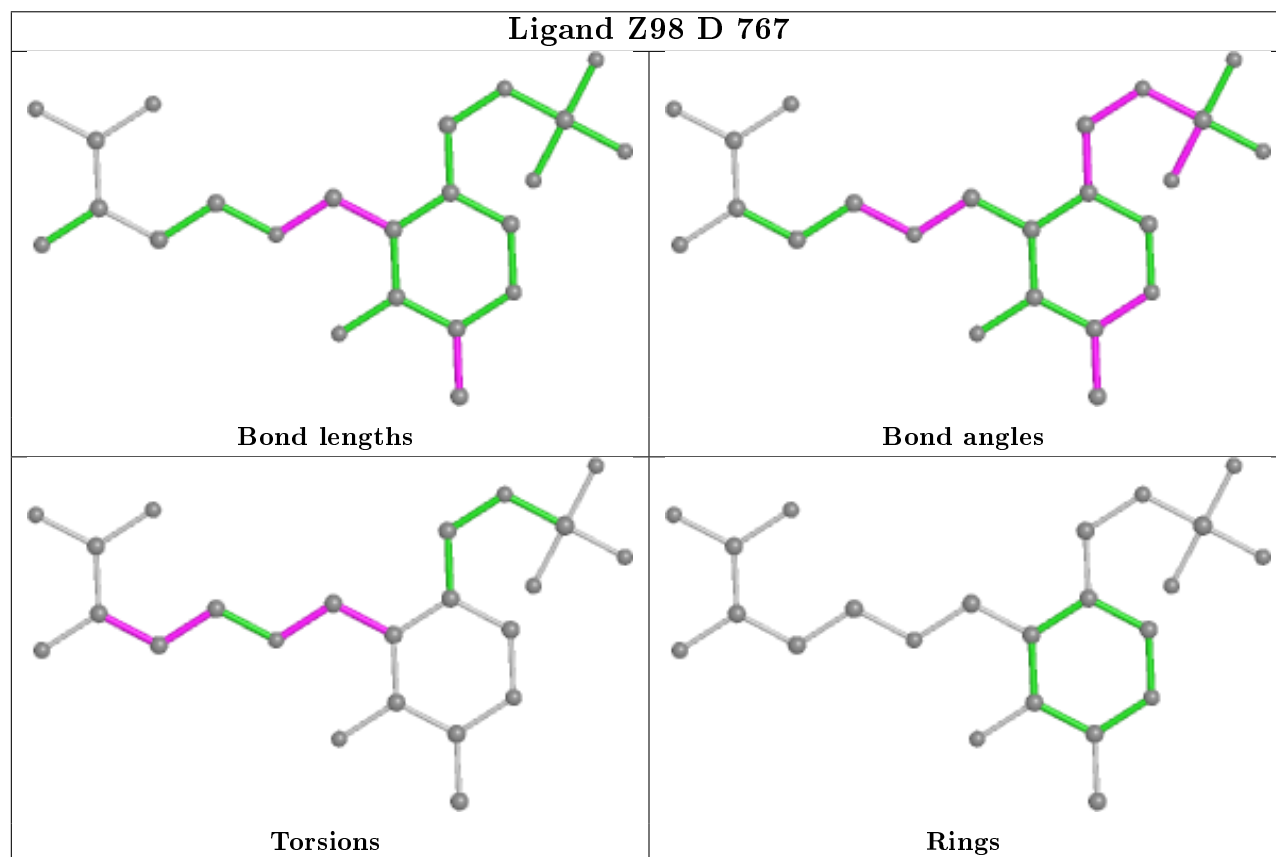
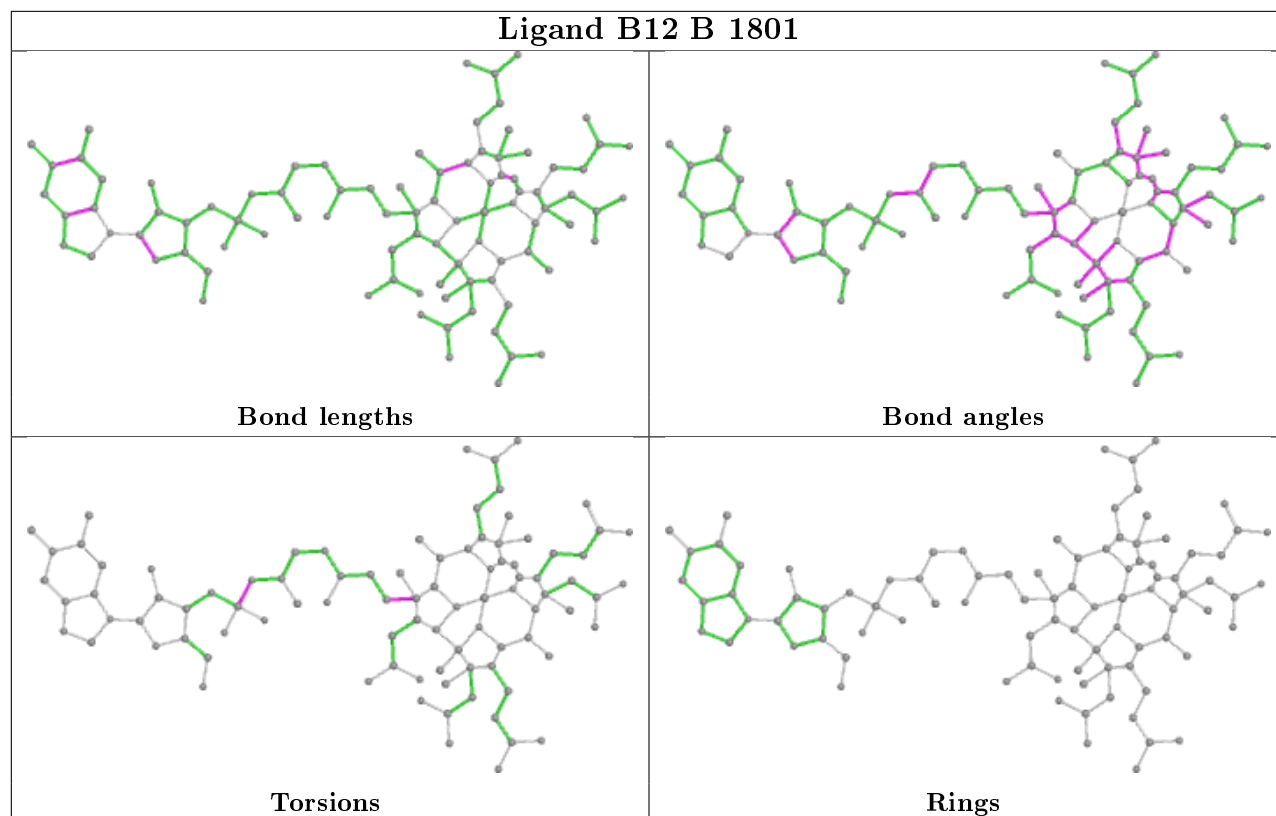
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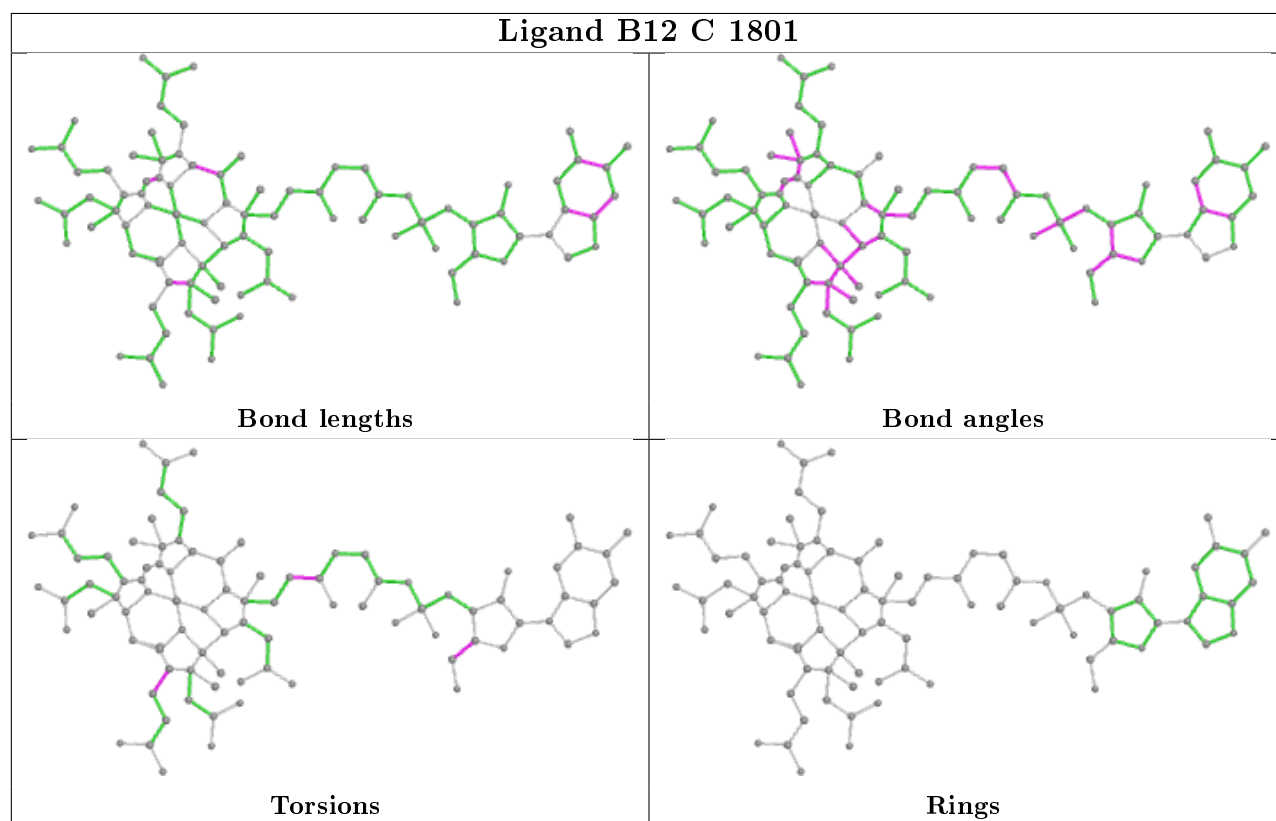
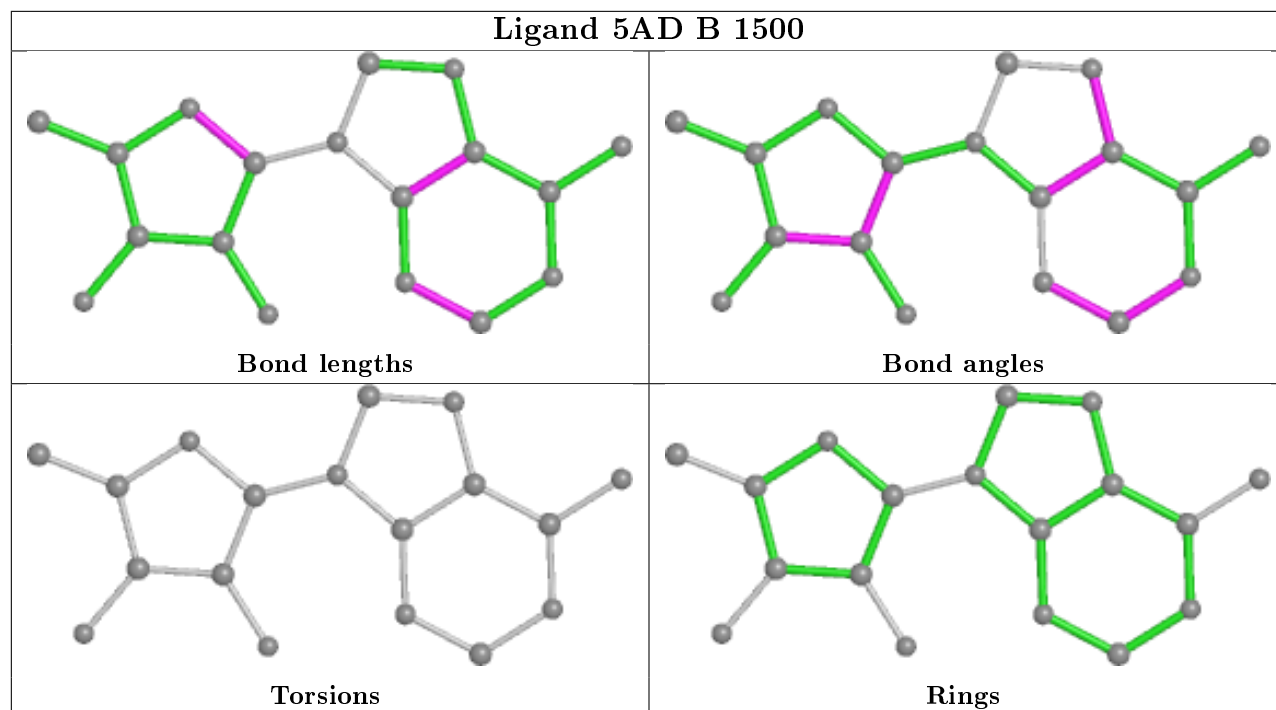
