wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 11:18 AM EDT

PDB ID	:	3KOX / pdb_00003kox
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

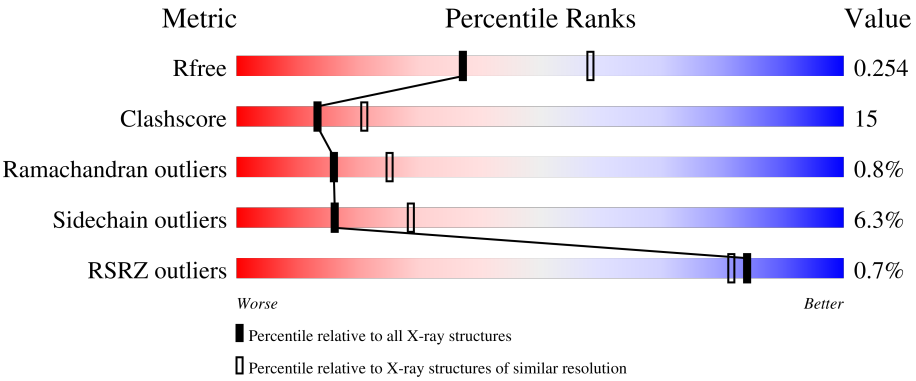
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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.



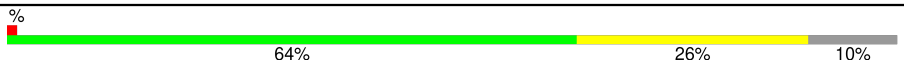
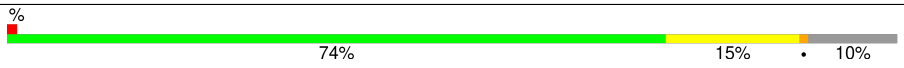
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 70% 23% • 5%
1	B	763	71% 22% • 5%
1	C	763	68% 24% • 5%
1	D	763	71% 21% • 5%
2	E	121	69% 19% • 10%

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Mol	Chain	Length	Quality of chain
2	F	121	
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	-

2 Entry composition (i)

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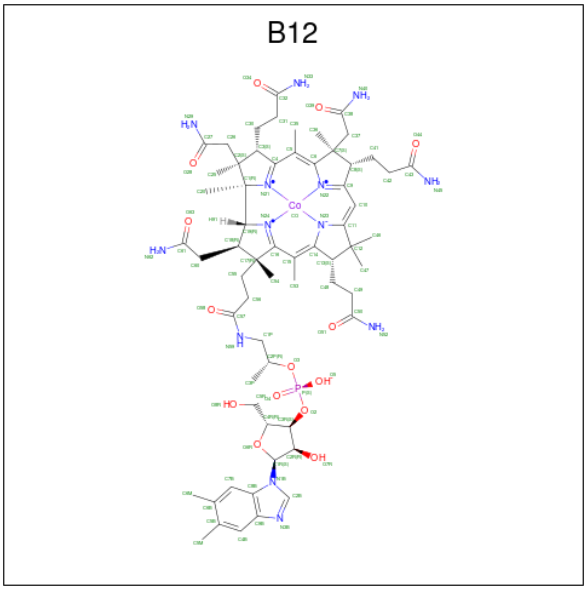
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Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA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

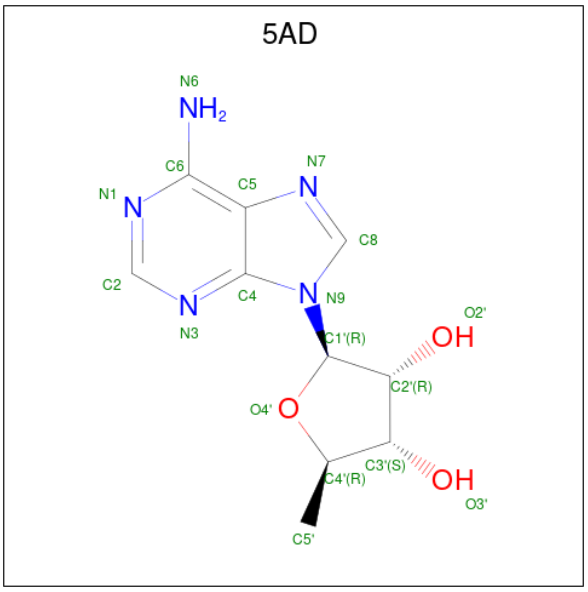
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	F	109	Total	C	N	O	S	0	0	0
			858	539	152	163	4			
2	G	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	H	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			

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



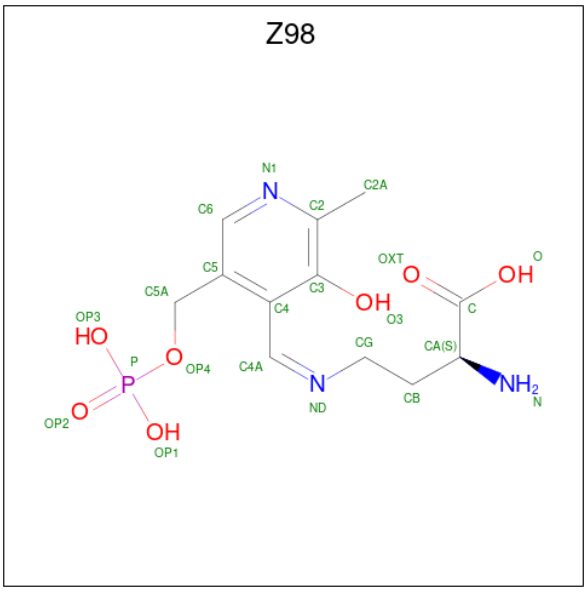
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	D	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is 5'-DEOXYADENOSINE (CCD ID: 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-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}butanoic acid (CCD ID: Z98) (formula: $C_{12}H_{18}N_3O_7P$).



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

- Molecule 6 is water.

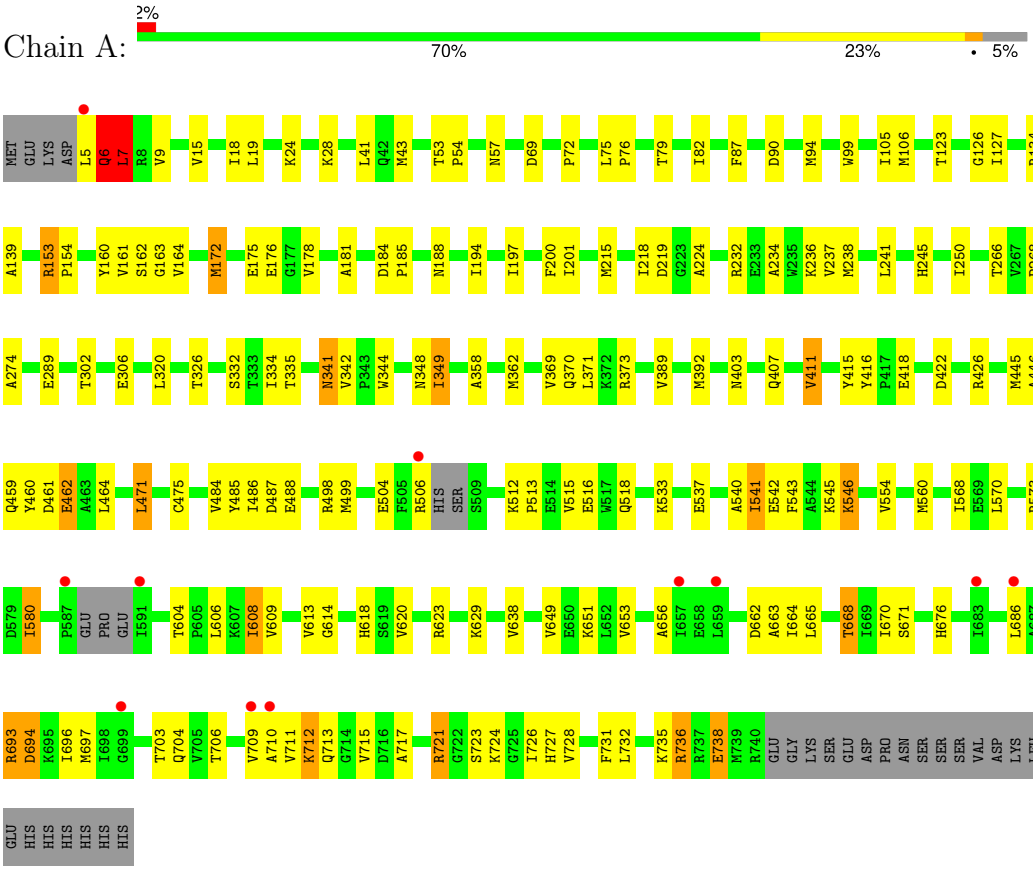
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	144	Total O 144 144	0	0
6	E	15	Total O 15 15	0	0
6	B	199	Total O 199 199	0	0
6	F	33	Total O 33 33	0	0
6	C	145	Total O 145 145	0	0
6	G	17	Total O 17 17	0	0
6	D	217	Total O 217 217	0	0
6	H	17	Total O 17 17	0	0

3 Residue-property plots (i)

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

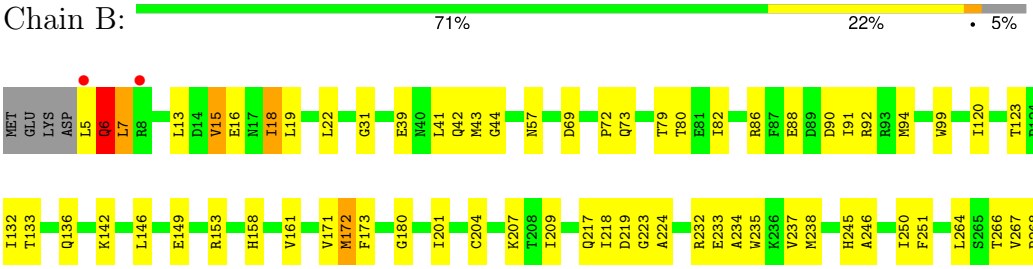
• Molecule 1: D-ornithine aminomutase E component

