



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:58 pm BST

PDB ID : 3KP1
Title : Crystal structure of ornithine 4,5 aminomutase (Resting State)
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.
Deposited on : 2009-11-14
Resolution : 2.01 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

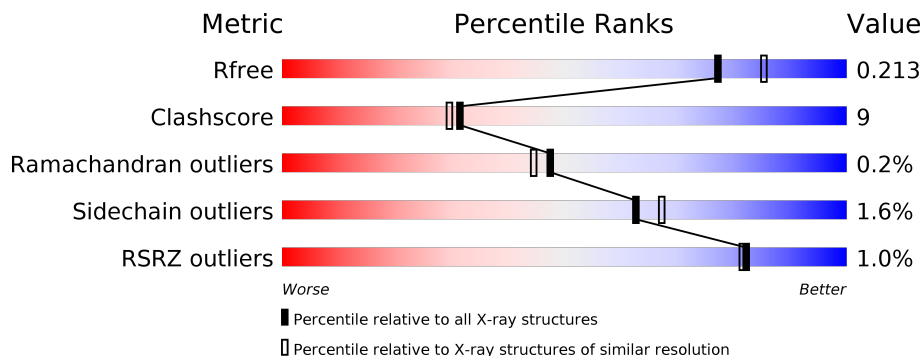
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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	2% 76% 19% 5%
1	B	763	81% 14% • 5%
1	C	763	% 82% 13% • 5%
1	D	763	% 80% 15% • 5%
2	E	121	74% 16% 10%
2	F	121	76% 13% • 10%

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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
4	B12	A	1801	X	-	X	-
4	B12	B	1801	X	-	-	-
4	B12	D	1801	X	-	X	-
5	5AD	A	767	X	-	-	-
5	5AD	B	767	X	-	-	-
5	5AD	C	767	X	-	-	-
5	5AD	D	767	X	-	-	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 29625 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
			Total	C	N	O	S			
1	A	726	5634	3550	978	1072	34	0	0	0
1	B	726	5655	3568	981	1072	34	0	0	0
1	D	726	5647	3564	981	1068	34	0	0	0
1	C	726	5633	3557	978	1064	34	0	0	0

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
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

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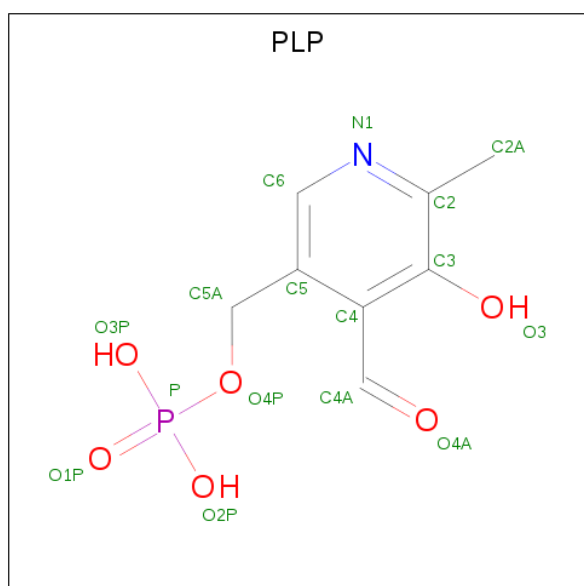
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Chain	Residue	Modelled	Actual	Comment	Reference
D	752	VAL	-	expression tag	UNP Q8VPJ5
D	753	ASP	-	expression tag	UNP Q8VPJ5
D	754	LYS	-	expression tag	UNP Q8VPJ5
D	755	LEU	-	expression tag	UNP Q8VPJ5
D	756	ALA	-	expression tag	UNP Q8VPJ5
D	757	ALA	-	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
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
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

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

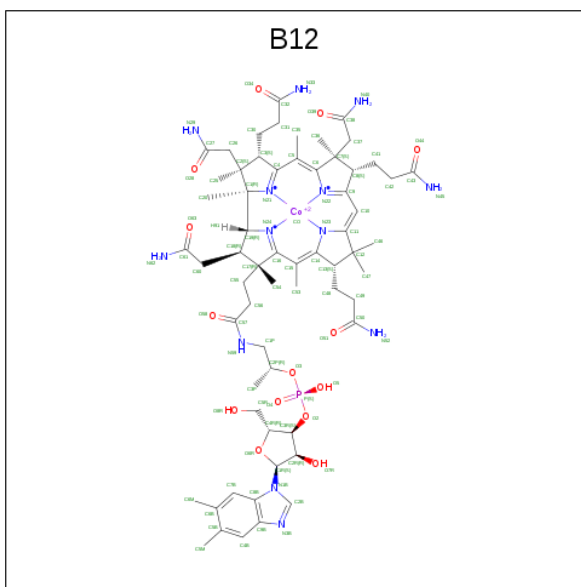
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	109	Total 855	C 538	N 152	O 161	S 4	0	0	0
2	F	109	Total 858	C 539	N 152	O 163	S 4	0	0	0
2	H	109	Total 855	C 538	N 152	O 161	S 4	0	0	0
2	G	109	Total 855	C 538	N 152	O 161	S 4	0	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



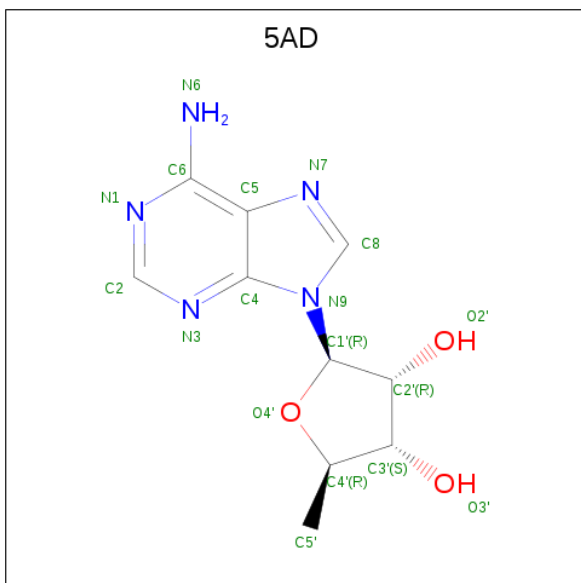
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	B	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	D	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	C	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



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

- 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	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	D	1	Total	C	N	O	0	0
			18	10	5	3		
5	C	1	Total	C	N	O	0	0
			18	10	5	3		

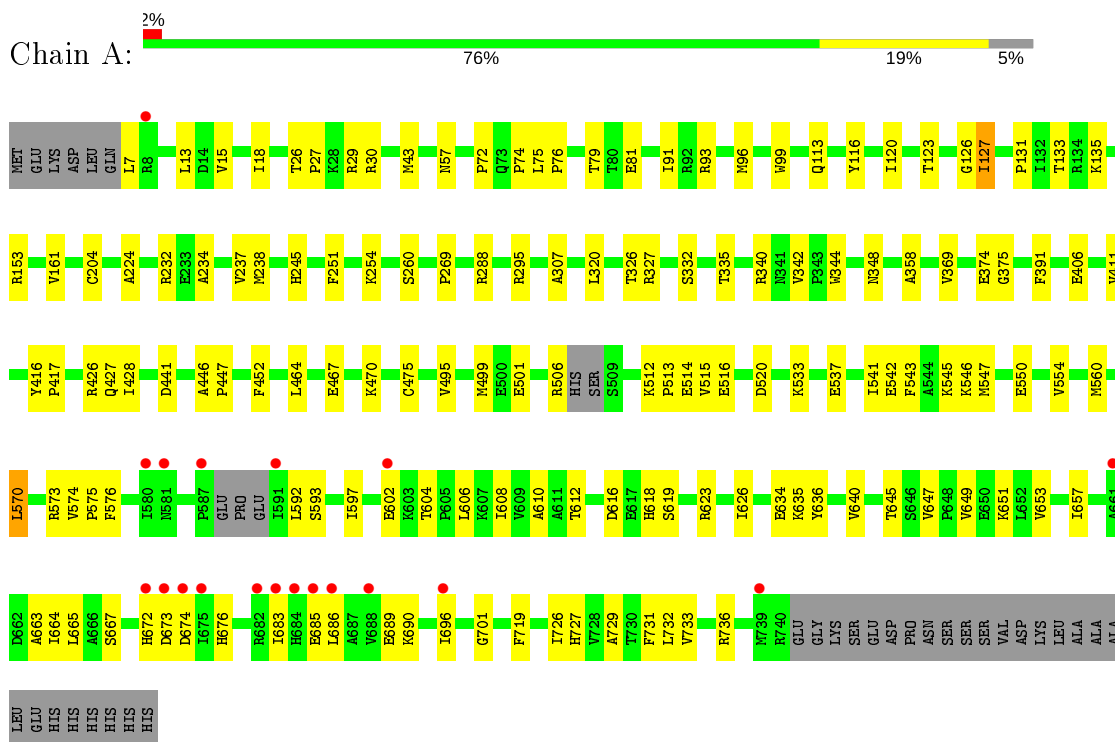
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	618	Total	O	0	0
			618	618		
6	E	108	Total	O	0	0
			108	108		
6	B	722	Total	O	0	0
			722	722		
6	F	139	Total	O	0	0
			139	139		
6	D	731	Total	O	0	0
			731	731		
6	H	111	Total	O	0	0
			111	111		
6	C	633	Total	O	0	0
			633	633		
6	G	75	Total	O	0	0
			75	75		