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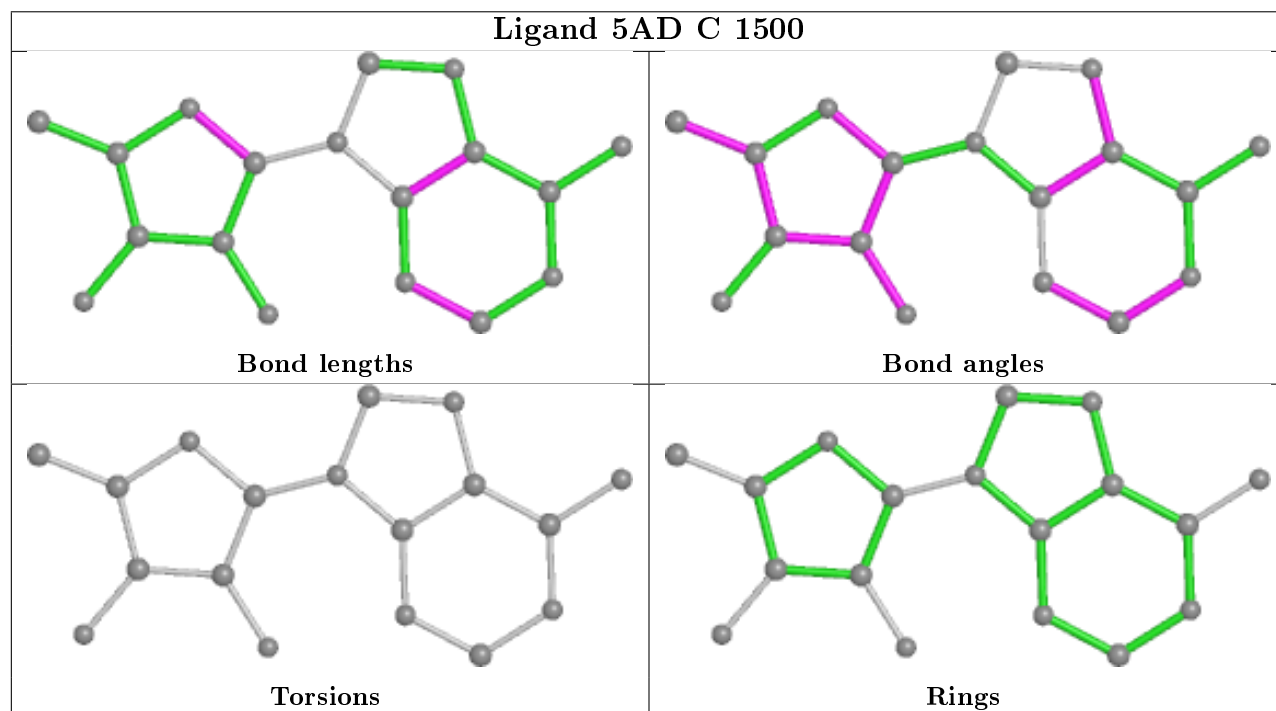
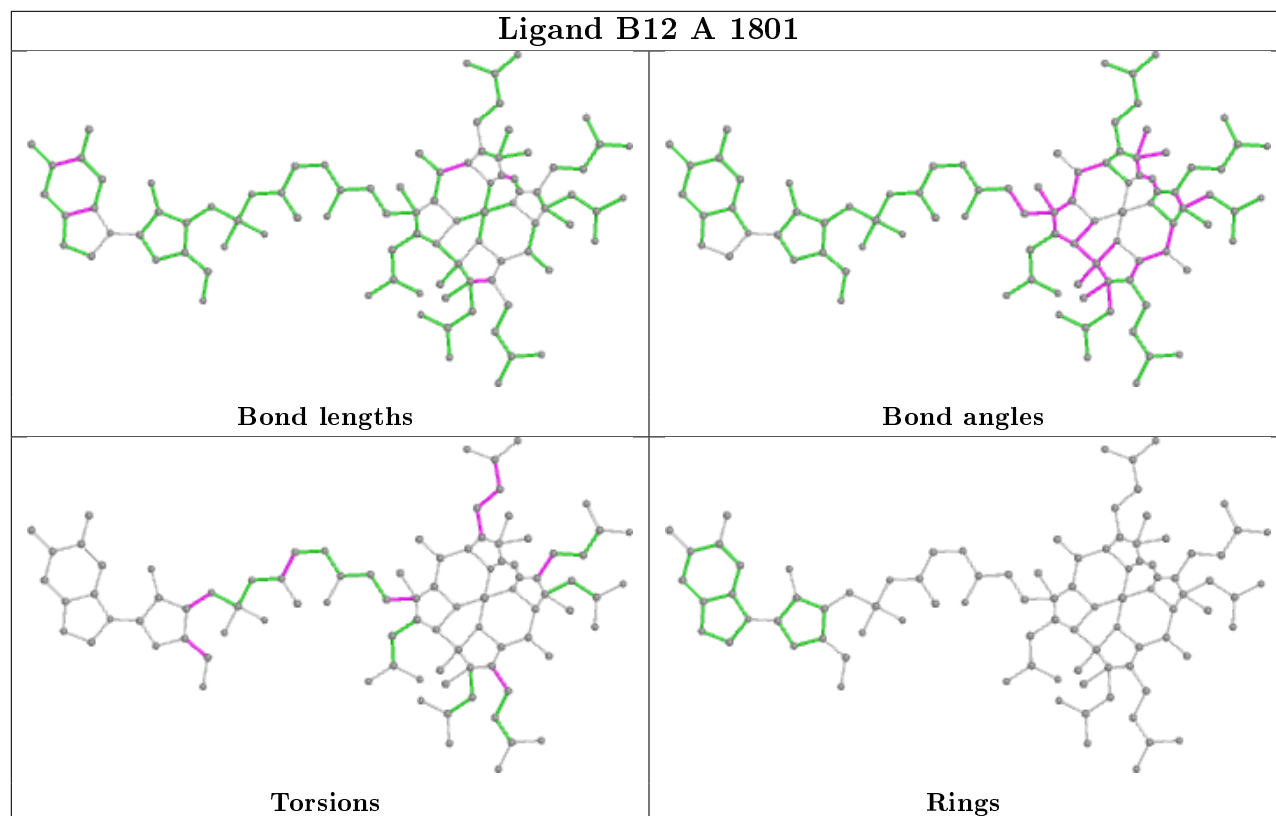
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1500	5AD	4	0
4	A	1500	5AD	2	0
3	D	1801	B12	14	0
5	C	767	Z98	8	0
5	A	767	Z98	10	0