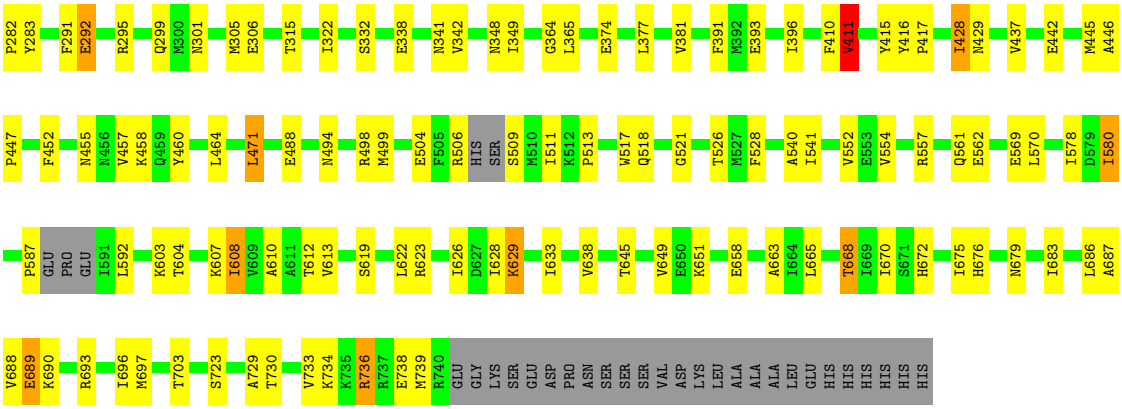
Chain A:



• Molecule 1: D-ornithine aminomutase E component

Chain B:

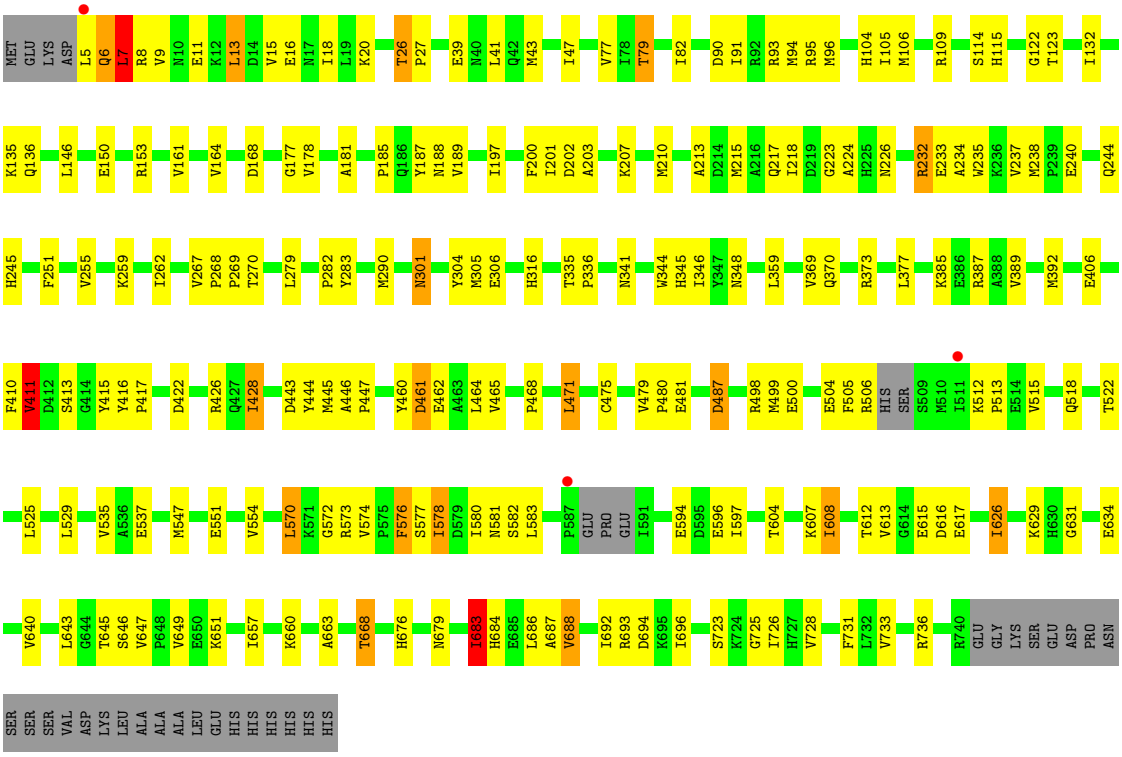




• Molecule 1: D-ornithine aminomutase E component

Chain C:

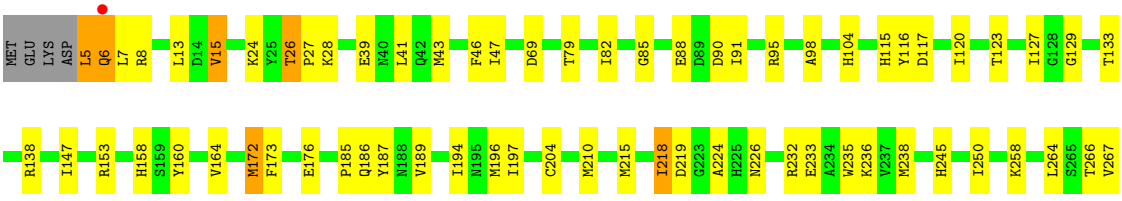


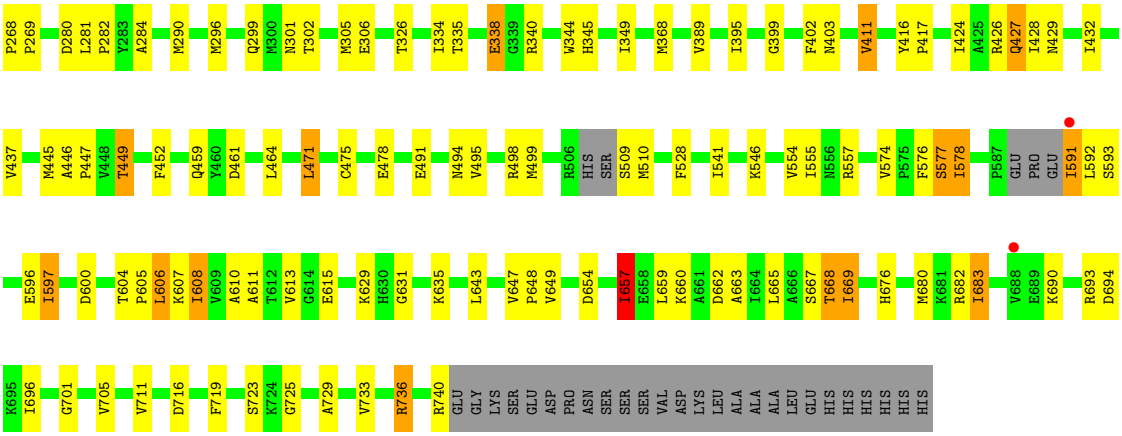


• Molecule 1: D-ornithine aminomutase E component

Chain D:







• Molecule 2: D-ornithine aminomutase S component

Chain E:

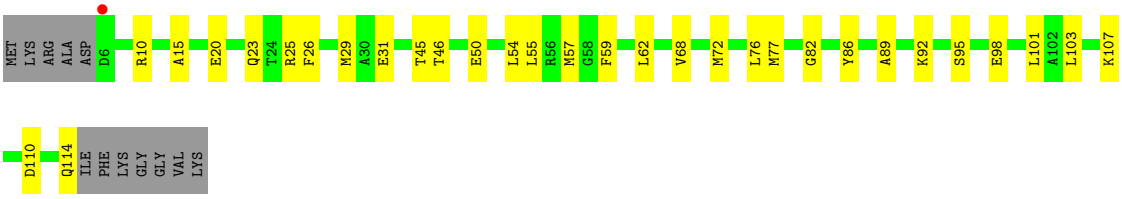




• Molecule 2: D-ornithine aminomutase S component

Chain F:





• Molecule 2: D-ornithine aminomutase S component

Chain G:

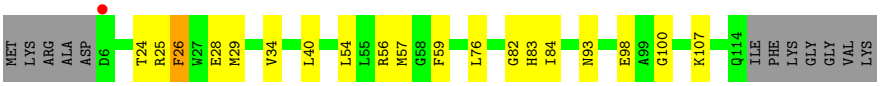




• Molecule 2: D-ornithine aminomutase S component

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.96Å 231.69Å 123.89Å 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
$< I/\sigma(I) >$ [1]	2.46 (at 2.40Å)	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 (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 5AD, B12, 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	0.95	4/5756 (0.1%)	1.01	8/7794 (0.1%)
1	B	1.03	3/5777 (0.1%)	1.04	8/7818 (0.1%)
1	C	0.93	2/5759 (0.0%)	0.99	8/7796 (0.1%)
1	D	1.04	5/5769 (0.1%)	1.02	4/7808 (0.1%)
2	E	0.89	0/867	0.95	1/1163 (0.1%)
2	F	1.08	0/870	1.08	0/1167
2	G	0.81	0/867	1.02	0/1163
2	H	0.97	0/867	0.97	1/1163 (0.1%)
All	All	0.98	14/26532 (0.1%)	1.02	30/35872 (0.1%)

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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	GLY	C-O	-8.06	1.18	1.24
1	A	326	THR	CA-C	7.54	1.56	1.52
1	D	194	ILE	CA-CB	-7.37	1.46	1.54
1	B	223	GLY	C-O	-7.24	1.19	1.24
1	D	326	THR	CA-C	6.23	1.55	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	647	VAL	CA-C-N	-8.31	111.46	119.85
1	C	647	VAL	C-N-CA	-8.31	111.46	119.85
1	C	683	ILE	CB-CA-C	-7.66	101.98	112.24
1	B	629	LYS	N-CA-C	7.01	119.52	111.11
1	B	342	VAL	N-CA-C	-6.96	102.54	109.02

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	164	0
1	B	5672	0	5644	185	0
1	C	5654	0	5621	182	0
1	D	5664	0	5636	161	0
2	E	855	0	863	17	0
2	F	858	0	865	24	0
2	G	855	0	863	23	0
2	H	855	0	863	16	0
3	A	91	0	87	17	0
3	B	91	0	87	20	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	11	0
5	B	23	0	14	8	0
5	C	23	0	14	8	0
5	D	23	0	14	8	0
6	A	144	0	0	8	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	14	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	782	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 15.