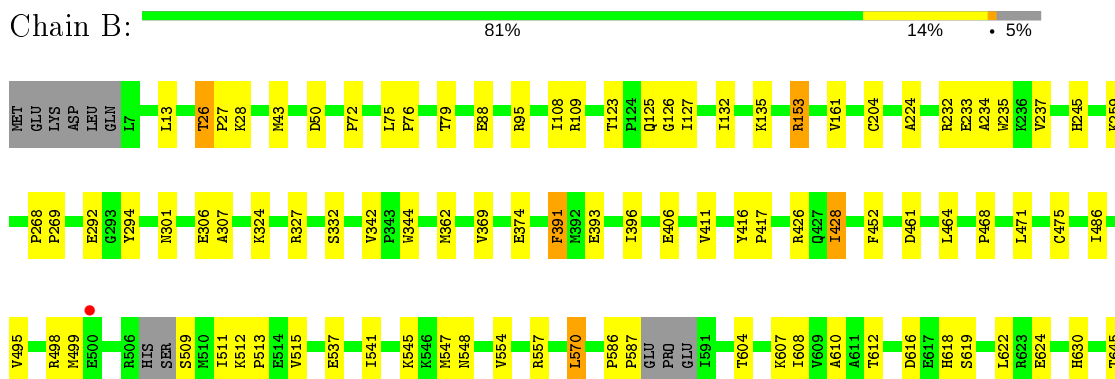
3 Residue-property plots [i](#)

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

- Molecule 1: D-ornithine aminomutase E component

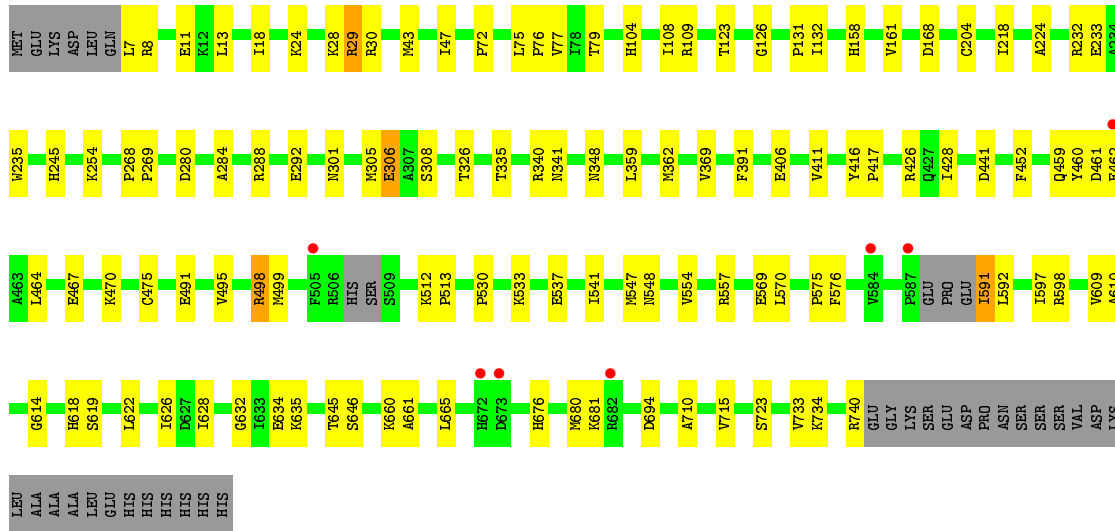
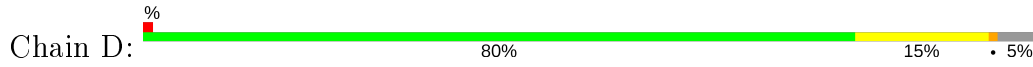


- Molecule 1: D-ornithine aminomutase E component

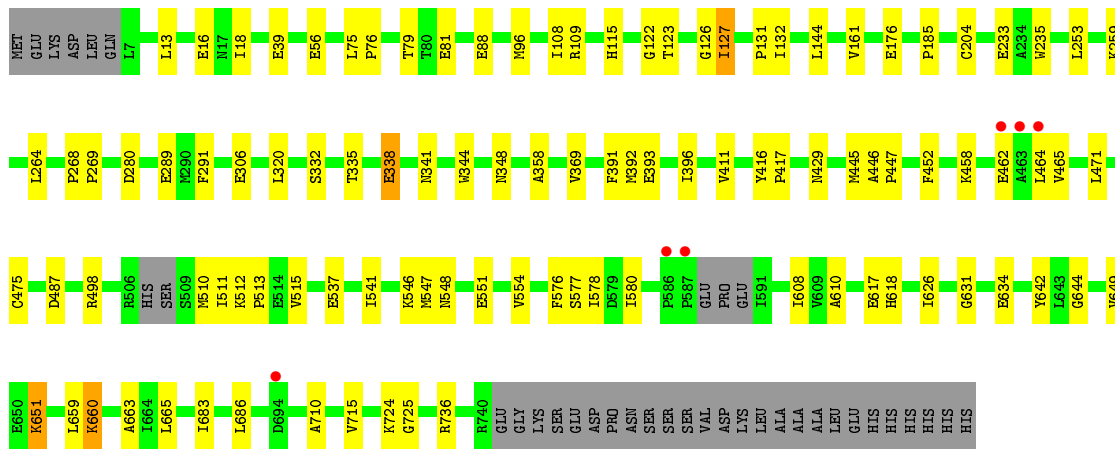
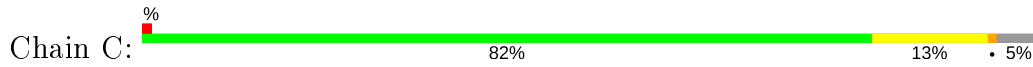




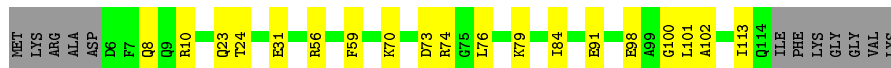
Molecule 1: D-ornithine aminomutase E component




Molecule 1: D-ornithine aminomutase E component



Molecule 2: D-ornithine aminomutase S component




Molecule 2: D-ornithine aminomutase S component

Chain F:  76% 13% 10%



• Molecule 2: D-ornithine aminomutase S component

Chain H:  80% 10% 10%



• Molecule 2: D-ornithine aminomutase S component

Chain G:  71% 19% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.43Å 234.51Å 124.56Å 90.00° 103.51° 90.00°	Depositor
Resolution (Å)	43.74 – 2.01 49.28 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.74-2.01) 99.3 (49.28-2.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0066	Depositor
R, R_{free}	0.163 , 0.216 0.162 , 0.213	Depositor DCC
R_{free} test set	12201 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtrriage
Anisotropy	0.573	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29625	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% 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: B12, 5AD, PLP

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	0.36	0/5739	0.52	0/7771
1	B	0.40	0/5760	0.55	1/7795 (0.0%)
1	C	0.33	0/5738	0.51	0/7768
1	D	0.38	0/5752	0.54	1/7785 (0.0%)
2	E	0.36	0/867	0.46	0/1163
2	F	0.40	0/870	0.51	0/1167
2	G	0.30	0/867	0.43	0/1163
2	H	0.37	0/867	0.47	0/1163
All	All	0.37	0/26460	0.52	2/35775 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	498	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	153	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	5563	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5655	0	5622	91	0
1	C	5633	0	5596	84	0
1	D	5647	0	5616	84	0
2	E	855	0	863	13	0
2	F	858	0	865	20	0
2	G	855	0	863	24	0
2	H	855	0	863	18	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	0	0
3	D	15	0	7	0	0
4	A	91	0	87	23	0
4	B	91	0	87	10	0
4	C	91	0	87	15	0
4	D	91	0	87	23	0
5	A	18	0	10	1	0
5	B	18	0	10	0	0
5	C	18	0	10	1	0
5	D	18	0	10	0	0
6	A	618	0	0	17	0
6	B	722	0	0	17	0
6	C	633	0	0	14	0
6	D	731	0	0	15	1
6	E	108	0	0	6	0
6	F	139	0	0	10	1
6	G	75	0	0	2	0
6	H	111	0	0	8	0
All	All	29625	0	26267	473	1

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 9.