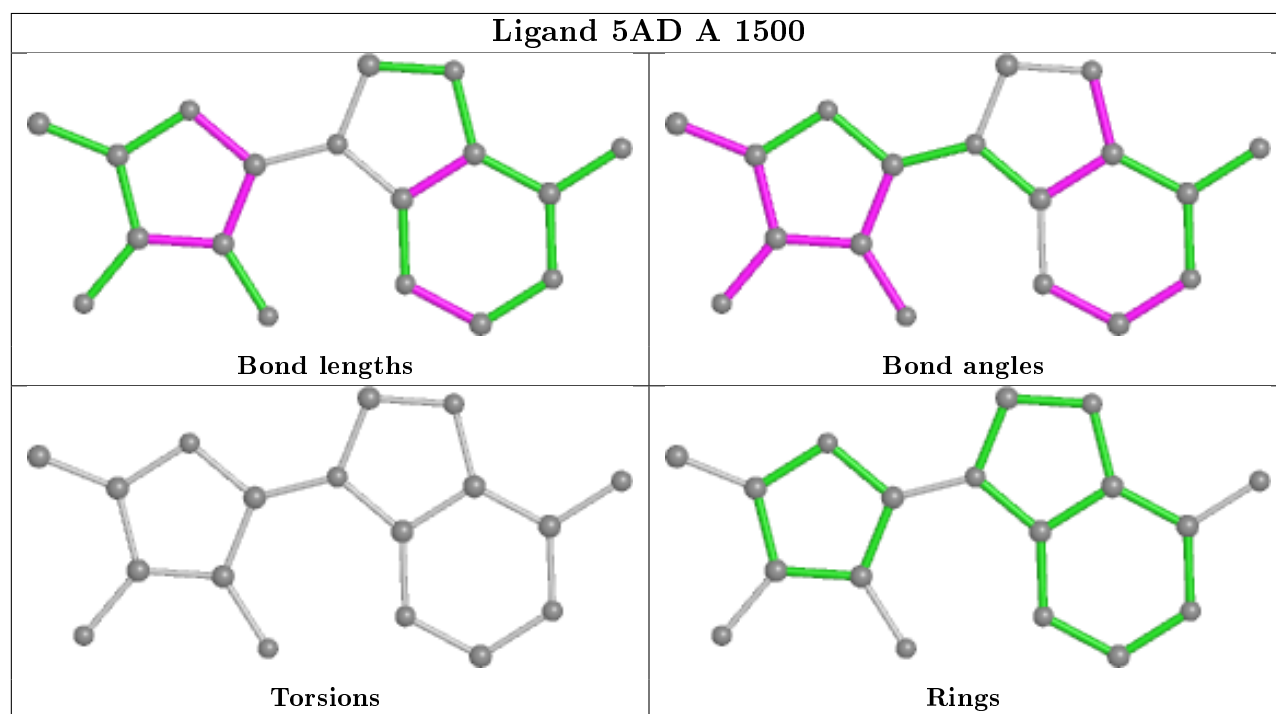
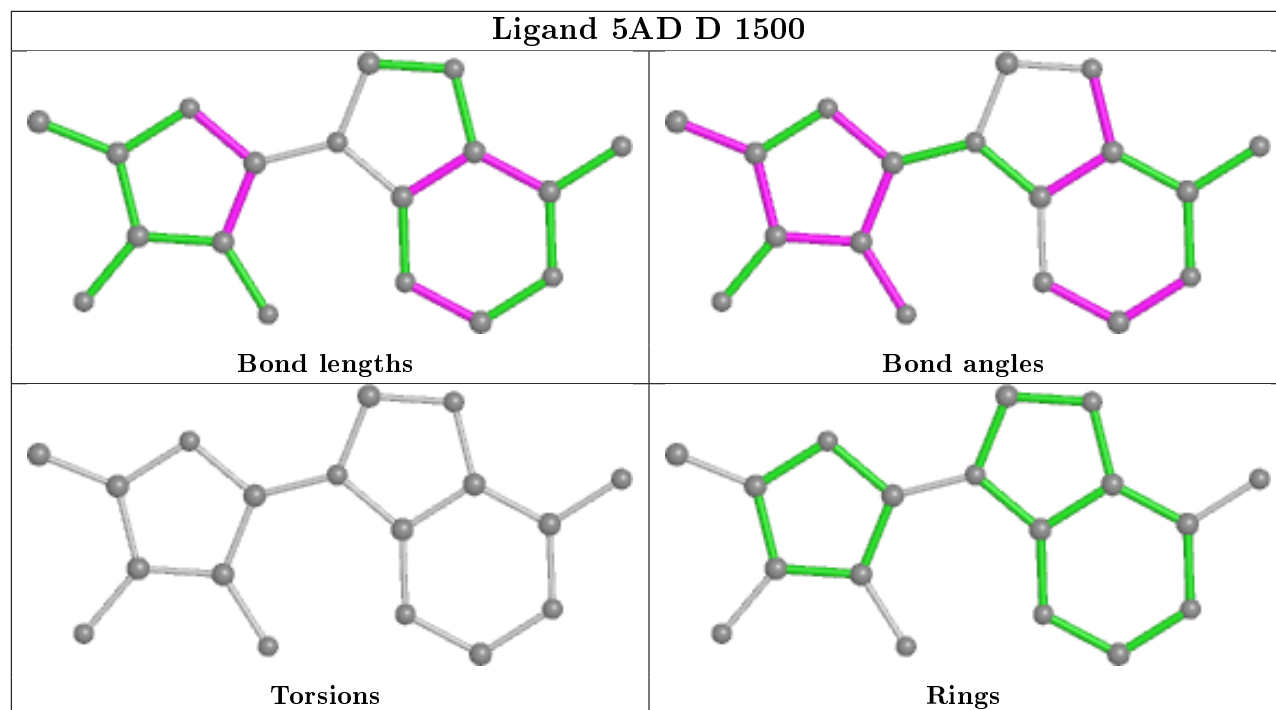
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