The worst 5 of 782 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:A:629:LYS:NZ	5:C:767:Z98:H4A	1.64	1.12
1:B:396:ILE:HD12	2:F:29:MET:HE3	1.26	1.12
2:F:54:LEU:HD23	2:F:57:MET:CE	1.78	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%)	16	25
1	B	722/763 (95%)	683 (95%)	32 (4%)	7 (1%)	12	20
1	C	722/763 (95%)	691 (96%)	22 (3%)	9 (1%)	10	16
1	D	722/763 (95%)	690 (96%)	30 (4%)	2 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	107/121 (88%)	101 (94%)	5 (5%)	1 (1%)	14	22
2	F	107/121 (88%)	103 (96%)	3 (3%)	1 (1%)	14	22
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%)	16	25

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 (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	598/644 (93%)	559 (94%)	39 (6%)	15	27
1	B	604/644 (94%)	574 (95%)	30 (5%)	22	38
1	C	600/644 (93%)	565 (94%)	35 (6%)	18	32
1	D	602/644 (94%)	556 (92%)	46 (8%)	12	21
2	E	89/100 (89%)	82 (92%)	7 (8%)	11	19
2	F	90/100 (90%)	85 (94%)	5 (6%)	19	33
2	G	89/100 (89%)	82 (92%)	7 (8%)	11	19
2	H	89/100 (89%)	84 (94%)	5 (6%)	19	33
All	All	2761/2976 (93%)	2587 (94%)	174 (6%)	16	29

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	736	ARG
1	D	449	THR
2	G	76	LEU
1	D	39	GLU
1	D	591	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	8	GLN
1	D	341	ASN
2	G	16	ASN
1	D	36	GLN
1	D	403	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (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	$\#\|Z\|>2$
3	B12	D	1801	1	94,101,101	1.48	12 (12%)	149,166,166	2.39	36 (24%)
4	5AD	D	1500	-	20,20,20	1.72	4 (20%)	28,30,30	3.14	13 (46%)
5	Z98	A	767	-	22,23,23	1.96	8 (36%)	27,32,32	2.32	5 (18%)
5	Z98	B	767	-	22,23,23	1.55	6 (27%)	27,32,32	1.82	7 (25%)
4	5AD	C	1500	-	20,20,20	1.74	3 (15%)	28,30,30	2.75	13 (46%)
5	Z98	C	767	-	22,23,23	1.55	2 (9%)	27,32,32	1.73	6 (22%)
3	B12	B	1801	1	94,101,101	1.77	11 (11%)	149,166,166	2.41	34 (22%)
4	5AD	A	1500	-	20,20,20	1.80	5 (25%)	28,30,30	2.85	15 (53%)
3	B12	C	1801	1	94,101,101	1.75	13 (13%)	149,166,166	2.56	37 (24%)
5	Z98	D	767	-	22,23,23	1.53	3 (13%)	27,32,32	1.61	4 (14%)
4	5AD	B	1500	-	20,20,20	1.73	4 (20%)	28,30,30	2.55	12 (42%)
3	B12	A	1801	1	94,101,101	1.47	11 (11%)	149,166,166	2.49	39 (26%)

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
3	B12	D	1801	1	-	6/56/223/223	0/3/11/11
4	5AD	D	1500	-	1/1/4/4	0/4/20/20	0/3/3/3
5	Z98	A	767	-	-	10/17/17/17	0/1/1/1
5	Z98	B	767	-	-	7/17/17/17	0/1/1/1
4	5AD	C	1500	-	-	0/4/20/20	0/3/3/3
5	Z98	C	767	-	-	7/17/17/17	0/1/1/1
3	B12	B	1801	1	1/1/36/38	7/56/223/223	0/3/11/11
4	5AD	A	1500	-	1/1/4/4	0/4/20/20	0/3/3/3
3	B12	C	1801	1	1/1/36/38	10/56/223/223	0/3/11/11
5	Z98	D	767	-	-	8/17/17/17	0/1/1/1
4	5AD	B	1500	-	-	0/4/20/20	0/3/3/3
3	B12	A	1801	1	1/1/36/38	18/56/223/223	0/3/11/11

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C19-N24	-9.96	1.36	1.49
3	B	1801	B12	C19-N24	-9.45	1.37	1.49
3	B	1801	B12	C14-N23	6.99	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1801	B12	C14-N23	6.71	1.44	1.35
3	A	1801	B12	C14-N23	5.93	1.43	1.35

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1801	B12	C20-C1-C19	-11.59	98.19	109.35
3	A	1801	B12	C20-C1-C19	-10.08	99.64	109.35
3	A	1801	B12	C1-C19-N24	9.38	116.69	106.25
3	C	1801	B12	C20-C1-C19	-9.37	100.33	109.35
3	C	1801	B12	C12-C11-C10	-9.11	111.66	123.40

All (5) chirality outliers are listed below:

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

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C2R-C1R-N1B-C2B
5	A	767	Z98	C5A-OP4-P-OP1
5	A	767	Z98	C5A-OP4-P-OP2
5	A	767	Z98	C5A-OP4-P-OP3

There are no ring outliers.

12 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1801	B12	14	0
4	D	1500	5AD	4	0
5	A	767	Z98	11	0
5	B	767	Z98	8	0
4	C	1500	5AD	3	0
5	C	767	Z98	8	0
3	B	1801	B12	20	0

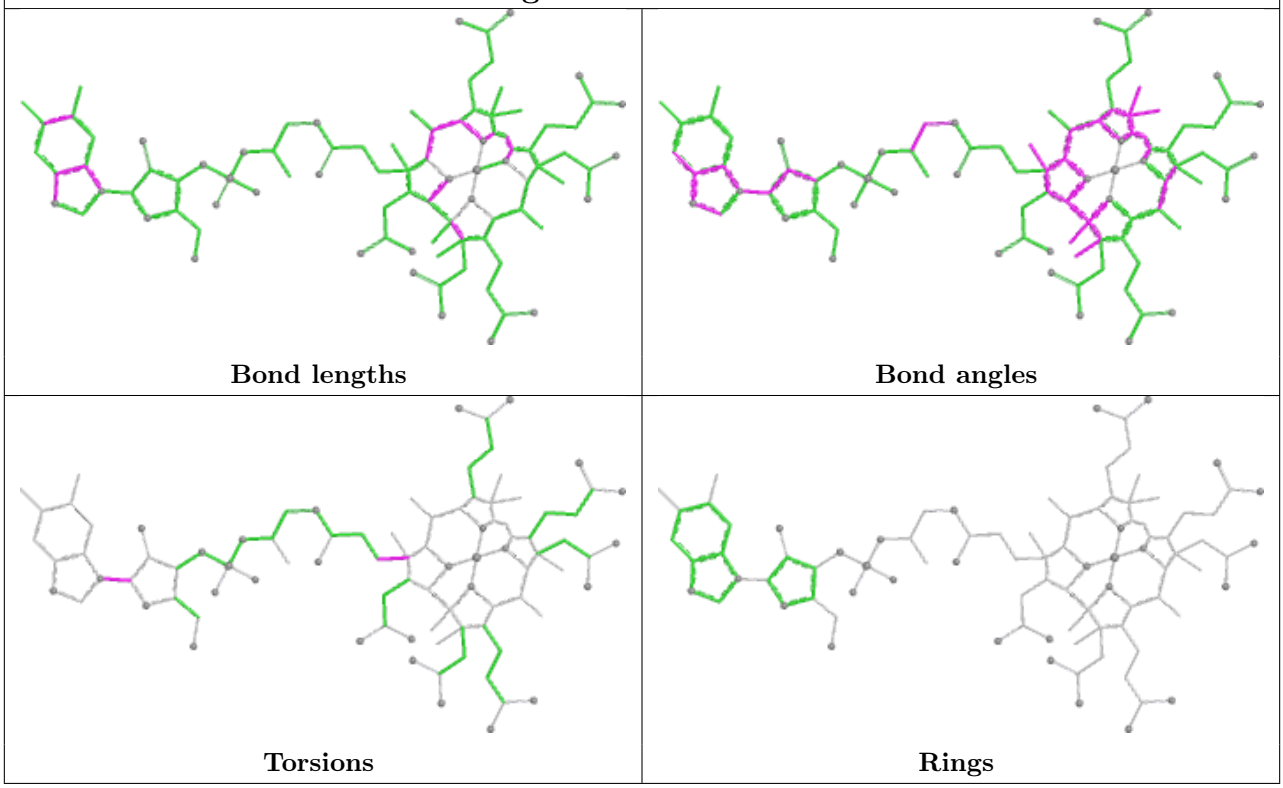
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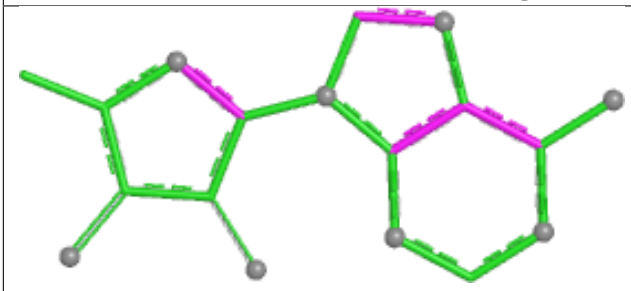
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1500	5AD	2	0
3	C	1801	B12	16	0
5	D	767	Z98	8	0
4	B	1500	5AD	2	0
3	A	1801	B12	17	0

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 then 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.