The worst 5 of 473 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HA	1:A:96:MET:HE2	1.18	1.12
2:H:54:LEU:HD23	2:H:57:MET:HE1	1.29	1.09
1:D:43:MET:SD	6:D:3158:HOH:O	2.21	0.98
1:D:428:ILE:HB	6:D:1191:HOH:O	1.65	0.96
1:B:393:GLU:HG2	2:F:29:MET:HE2	1.48	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:3045:HOH:O	6:D:834:HOH:O[1_656]	1.99	0.21

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	720/763 (94%)	703 (98%)	16 (2%)	1 (0%)	51	49
1	B	720/763 (94%)	704 (98%)	14 (2%)	2 (0%)	41	37
1	C	720/763 (94%)	705 (98%)	14 (2%)	1 (0%)	51	49
1	D	720/763 (94%)	705 (98%)	14 (2%)	1 (0%)	51	49
2	E	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
2	F	107/121 (88%)	107 (100%)	0	0	100	100
2	G	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
2	H	107/121 (88%)	107 (100%)	0	0	100	100
All	All	3308/3536 (94%)	3242 (98%)	61 (2%)	5 (0%)	47	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	738	GLU
1	B	411	VAL
1	C	411	VAL
1	D	411	VAL
1	A	411	VAL

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	596/644 (92%)	586 (98%)	10 (2%)	60	65
1	B	602/644 (94%)	597 (99%)	5 (1%)	81	86
1	C	597/644 (93%)	586 (98%)	11 (2%)	59	63
1	D	600/644 (93%)	588 (98%)	12 (2%)	55	58
2	E	89/100 (89%)	86 (97%)	3 (3%)	37	36
2	F	90/100 (90%)	87 (97%)	3 (3%)	38	37
2	G	89/100 (89%)	88 (99%)	1 (1%)	73	78
2	H	89/100 (89%)	89 (100%)	0	100	100
All	All	2752/2976 (92%)	2707 (98%)	45 (2%)	62	67

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	97	ARG
1	D	341	ASN
1	C	651	LYS
1	D	168	ASP
1	D	391	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	9	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 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	767	4	17,20,20	2.42	6 (35%)	15,30,30	3.00	8 (53%)
3	PLP	C	1802	1	15,15,16	1.45	1 (6%)	20,22,23	1.04	1 (5%)
5	5AD	C	767	4	17,20,20	2.43	6 (35%)	15,30,30	3.12	8 (53%)
4	B12	D	1801	1,5	80,101,101	1.09	6 (7%)	101,166,166	2.07	20 (19%)
4	B12	B	1801	1,5	80,101,101	1.08	4 (5%)	101,166,166	2.01	18 (17%)
3	PLP	A	1802	1	15,15,16	1.42	1 (6%)	20,22,23	1.20	2 (10%)
5	5AD	B	767	4	17,20,20	2.48	6 (35%)	15,30,30	2.97	8 (53%)
4	B12	A	1801	1,5	80,101,101	1.10	5 (6%)	101,166,166	2.07	21 (20%)
3	PLP	B	1802	1	15,15,16	1.44	1 (6%)	20,22,23	1.21	3 (15%)
4	B12	C	1801	1,5	80,101,101	1.05	5 (6%)	101,166,166	2.06	18 (17%)
3	PLP	D	1802	1	15,15,16	1.44	1 (6%)	20,22,23	1.19	2 (10%)
5	5AD	D	767	4	17,20,20	2.47	6 (35%)	15,30,30	3.11	8 (53%)

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	767	4	1/1/4/4	0/0/20/20	0/3/3/3
3	PLP	C	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	C	767	4	1/1/4/4	0/0/20/20	0/3/3/3
4	B12	D	1801	1,5	1/1/36/38	8/51/223/223	0/3/11/11
4	B12	B	1801	1,5	1/1/36/38	2/51/223/223	0/3/11/11
3	PLP	A	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	B	767	4	1/1/4/4	0/0/20/20	0/3/3/3
4	B12	A	1801	1,5	1/1/36/38	7/51/223/223	0/3/11/11
3	PLP	B	1802	1	-	0/6/6/8	0/1/1/1
4	B12	C	1801	1,5	-	7/51/223/223	0/3/11/11
3	PLP	D	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	D	767	4	1/1/4/4	0/0/20/20	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	767	5AD	O4'-C1'	-7.54	1.30	1.41
5	C	767	5AD	O4'-C1'	-7.41	1.30	1.41
5	B	767	5AD	O4'-C1'	-7.40	1.30	1.41
5	A	767	5AD	O4'-C1'	-7.23	1.31	1.41
3	D	1802	PLP	C6-N1	4.67	1.44	1.34

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1801	B12	C20-C1-C19	-9.12	100.57	109.36
4	C	1801	B12	C20-C1-C19	-8.92	100.76	109.36
4	D	1801	B12	C1-C19-C18	7.89	134.98	121.93
4	A	1801	B12	C1-C19-N24	7.84	115.06	106.24
4	D	1801	B12	C20-C1-C19	-7.77	101.87	109.36

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	767	5AD	C1'
5	C	767	5AD	C1'
4	D	1801	B12	C19
4	B	1801	B12	C19
5	B	767	5AD	C1'

5 of 24 torsion outliers are listed below:

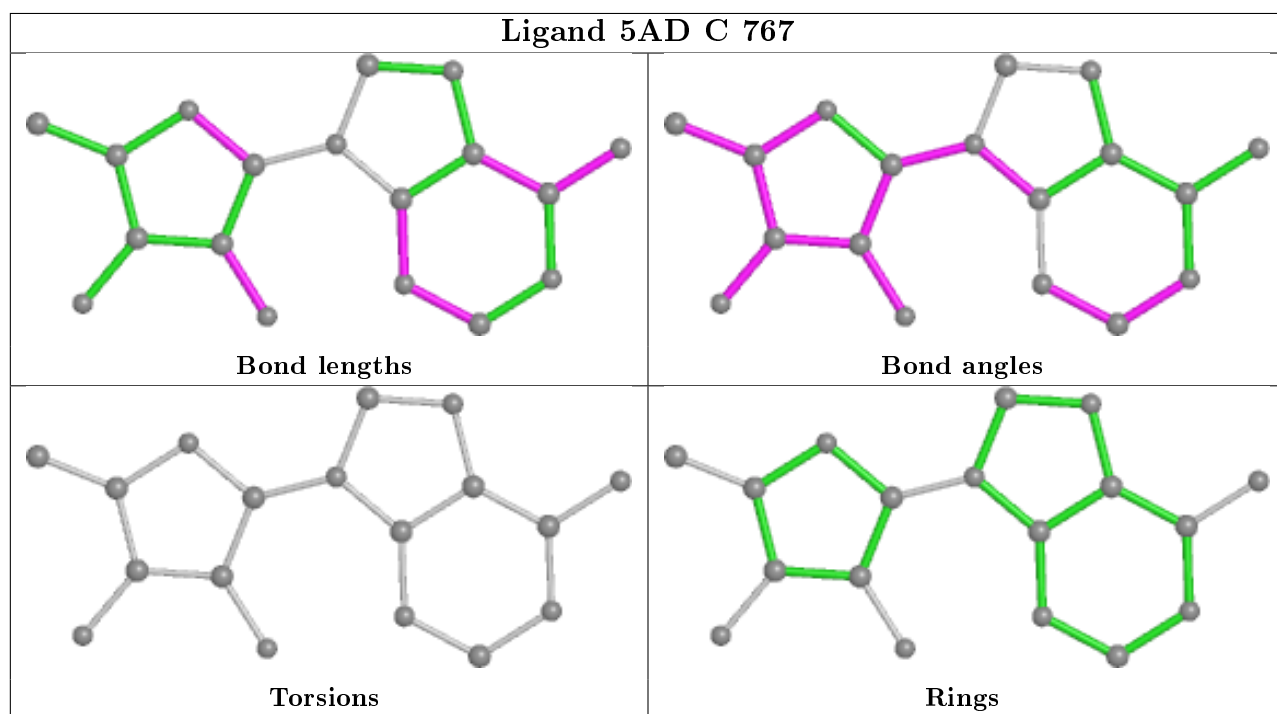
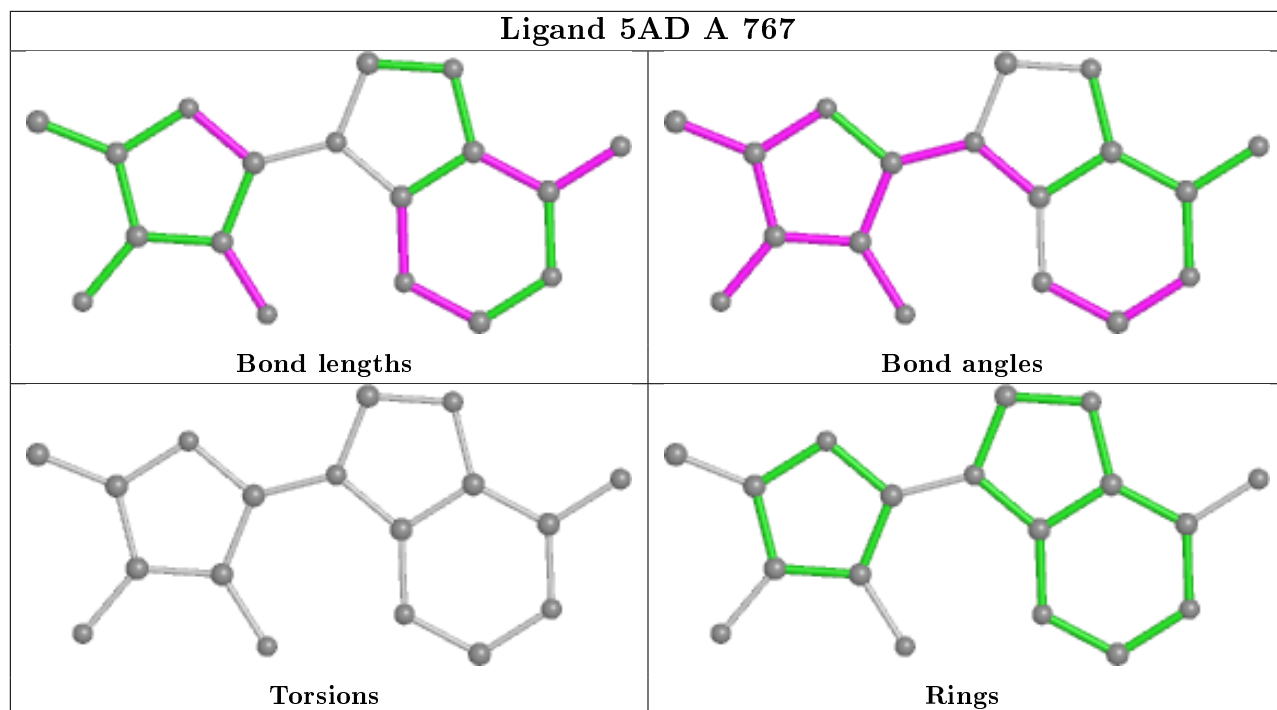
Mol	Chain	Res	Type	Atoms
4	D	1801	B12	C16-C17-C55-C56
4	D	1801	B12	C18-C17-C55-C56
4	A	1801	B12	C2-C3-C30-C31
4	A	1801	B12	C16-C17-C55-C56
4	A	1801	B12	C54-C17-C55-C56

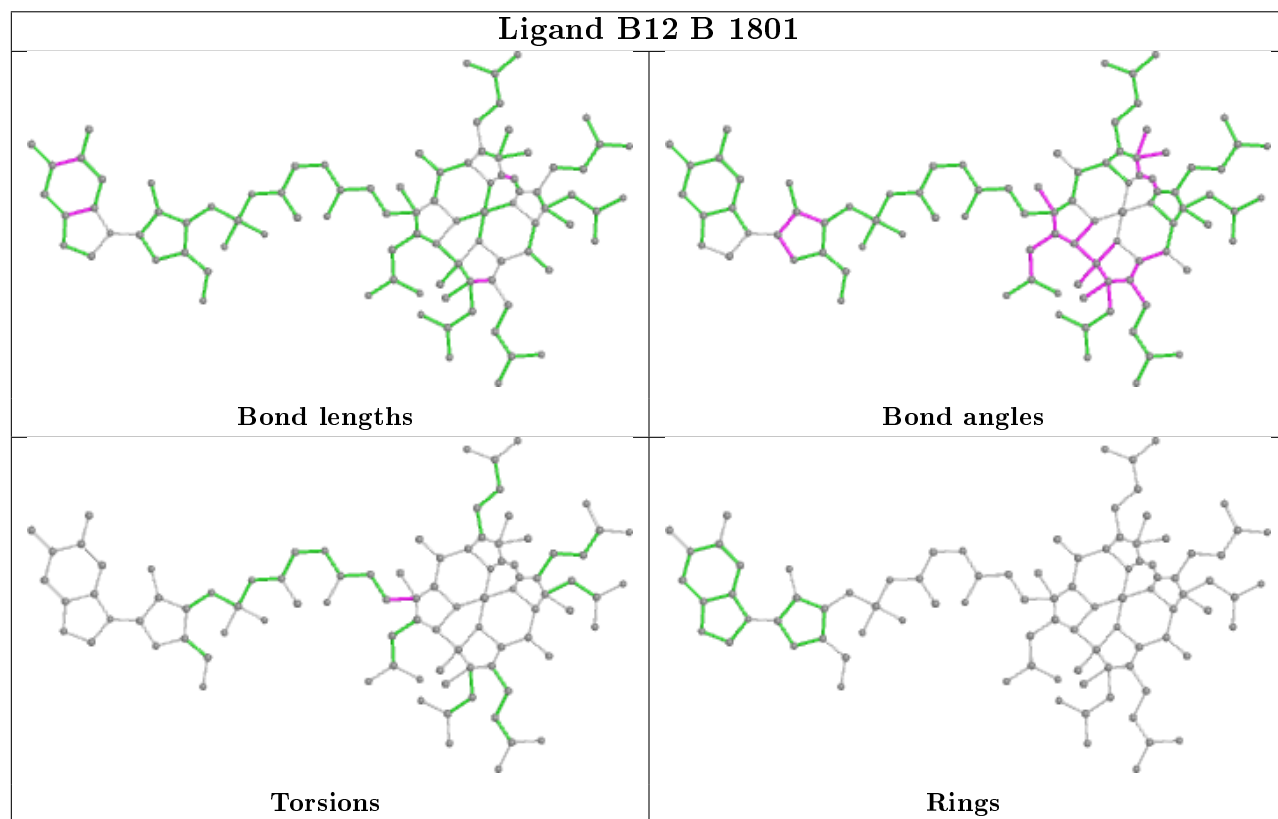
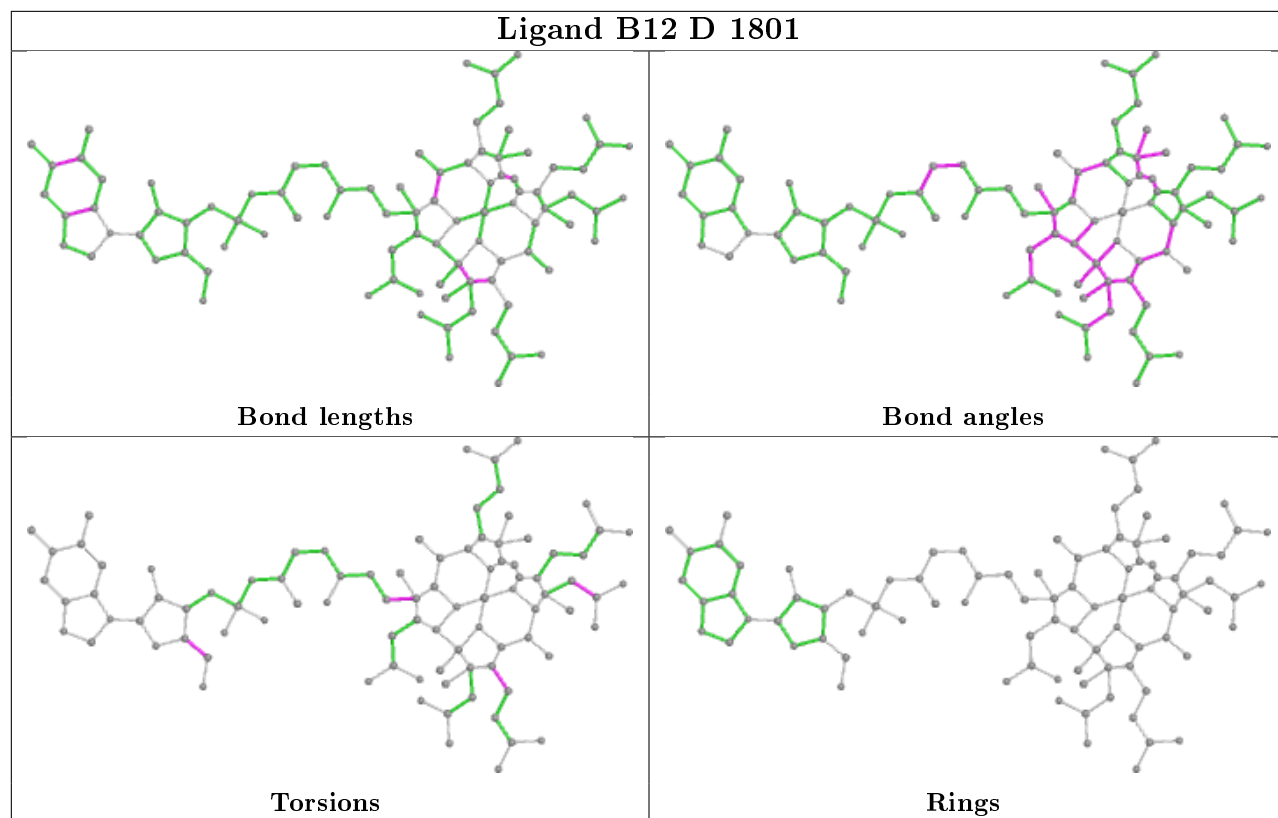
There are no ring outliers.