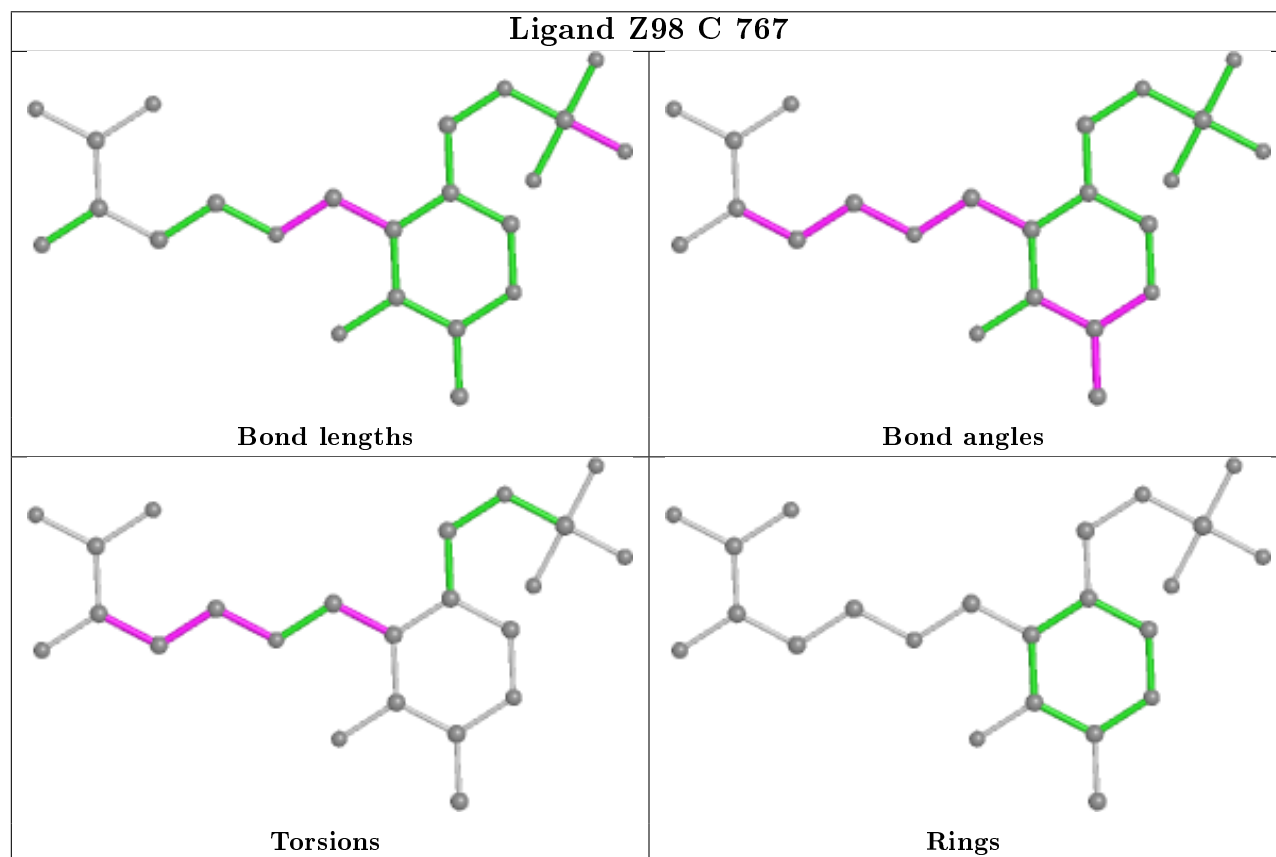
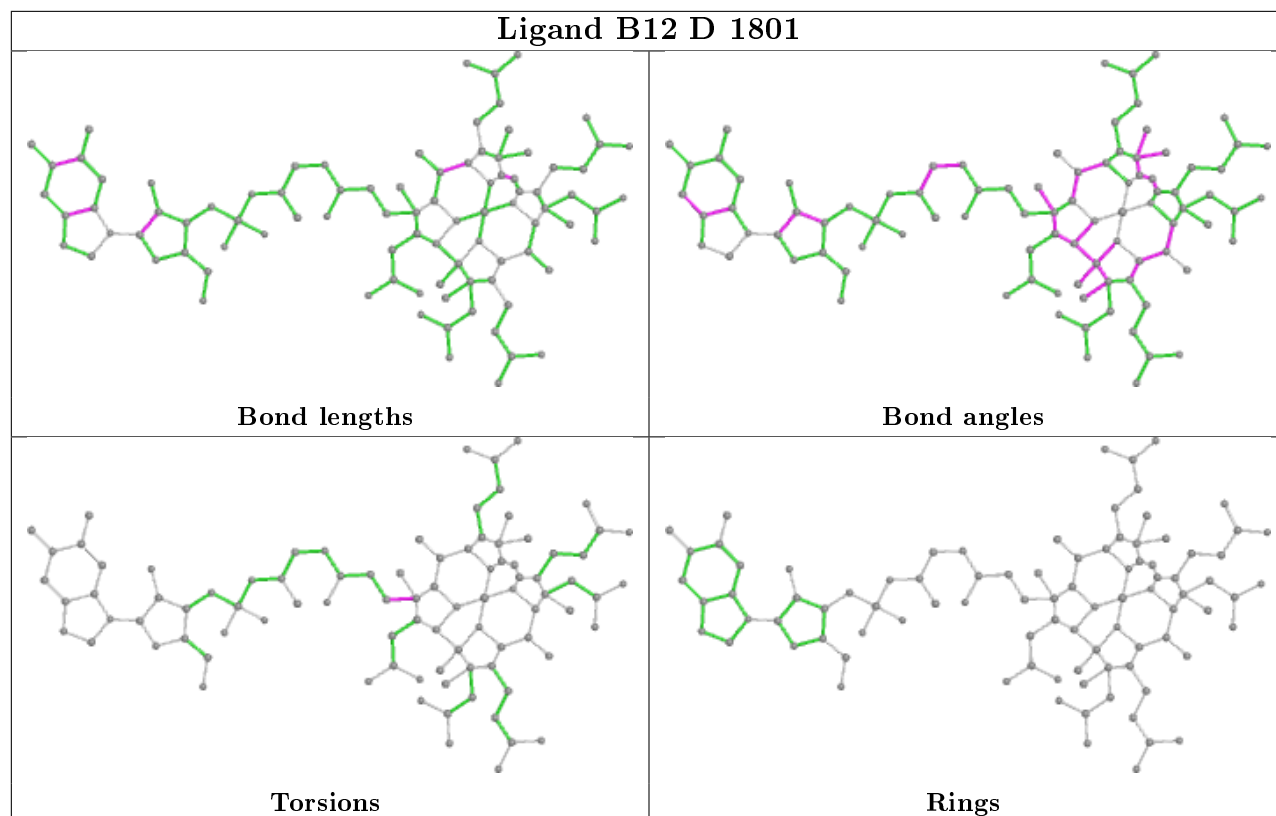