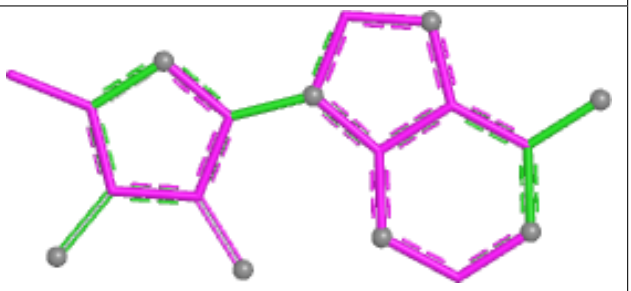
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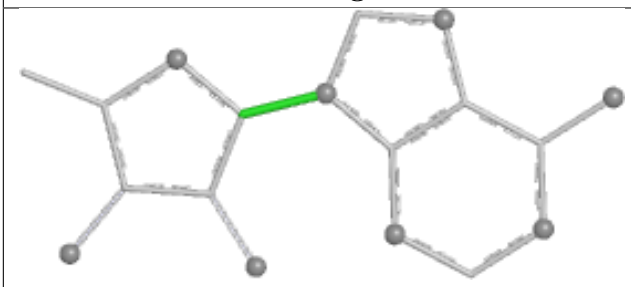
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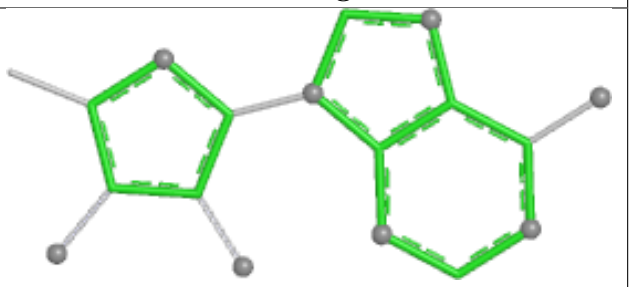
Bond lengths



Bond angles

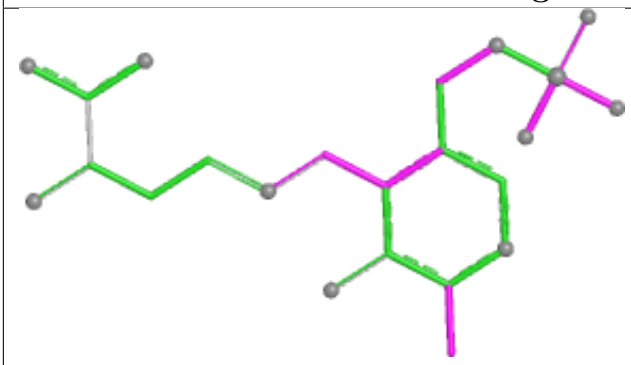


Torsions

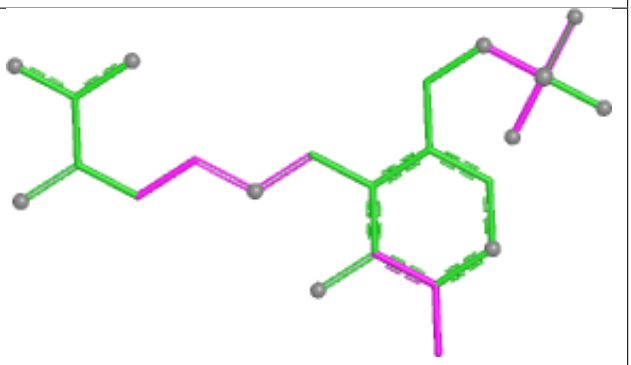


Rings

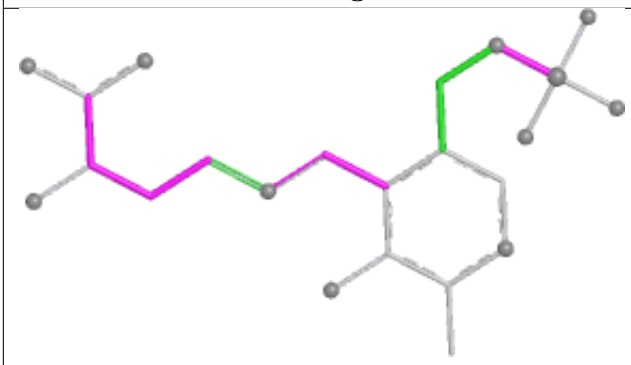
Ligand Z98 A 767



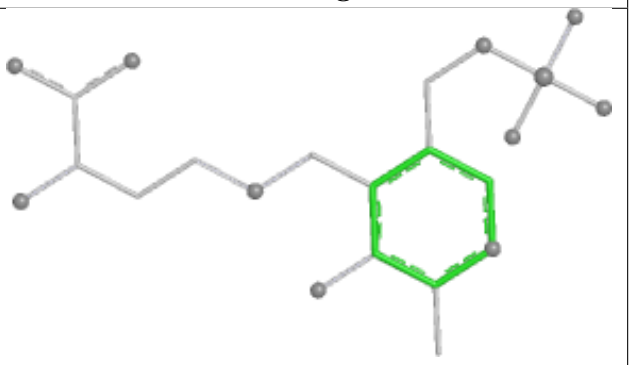
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Bond angles

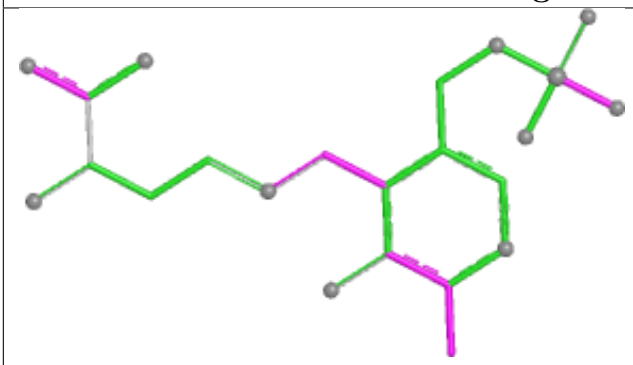


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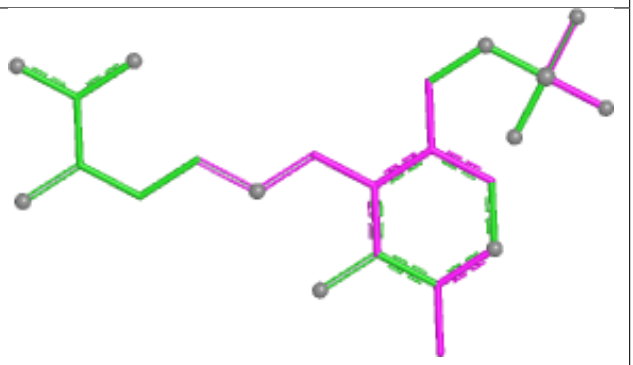


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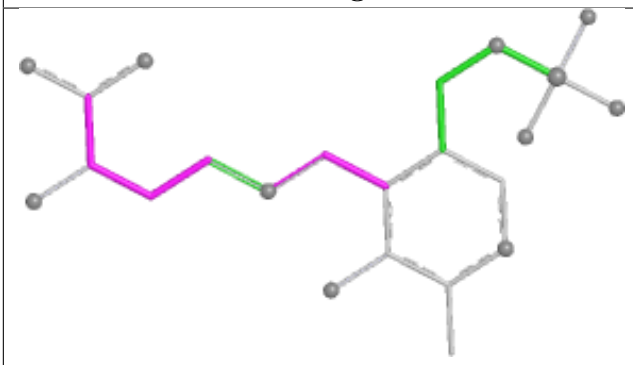
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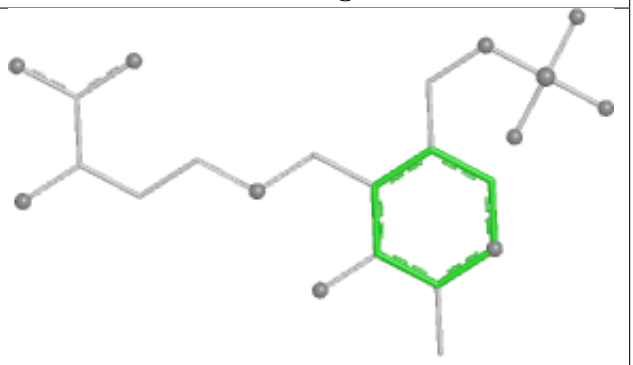
Bond lengths



Bond angles

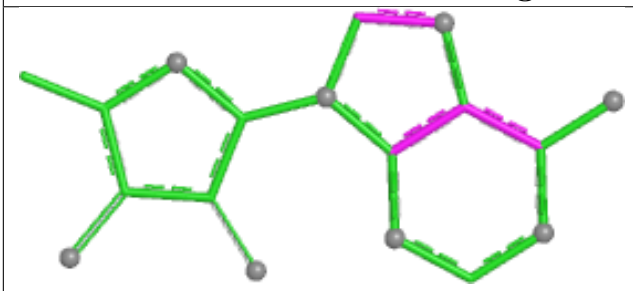


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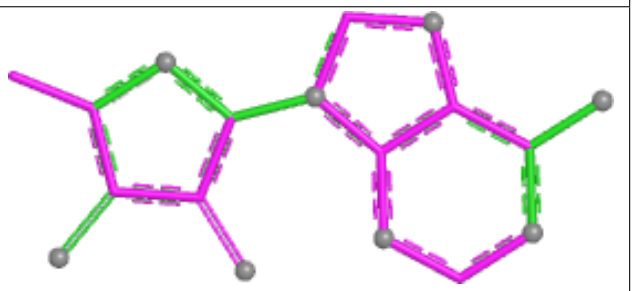


Rings

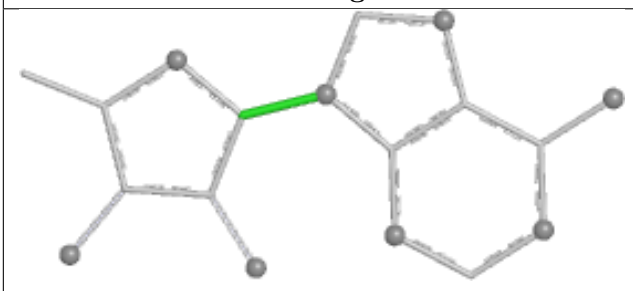
Ligand 5AD C 1500



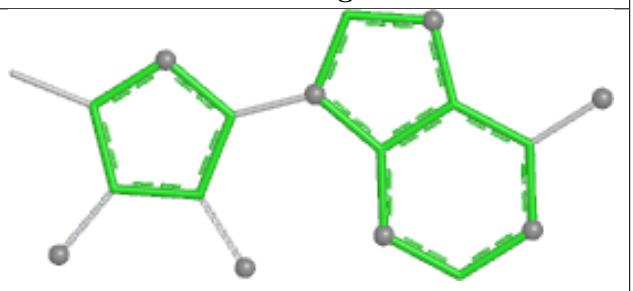
Bond lengths



Bond angles

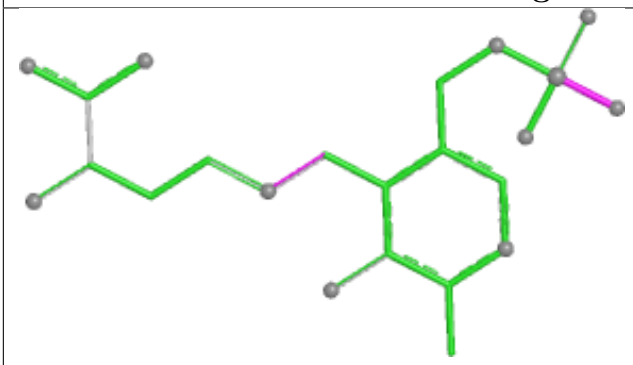


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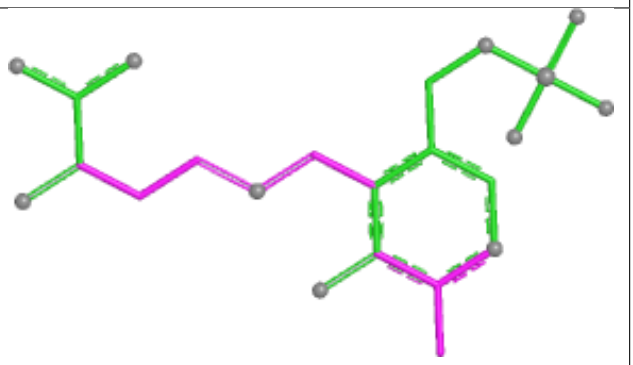