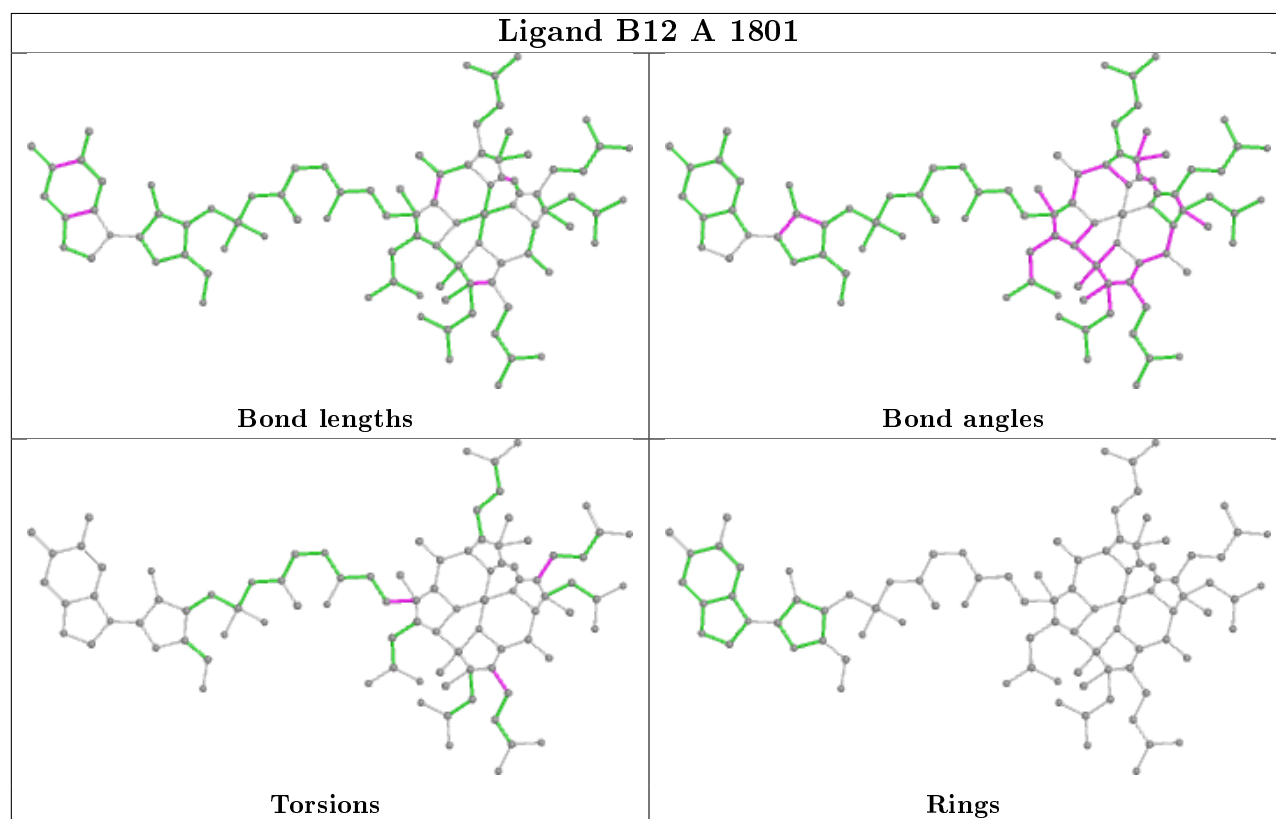
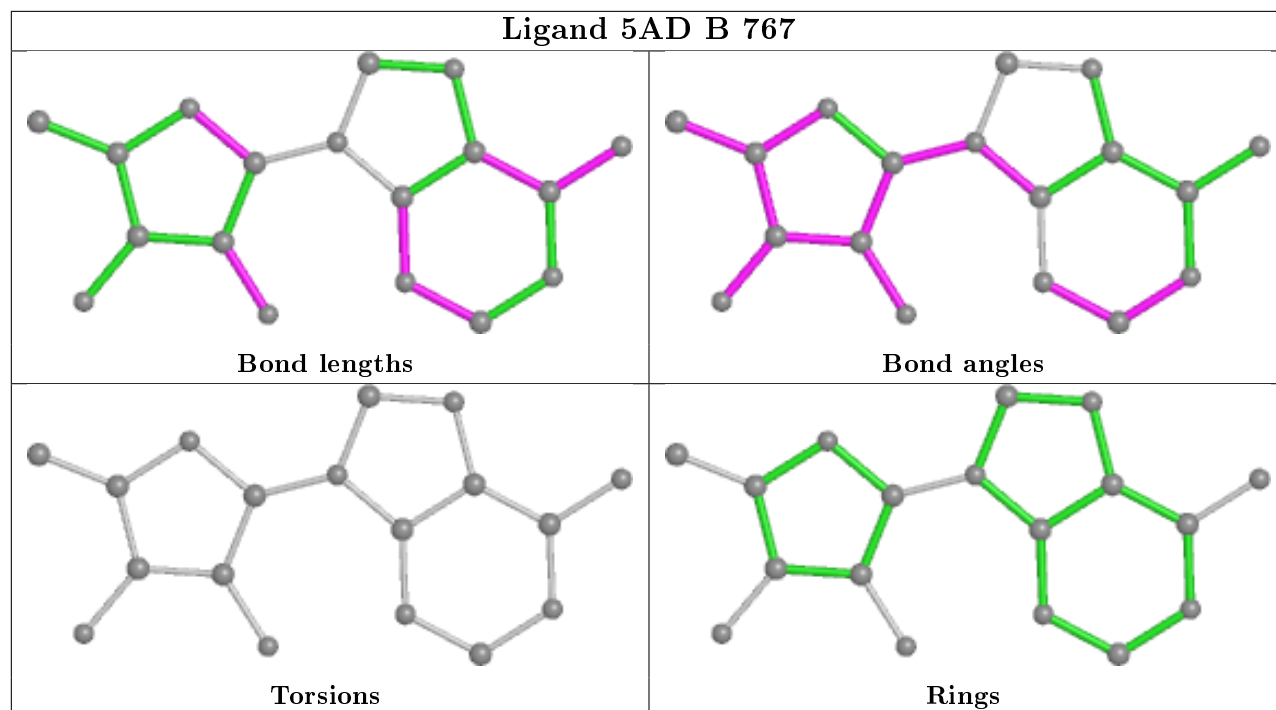
6 monomers are involved in 71 short contacts:

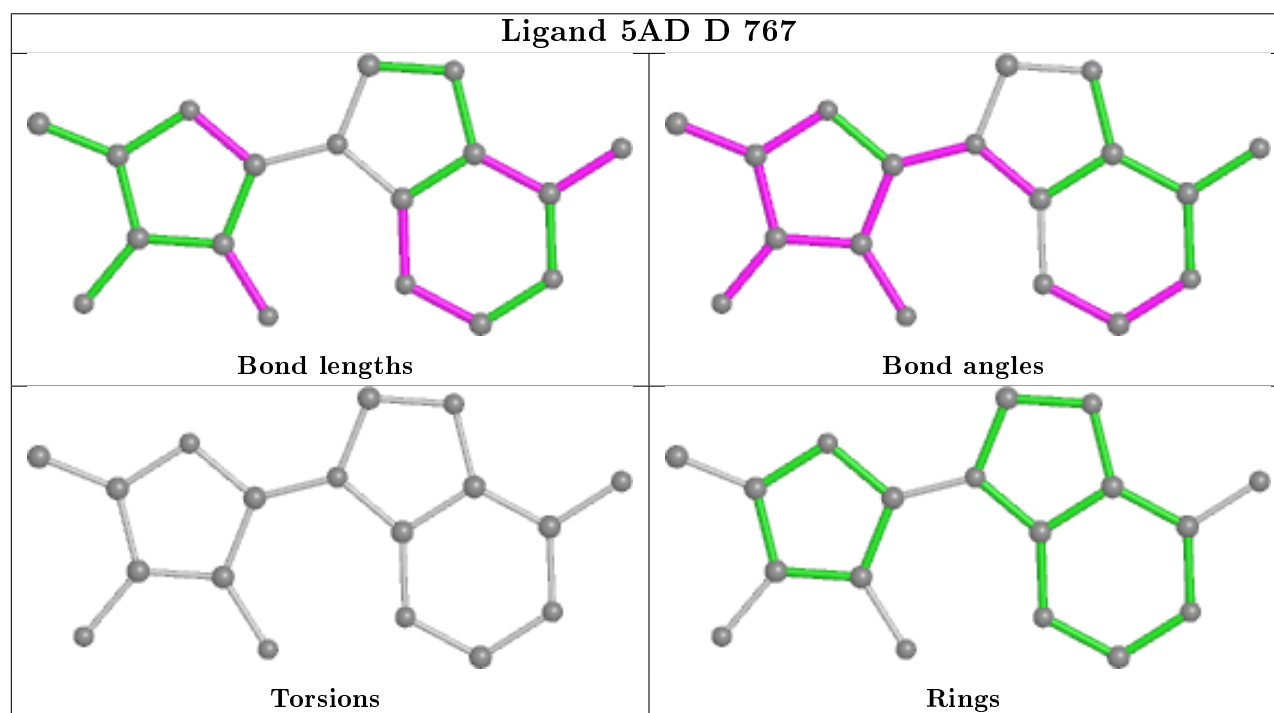
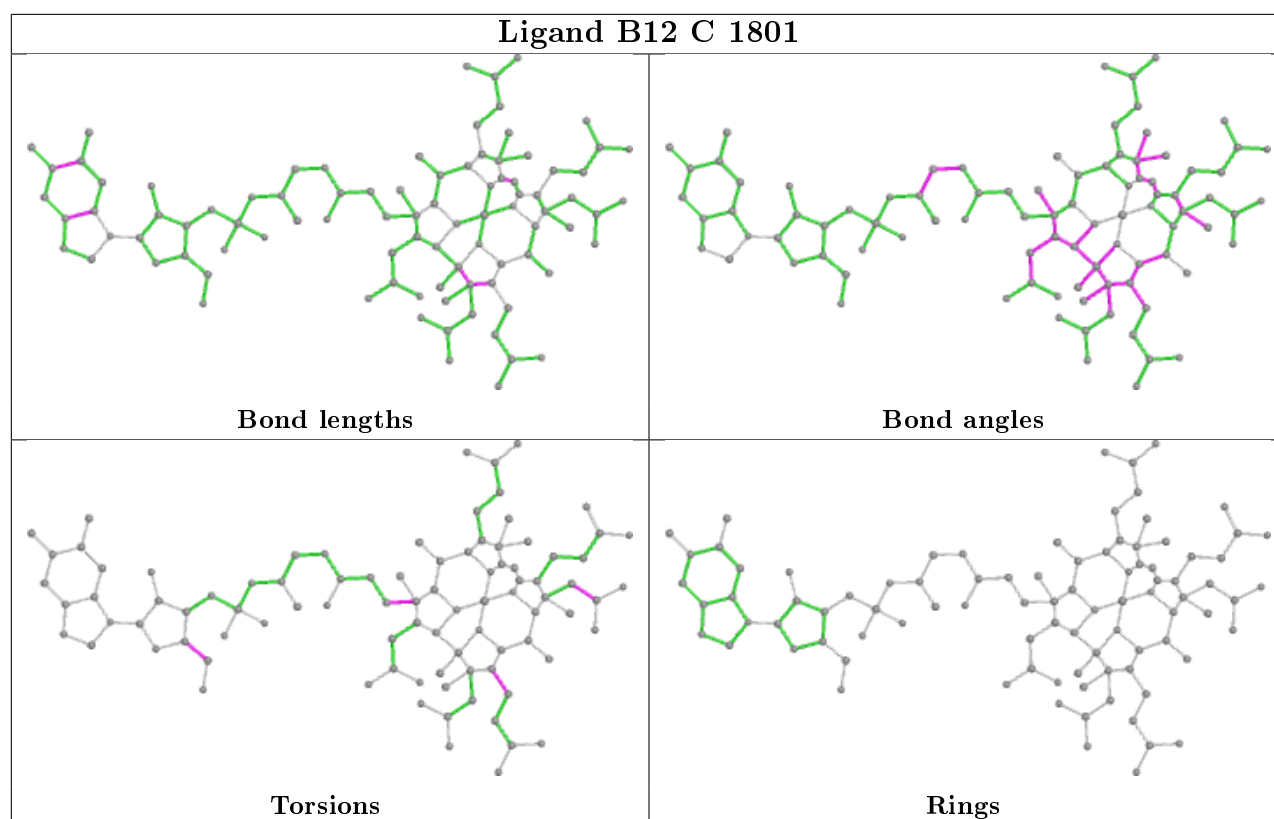
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	767	5AD	1	0
5	C	767	5AD	1	0
4	D	1801	B12	23	0
4	B	1801	B12	10	0
4	A	1801	B12	23	0
4	C	1801	B12	15	0

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

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, 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	726/763 (95%)	-0.13	19 (2%) 56 54	14, 26, 56, 73	0
1	B	726/763 (95%)	-0.41	1 (0%) 95 95	11, 23, 45, 63	0
1	C	726/763 (95%)	-0.33	6 (0%) 86 85	15, 28, 45, 61	0
1	D	726/763 (95%)	-0.39	7 (0%) 82 81	11, 23, 47, 61	0
2	E	109/121 (90%)	-0.45	0 100 100	20, 30, 47, 56	0
2	F	109/121 (90%)	-0.62	0 100 100	16, 25, 37, 47	0
2	G	109/121 (90%)	-0.10	0 100 100	24, 36, 49, 57	0
2	H	109/121 (90%)	-0.41	0 100 100	17, 29, 46, 56	0
All	All	3340/3536 (94%)	-0.33	33 (0%) 82 81	11, 26, 49, 73	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	HIS	4.0
1	C	463	ALA	3.5
1	A	587	PRO	3.5
1	A	673	ASP	3.4
1	D	587	PRO	3.1