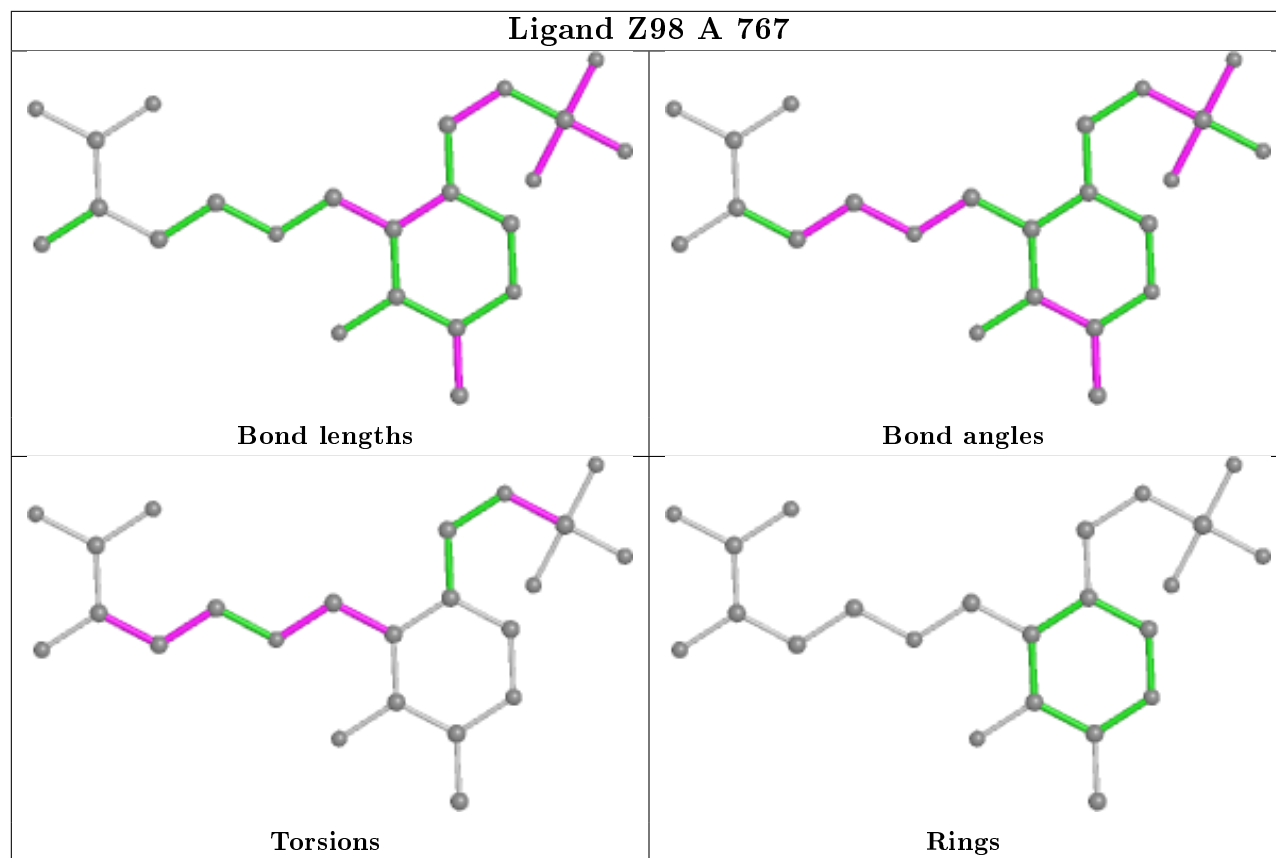












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.02	24 (3%) 46 45	13, 27, 68, 84	0
1	B	728/763 (95%)	-0.26	1 (0%) 95 95	10, 22, 42, 56	0
1	C	728/763 (95%)	-0.17	2 (0%) 94 93	12, 28, 49, 66	0
1	D	728/763 (95%)	-0.15	4 (0%) 91 89	10, 23, 50, 65	0
2	E	109/121 (90%)	0.07	1 (0%) 84 82	17, 32, 46, 50	0
2	F	109/121 (90%)	-0.06	1 (0%) 84 82	15, 24, 37, 45	0
2	G	109/121 (90%)	0.20	6 (5%) 25 24	24, 35, 50, 55	0
2	H	109/121 (90%)	-0.04	0 100 100	15, 27, 45, 61	0
All	All	3348/3536 (94%)	-0.11	39 (1%) 79 77	10, 26, 54, 84	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	ILE	4.1
1	D	692	ILE	3.4
1	A	717	ALA	3.2
1	C	511	ILE	3.0
1	A	705	VAL	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