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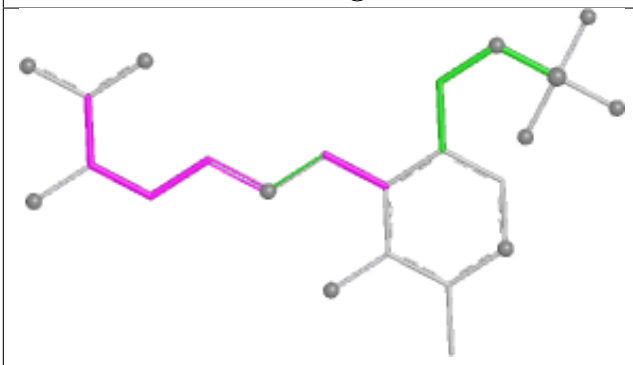
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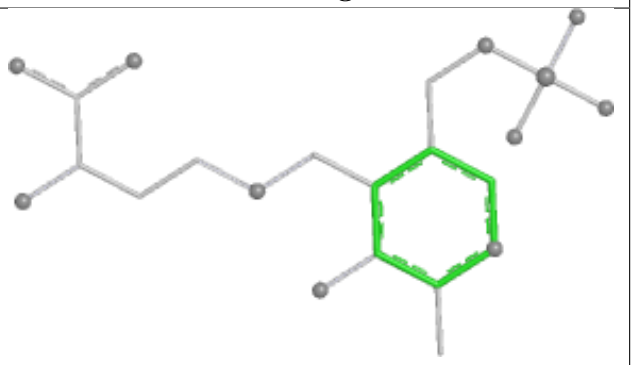
Bond lengths



Bond angles

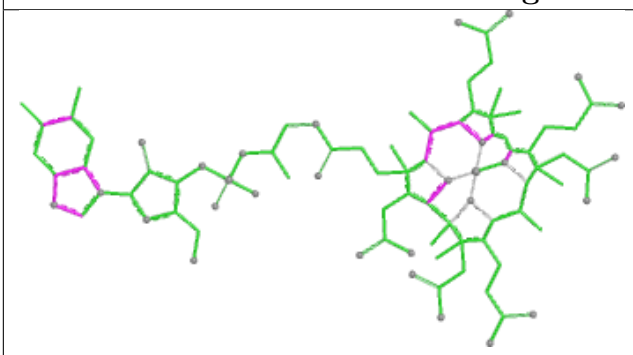


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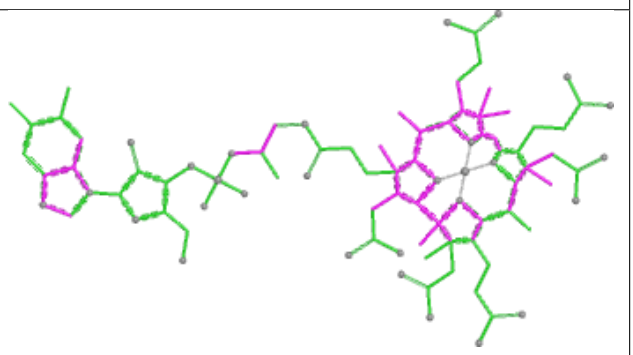


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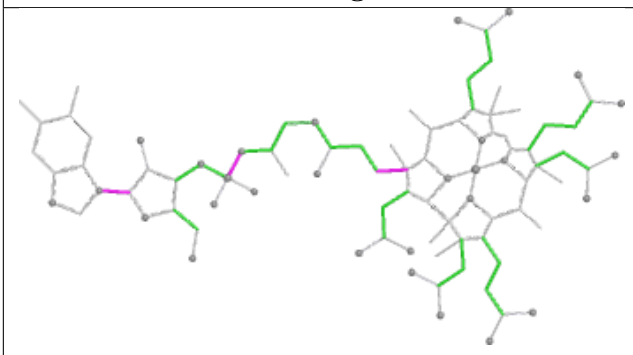
Ligand B12 B 1801



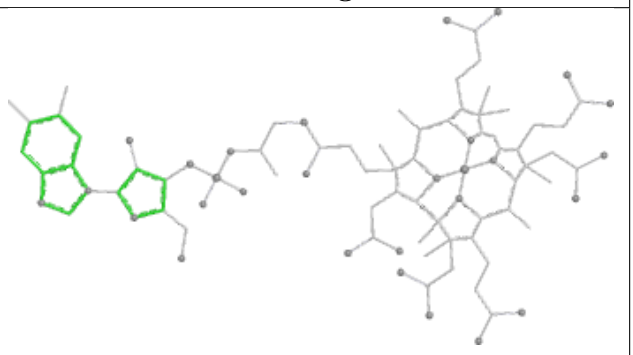
Bond lengths



Bond angles

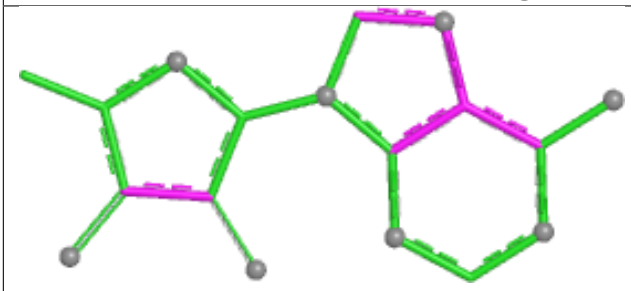


Torsions

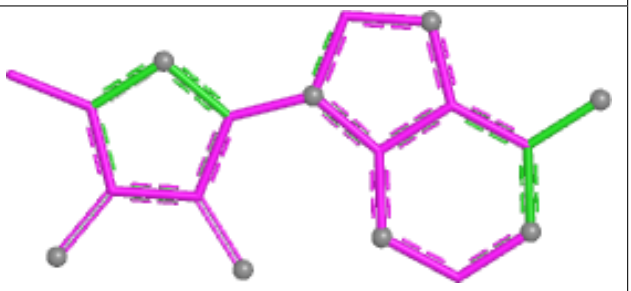


Rings

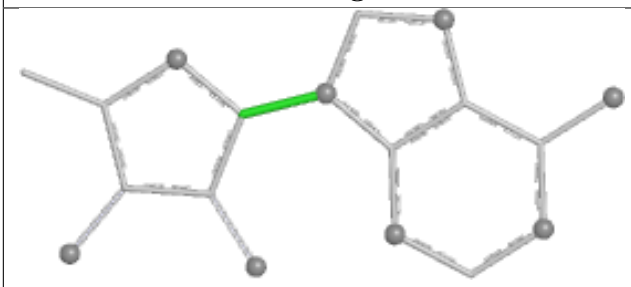
Ligand 5AD A 1500



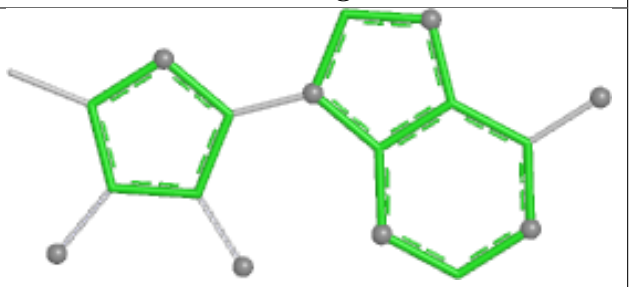
Bond lengths



Bond angles

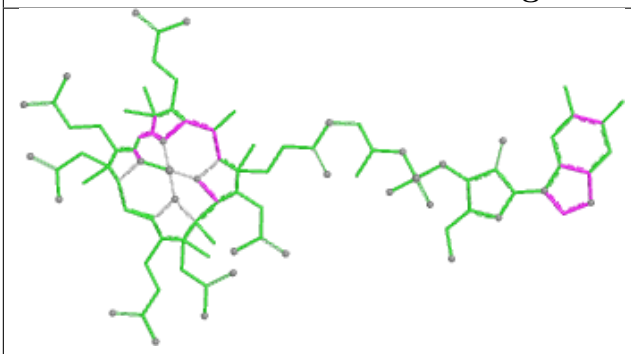


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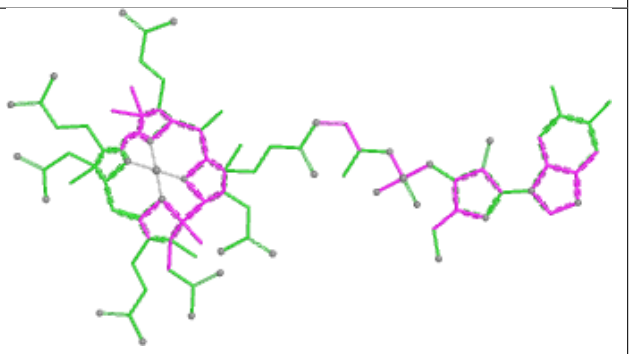