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

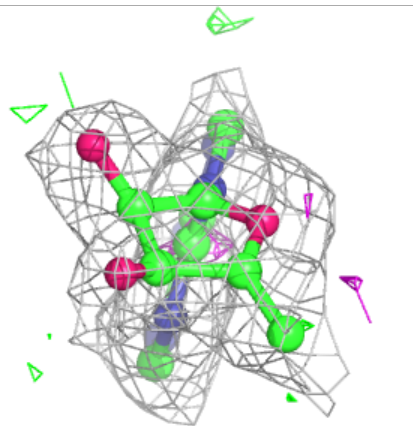
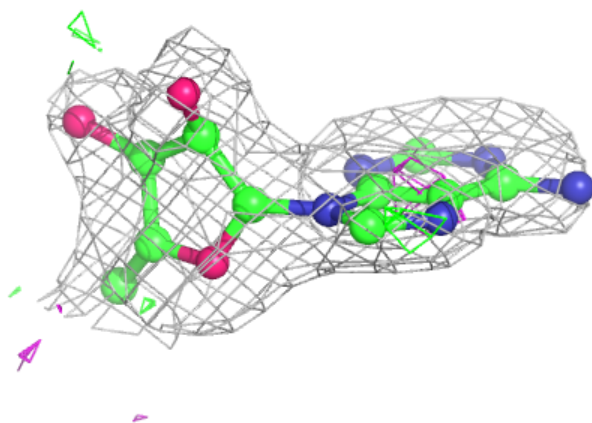
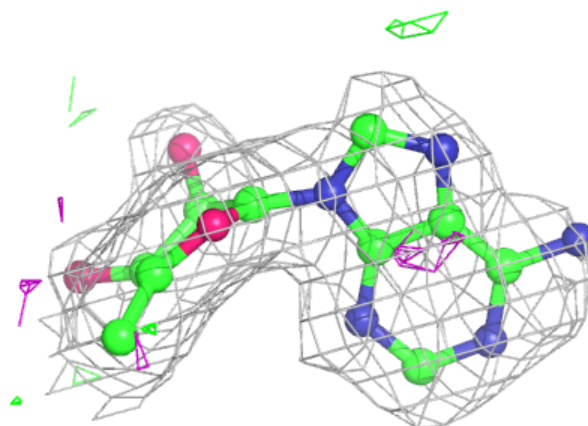
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	5AD	C	767	18/18	0.86	0.15	37,43,48,50	0
5	5AD	A	767	18/18	0.93	0.10	26,34,43,44	0
5	5AD	B	767	18/18	0.93	0.14	28,38,45,46	0
5	5AD	D	767	18/18	0.93	0.10	27,34,40,41	0
4	B12	A	1801	91/91	0.96	0.11	29,37,46,52	0
4	B12	C	1801	91/91	0.96	0.11	16,24,34,40	0
4	B12	D	1801	91/91	0.96	0.10	20,27,36,41	0
4	B12	B	1801	91/91	0.97	0.09	18,24,35,43	0
3	PLP	A	1802	15/16	0.98	0.14	22,26,33,34	0
3	PLP	D	1802	15/16	0.98	0.14	17,20,27,28	0
3	PLP	B	1802	15/16	0.98	0.13	14,20,24,25	0
3	PLP	C	1802	15/16	0.99	0.15	17,21,23,26	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.

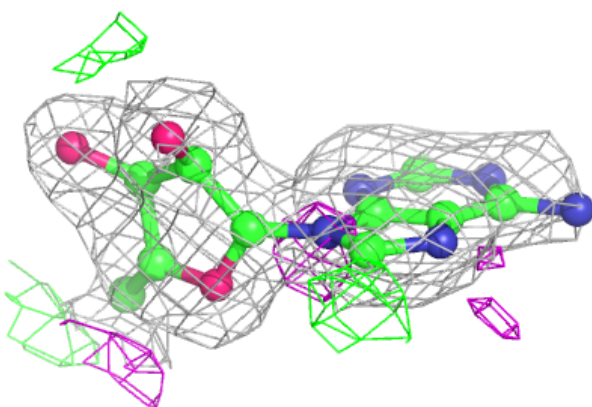
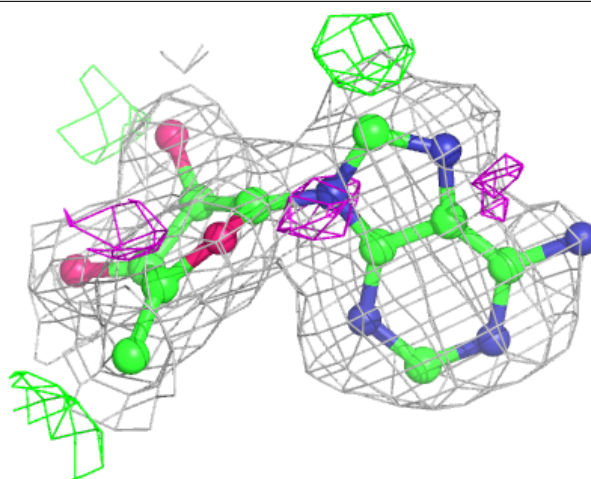
Electron density around 5AD C 767:

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



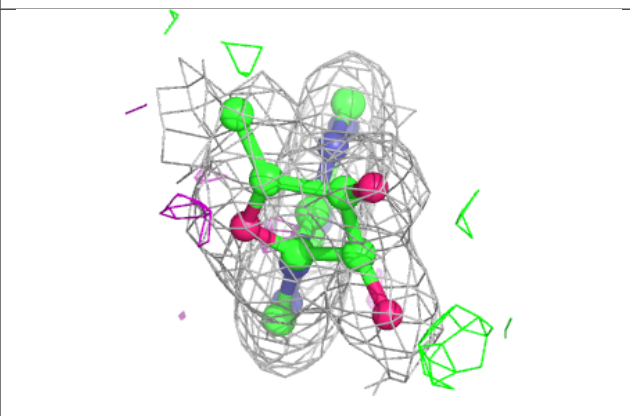
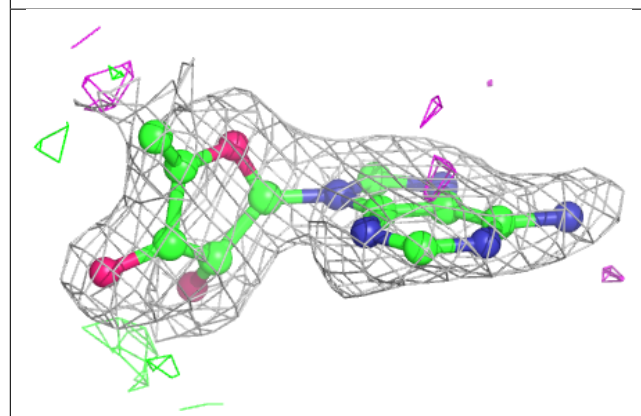
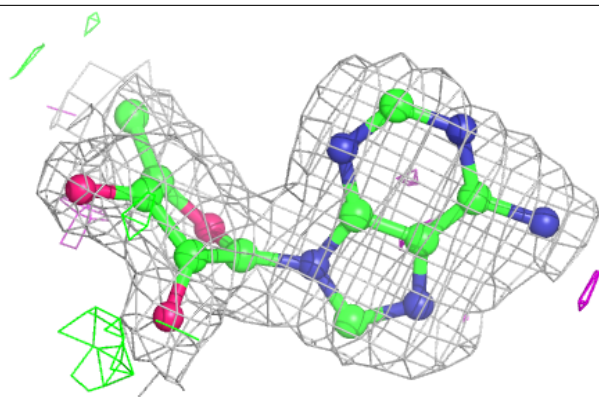
Electron density around 5AD A 767:

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



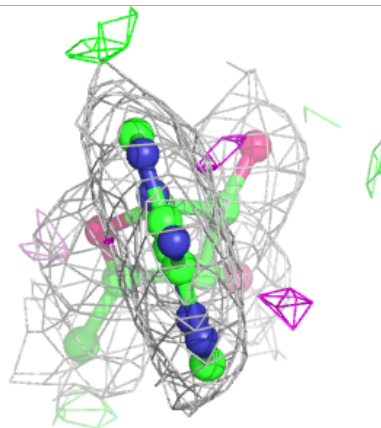
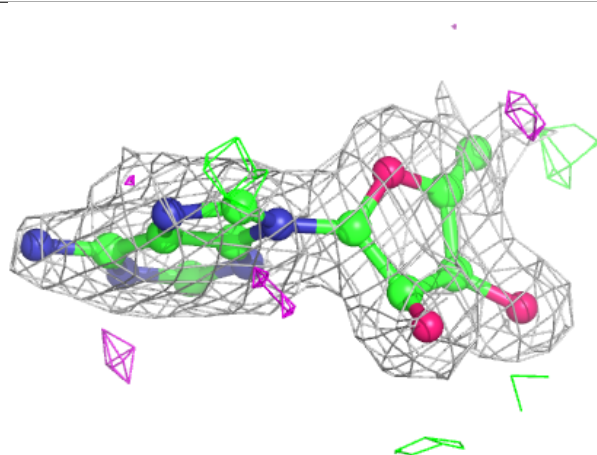
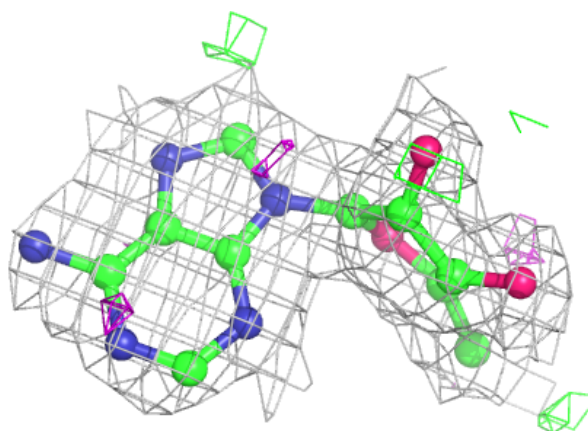
Electron density around 5AD B 767:

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



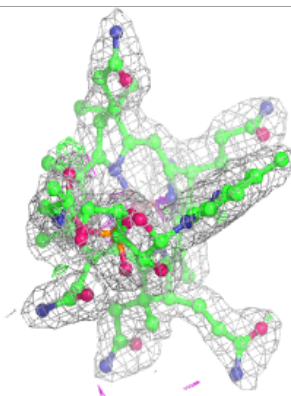
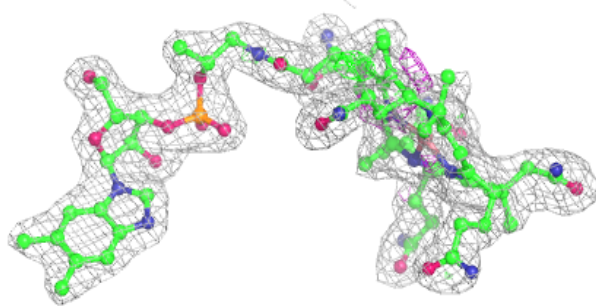
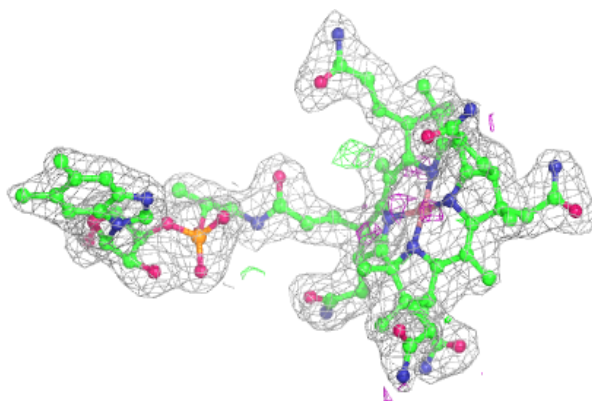
Electron density around 5AD D 767:

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

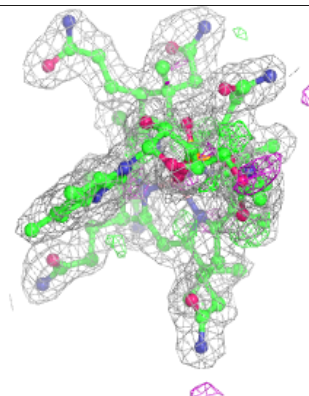
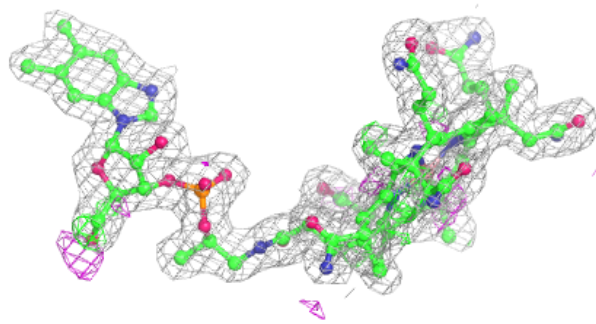
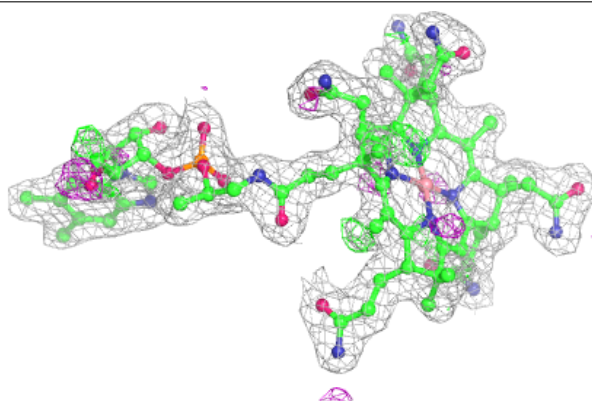


Electron density around B12 A 1801:

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

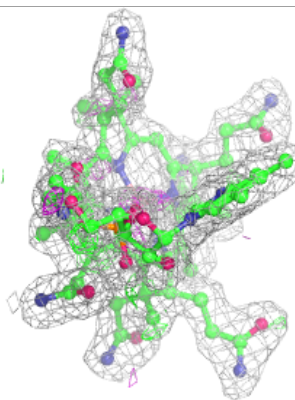
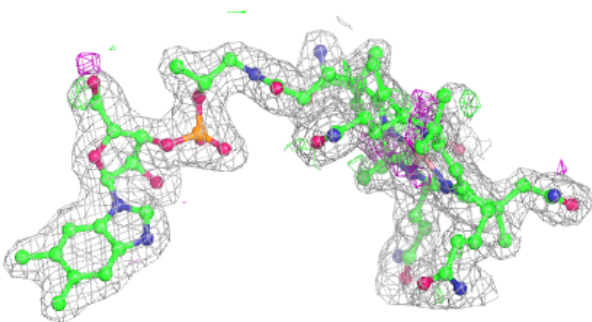
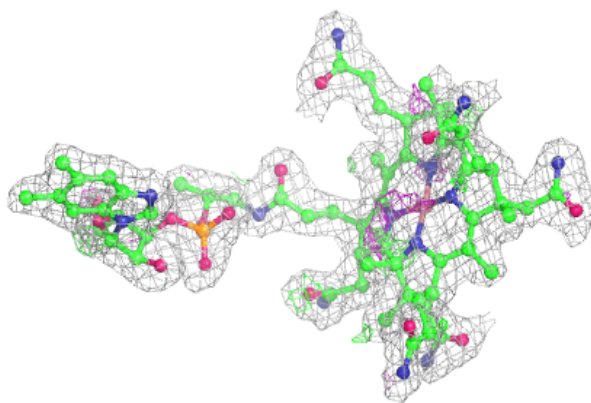
**Electron density around B12 C 1801:**

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

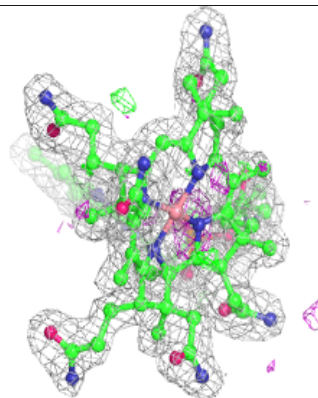
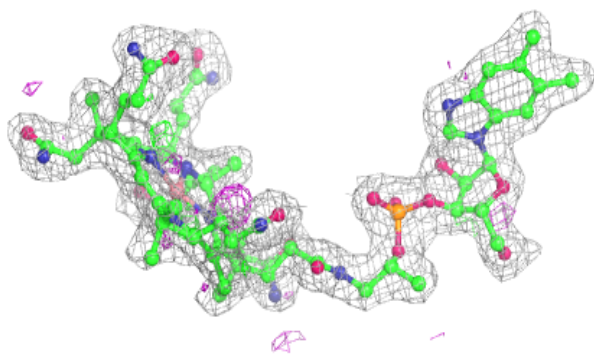
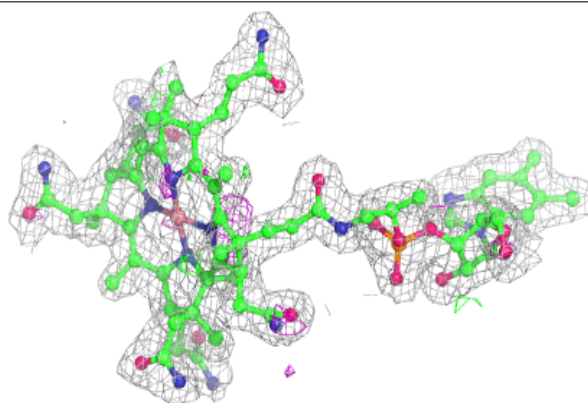


Electron density around B12 D 1801:

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

**Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.