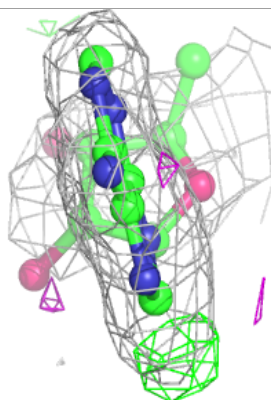
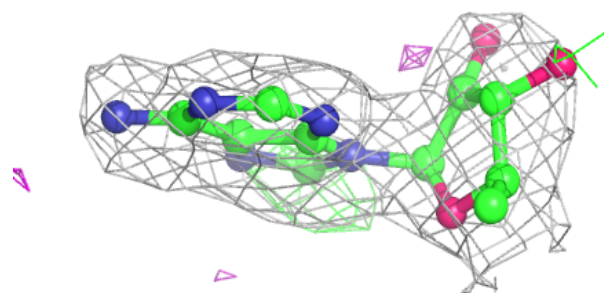
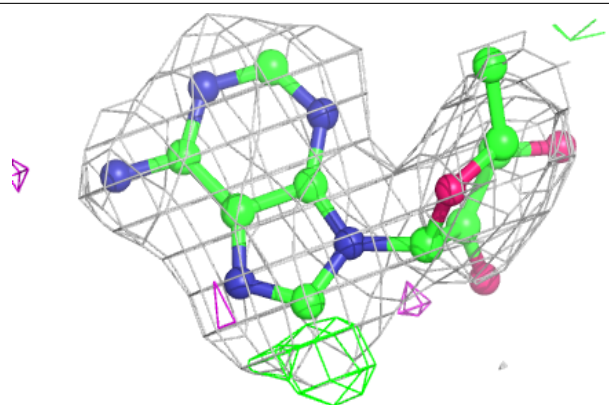
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	5AD	C	1500	18/18	0.87	0.22	53,54,55,57	0
4	5AD	A	1500	18/18	0.89	0.22	39,43,47,47	0
4	5AD	D	1500	18/18	0.90	0.20	38,40,45,45	0
4	5AD	B	1500	18/18	0.92	0.17	25,38,42,42	0
3	B12	A	1801	91/91	0.95	0.22	27,43,50,54	0
5	Z98	C	767	23/23	0.95	0.17	26,34,43,44	0
3	B12	D	1801	91/91	0.95	0.19	19,29,40,43	0
5	Z98	B	767	23/23	0.96	0.16	18,23,33,34	0
5	Z98	A	767	23/23	0.96	0.16	21,32,42,43	0
3	B12	B	1801	91/91	0.97	0.14	14,21,29,35	0
3	B12	C	1801	91/91	0.97	0.15	12,23,31,34	0
5	Z98	D	767	23/23	0.97	0.15	19,24,46,46	0

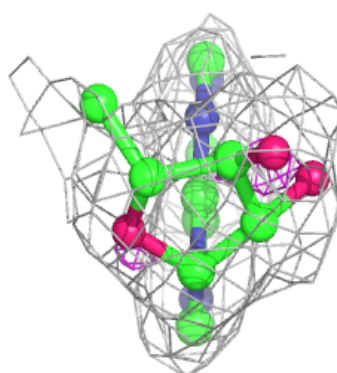
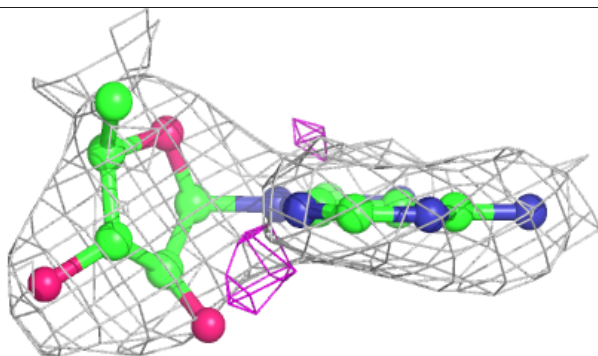
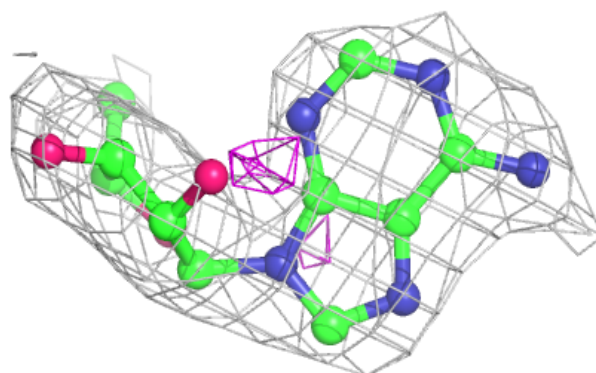
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

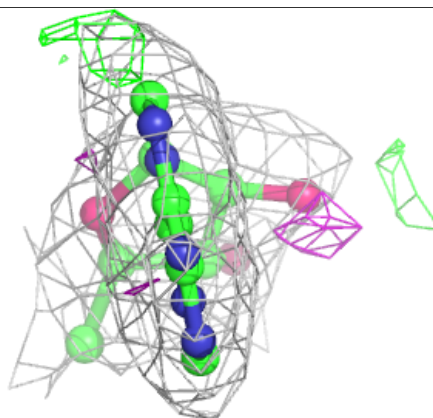
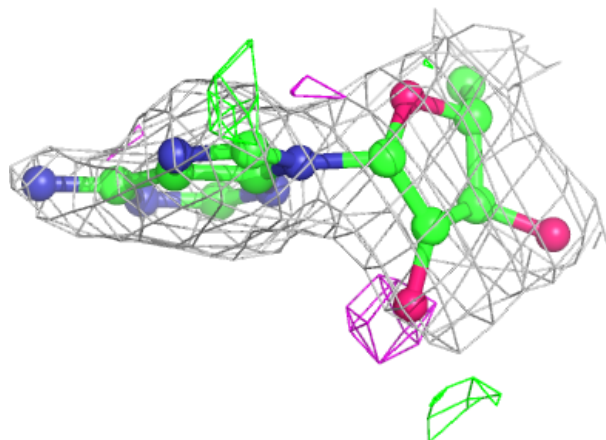
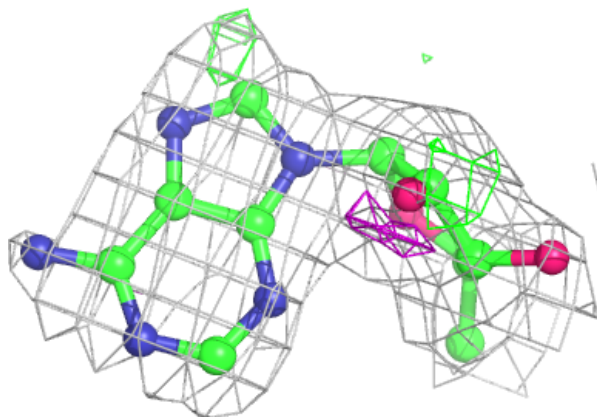
**Electron density around 5AD A 1500:**

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



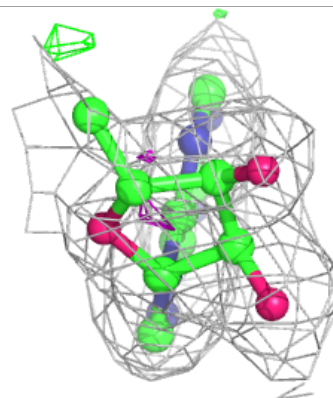
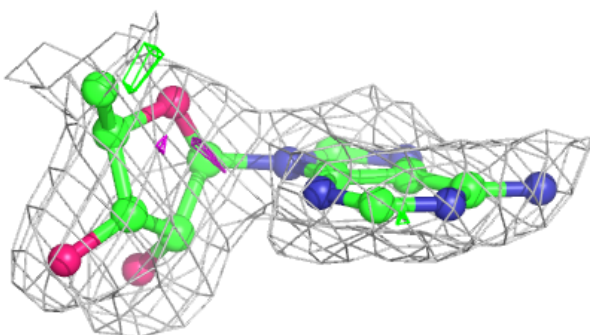
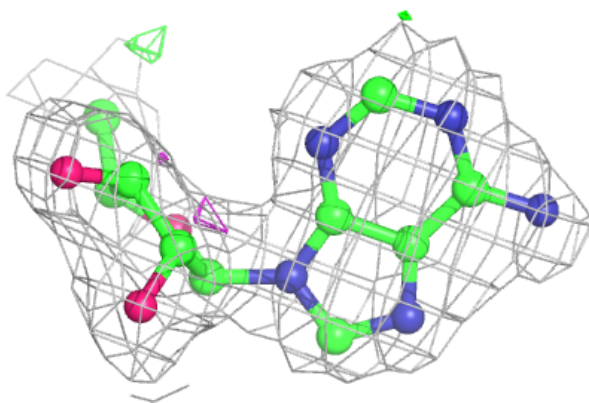
**Electron density around 5AD D 1500:**