Rings

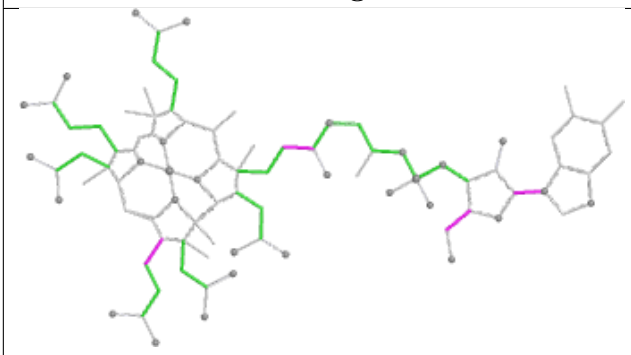
Ligand B12 C 1801



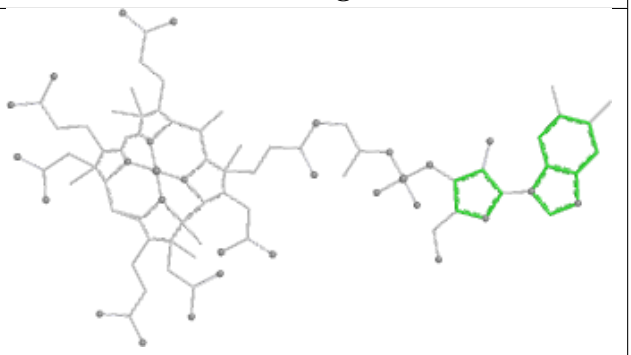
Bond lengths



Bond angles

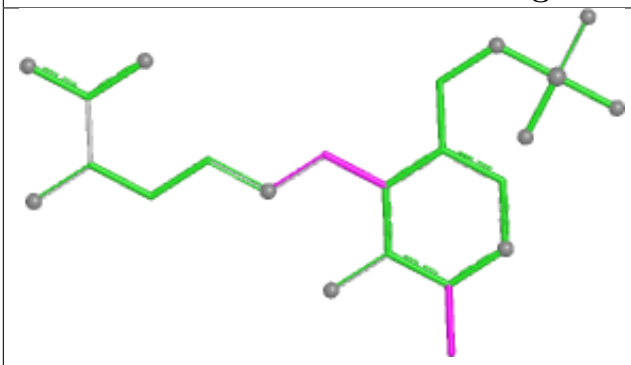


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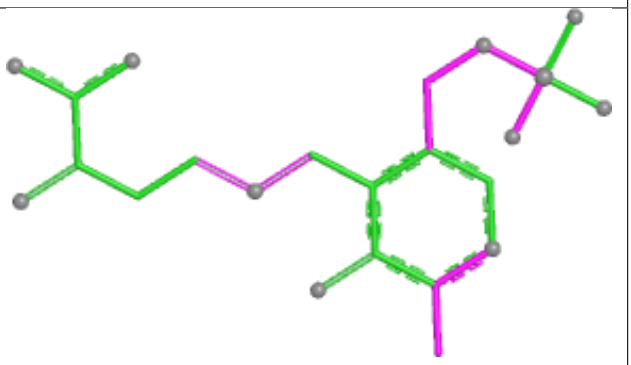


Rings

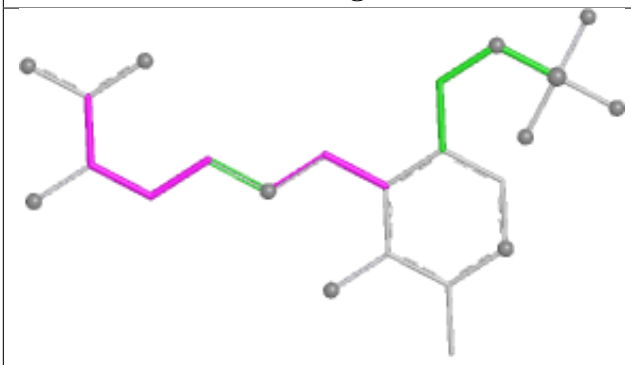
Ligand Z98 D 767



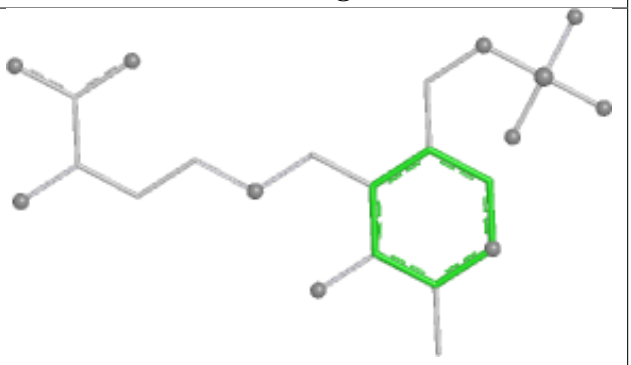
Bond lengths



Bond angles

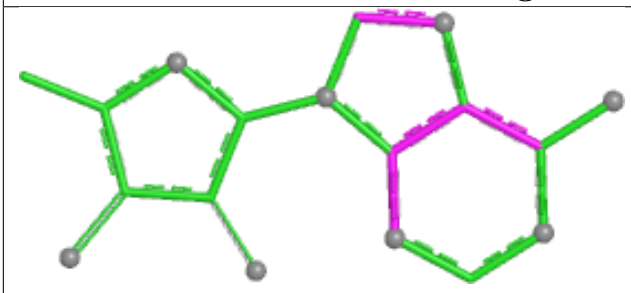


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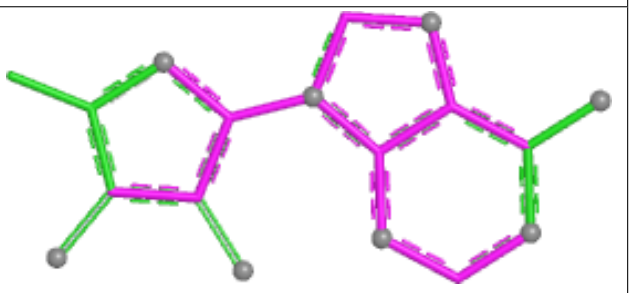


Rings

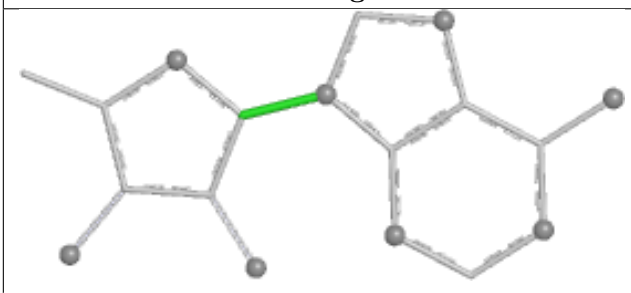
Ligand 5AD B 1500



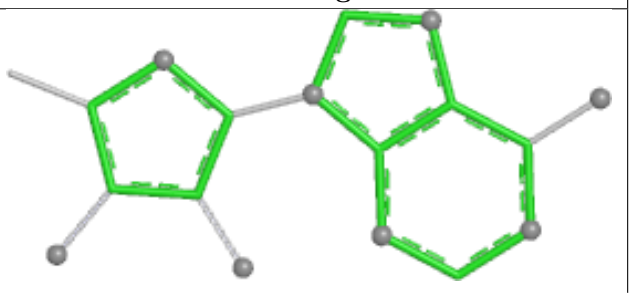
Bond lengths



Bond angles

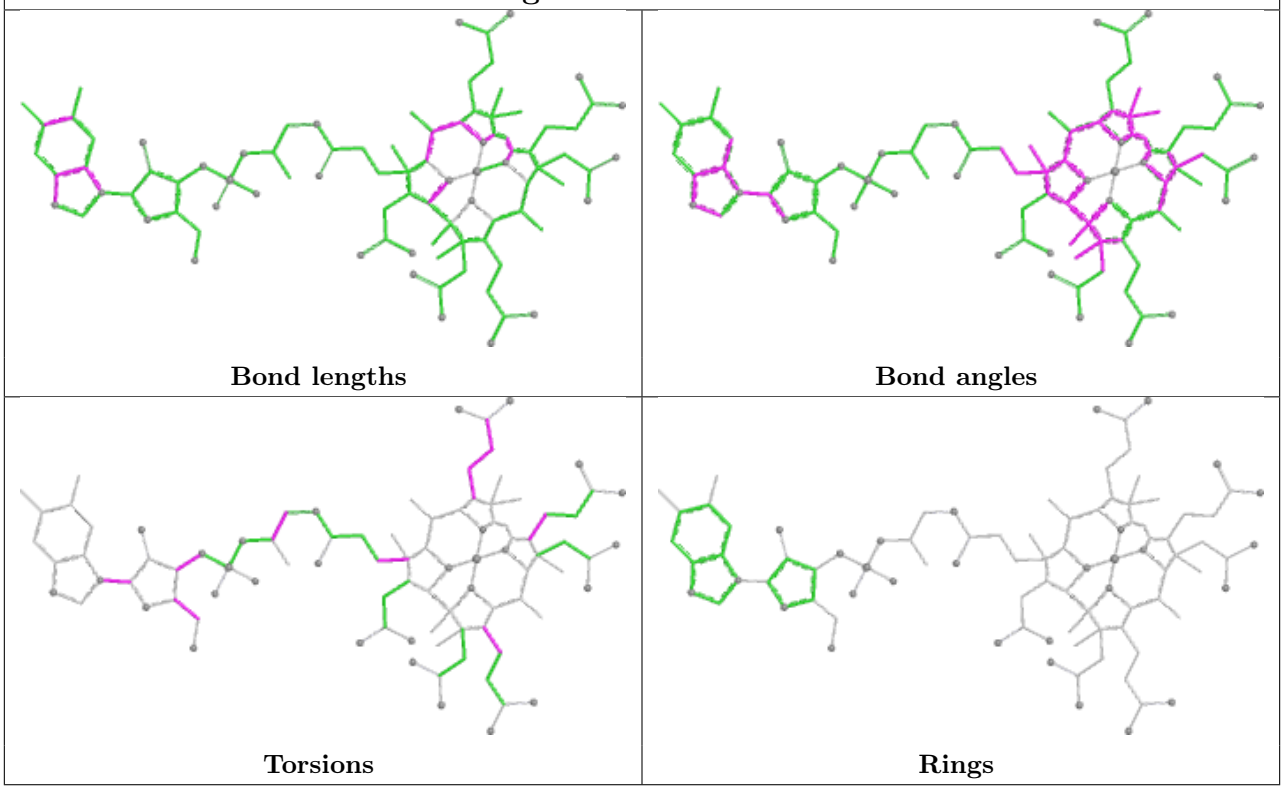


Torsions



Rings

Ligand B12 A 1801



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^{th} 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	728/763 (95%)	-0.11	13 (1%) 67 63	13, 27, 68, 84	0
1	B	728/763 (95%)	-0.46	2 (0%) 90 88	10, 22, 42, 56	0
1	C	728/763 (95%)	-0.30	3 (0%) 88 86	12, 28, 49, 66	0
1	D	728/763 (95%)	-0.37	3 (0%) 88 86	10, 23, 50, 65	0
2	E	109/121 (90%)	-0.17	0 100 100	17, 32, 46, 50	0
2	F	109/121 (90%)	-0.34	1 (0%) 81 78	15, 24, 37, 45	0
2	G	109/121 (90%)	-0.11	0 100 100	24, 35, 50, 55	0
2	H	109/121 (90%)	-0.20	1 (0%) 81 78	15, 27, 45, 61	0
All	All	3348/3536 (94%)	-0.30	23 (0%) 84 81	10, 26, 54, 84	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	591	ILE	3.9
1	A	683	ILE	3.2
1	B	5	LEU	3.0
1	A	692	ILE	2.7
1	A	688	VAL	2.7

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 oligosaccharides in this entry.