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

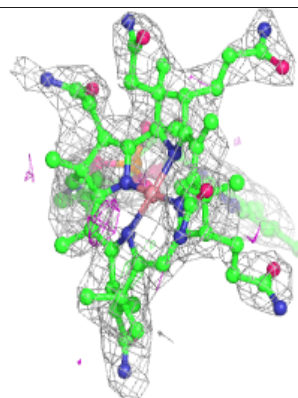
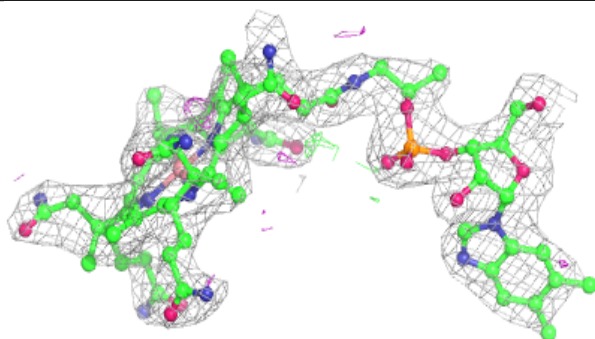
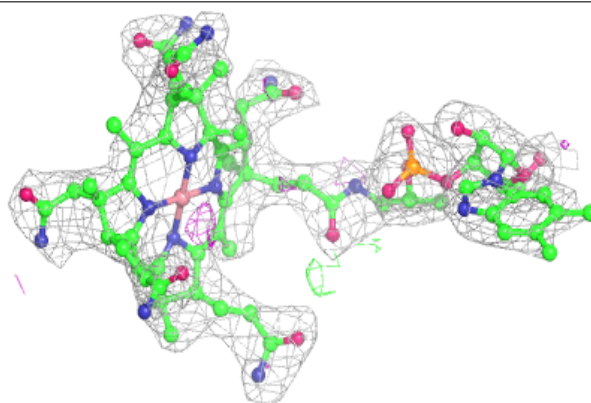


**Electron density around 5AD B 1500:**

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

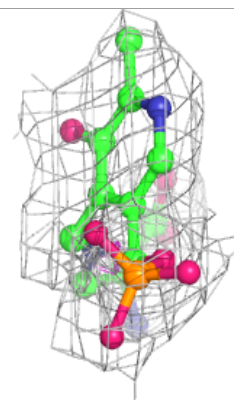
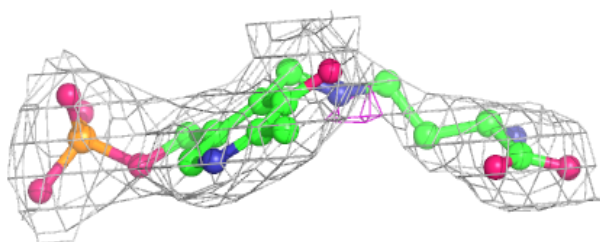
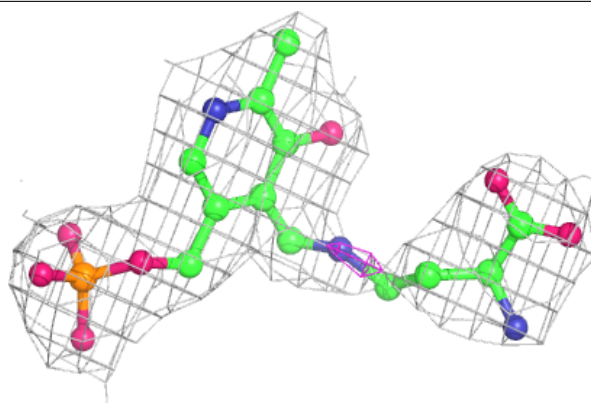
**Electron density around B12 A 1801:**

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

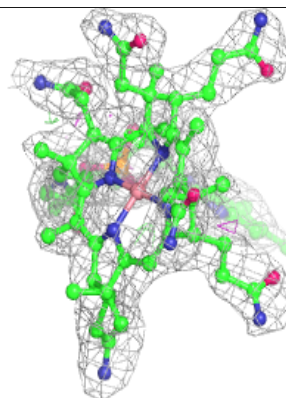
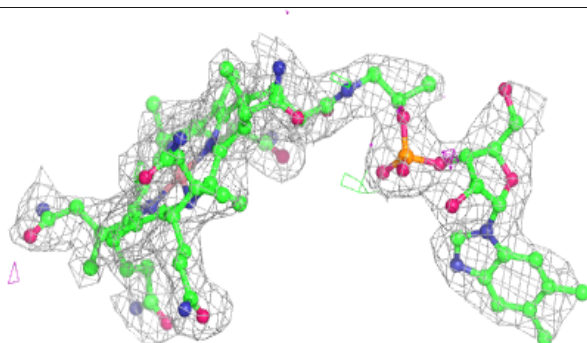
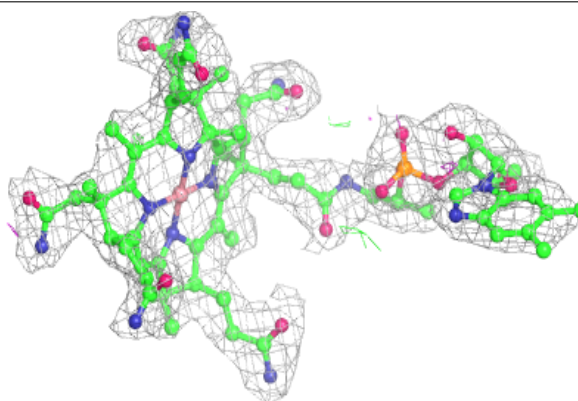


**Electron density around Z98 C 767:**

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

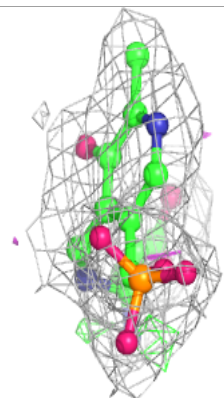
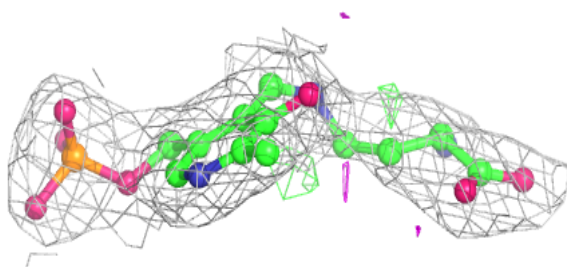
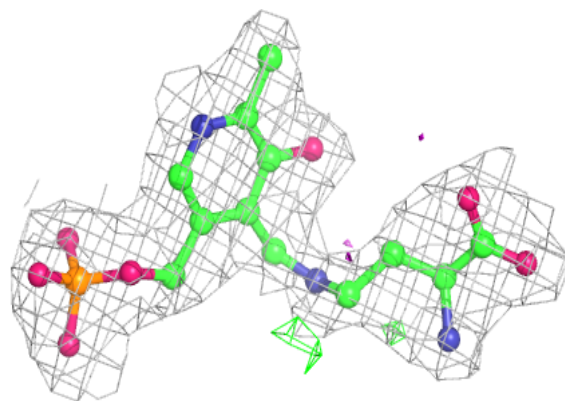
**Electron density around B12 D 1801:**