6.4 Ligands (i)

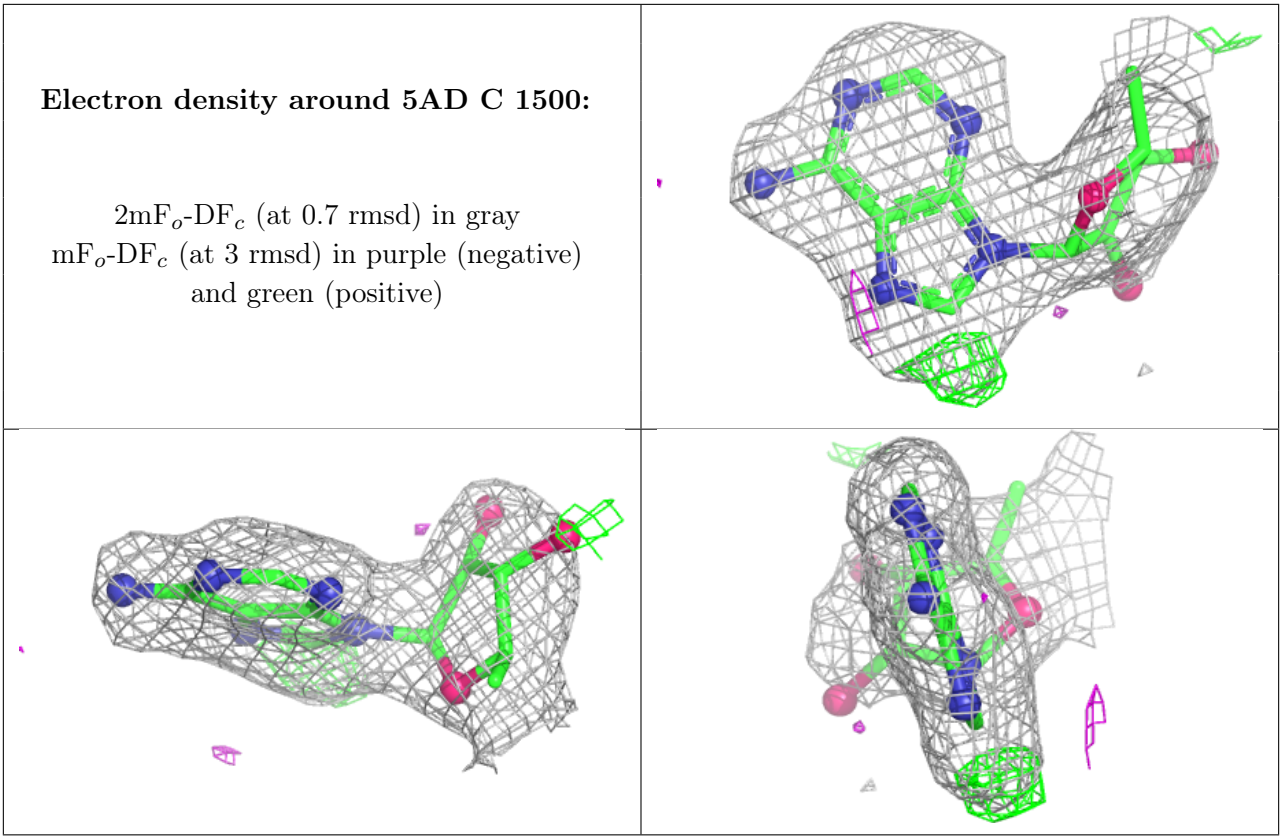
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	5AD	C	1500	18/18	0.80	0.13	53,54,55,57	0
4	5AD	D	1500	18/18	0.84	0.13	38,40,45,45	0
4	5AD	A	1500	18/18	0.86	0.13	39,43,47,47	0
4	5AD	B	1500	18/18	0.89	0.09	25,38,42,42	0
3	B12	A	1801	91/91	0.94	0.09	27,43,50,54	0
3	B12	D	1801	91/91	0.95	0.08	19,29,40,43	0
5	Z98	C	767	23/23	0.95	0.09	26,34,43,44	0
5	Z98	B	767	23/23	0.96	0.08	18,23,33,34	0
5	Z98	A	767	23/23	0.96	0.09	21,32,42,43	0
3	B12	B	1801	91/91	0.97	0.06	14,21,29,35	0
3	B12	C	1801	91/91	0.97	0.06	12,23,31,34	0
5	Z98	D	767	23/23	0.97	0.08	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.

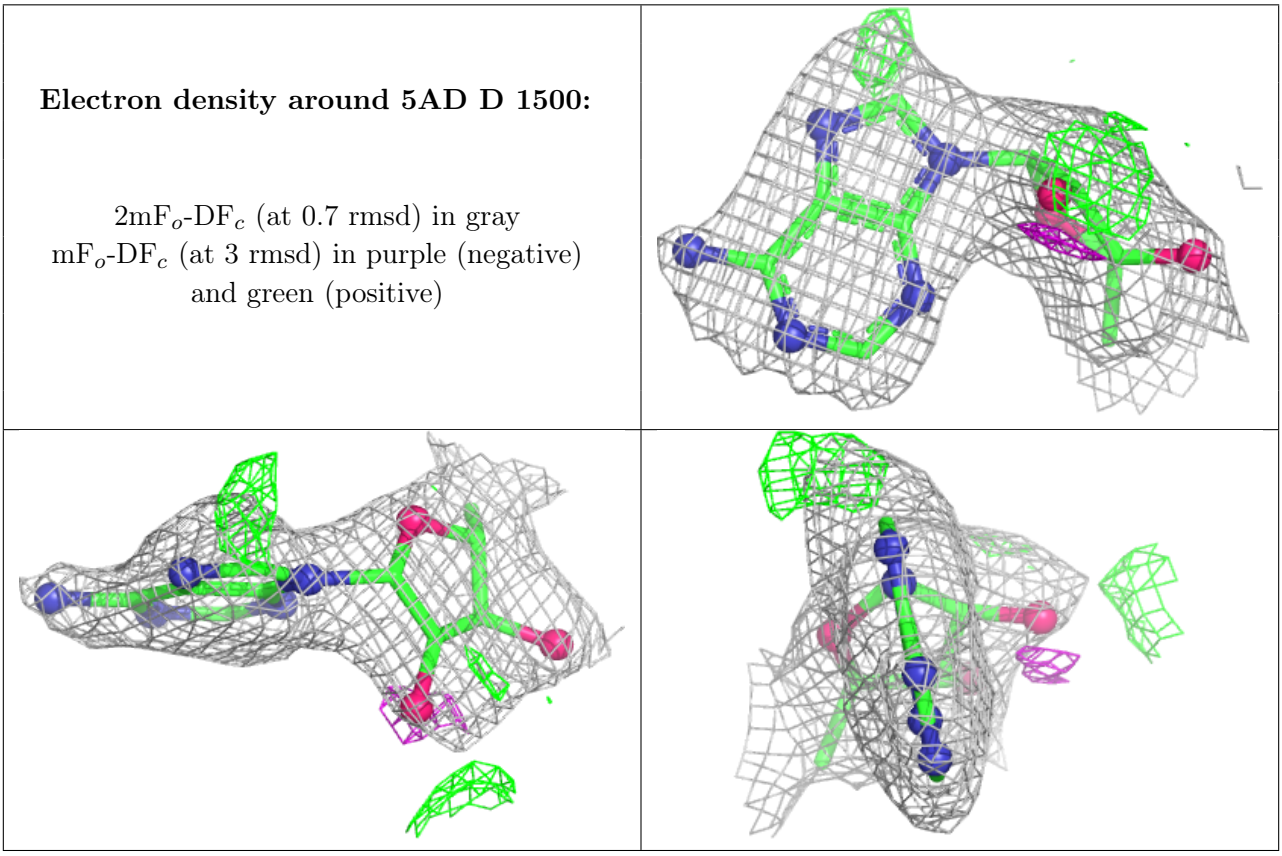
Electron density around 5AD C 1500:

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



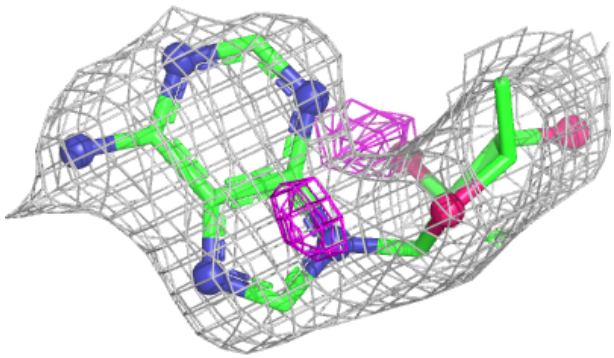
Electron density around 5AD D 1500:

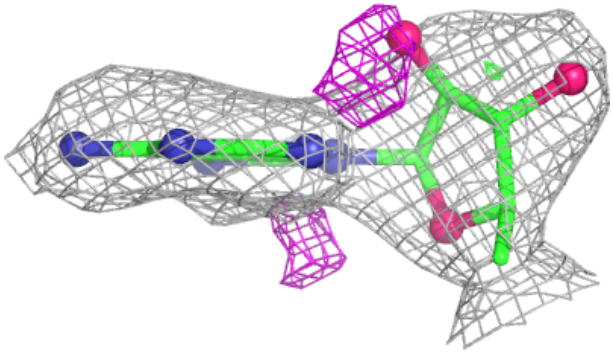
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