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

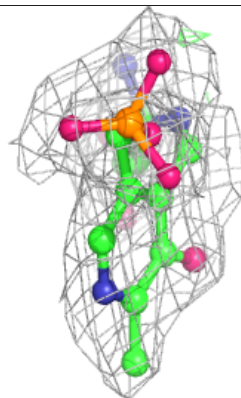
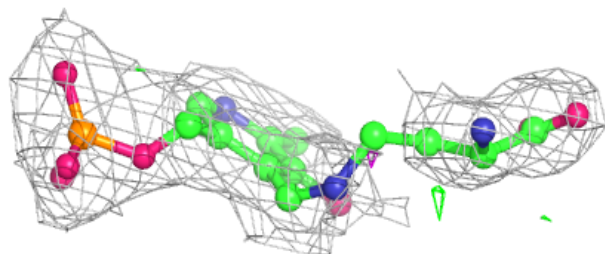
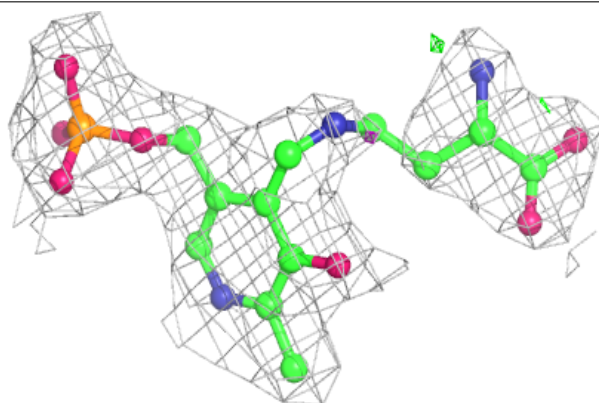


**Electron density around Z98 B 767:**

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

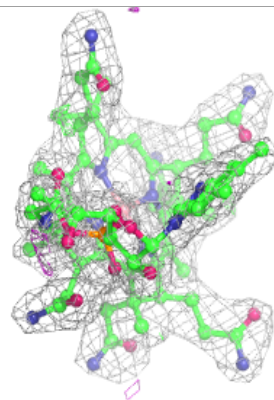
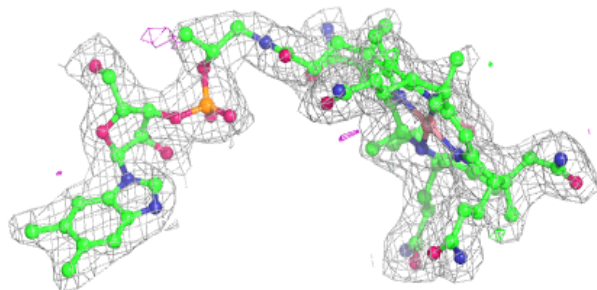
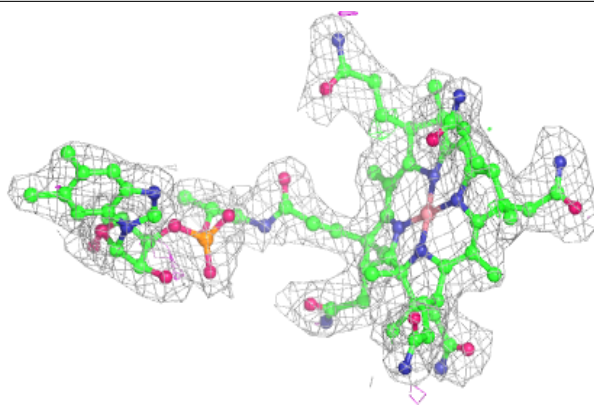
**Electron density around Z98 A 767:**

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

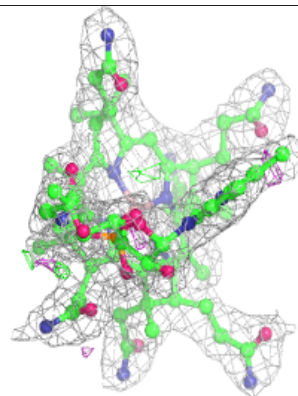
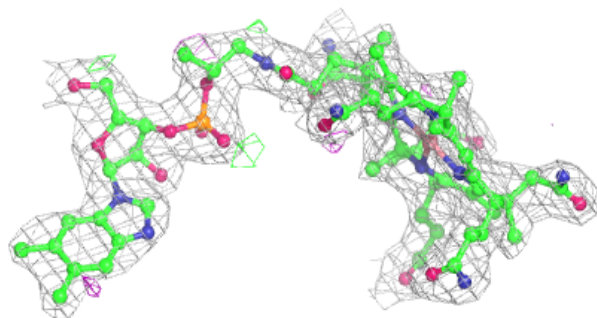
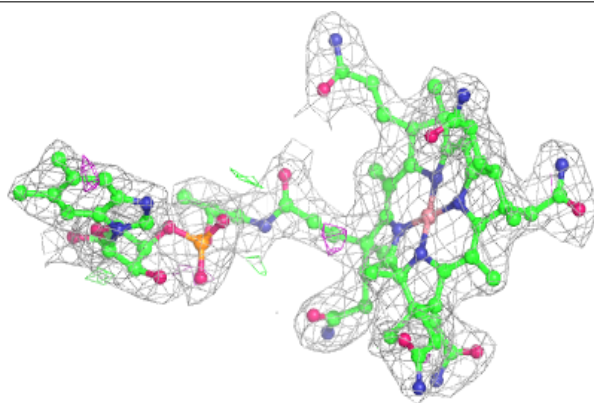


**Electron density around B12 B 1801:**

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

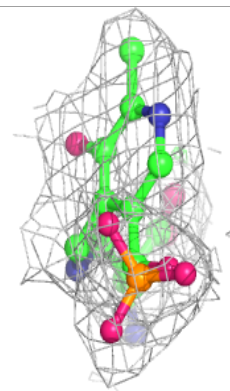
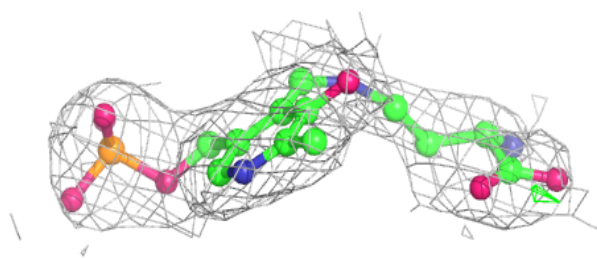
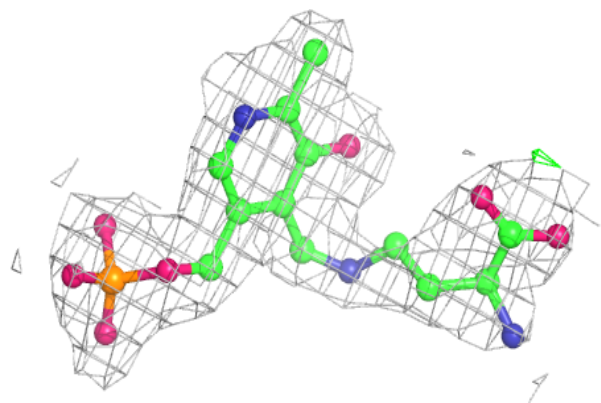
**Electron density around B12 C 1801:**

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



**Electron density around Z98 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.