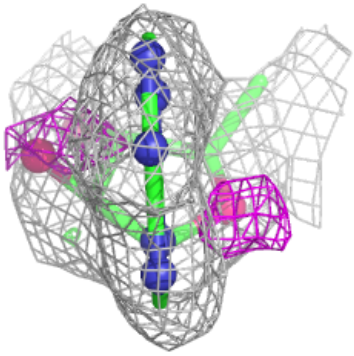


Electron density around 5AD A 1500:

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

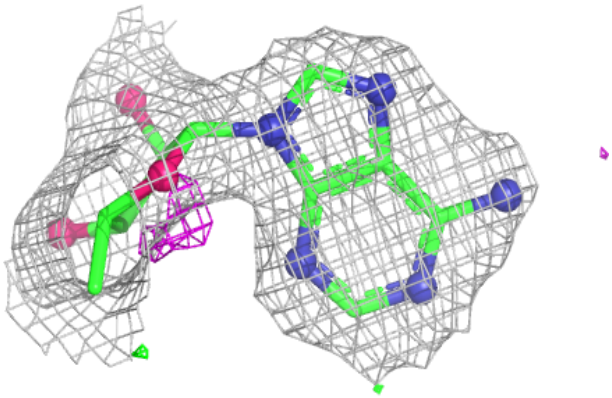


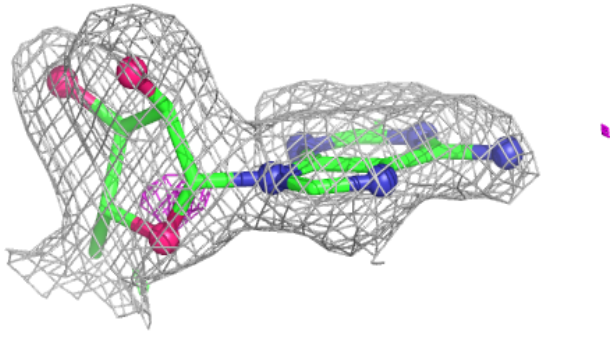


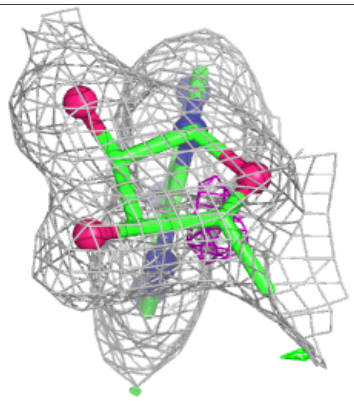


Electron density around 5AD B 1500:

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

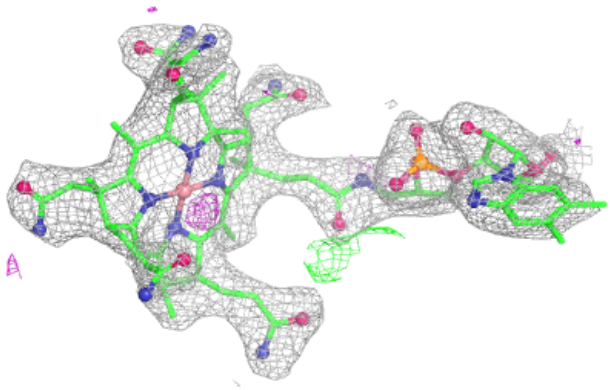


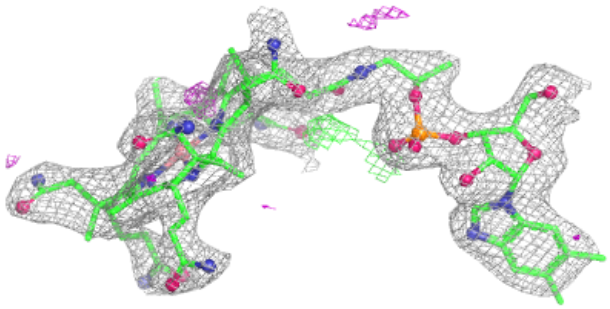


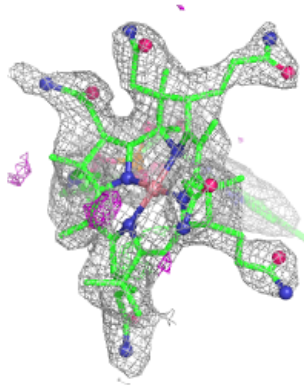


Electron density around B12 A 1801:

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

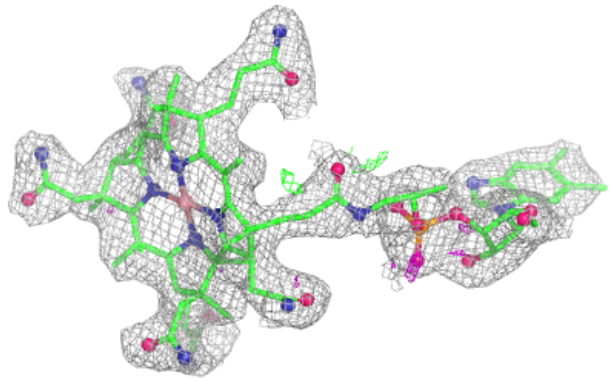


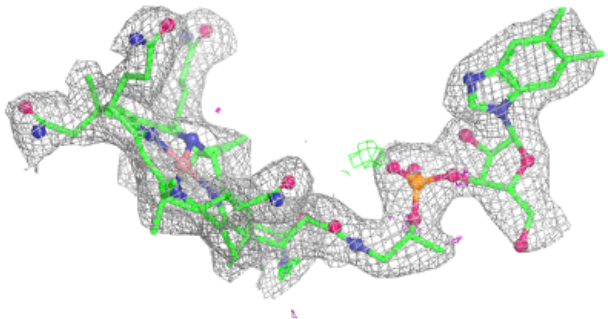


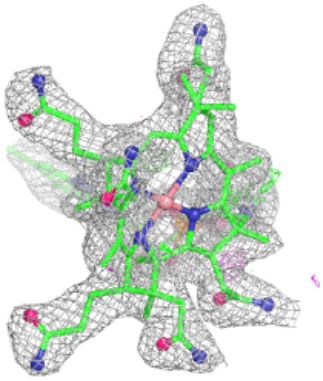


Electron density around B12 D 1801:

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

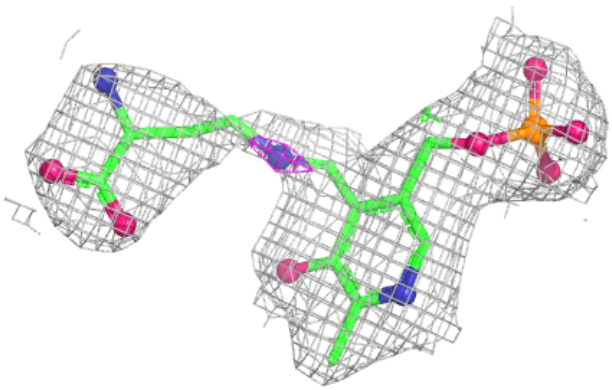


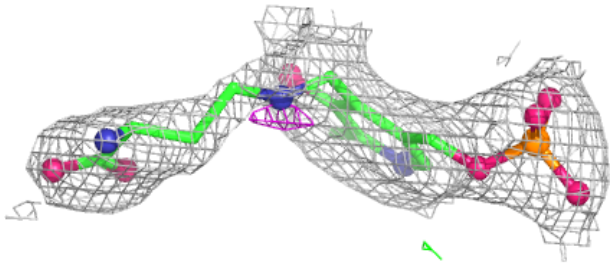


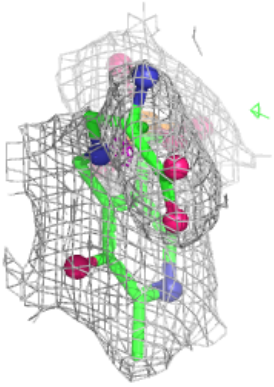


Electron density around Z98 C 767:

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

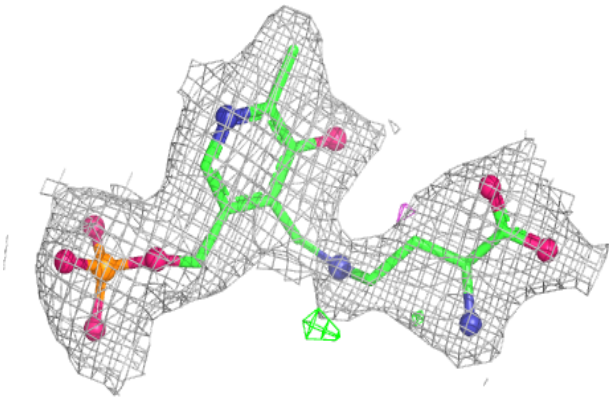


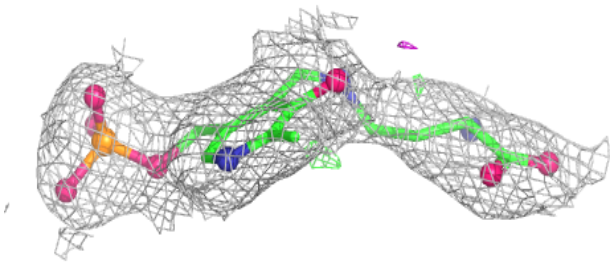


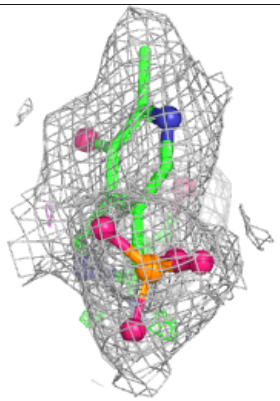


Electron density around Z98 B 767:

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

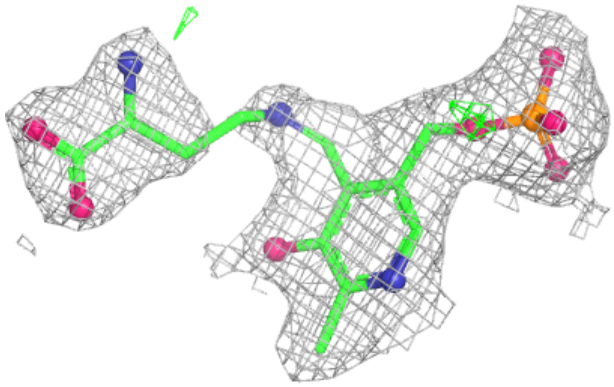


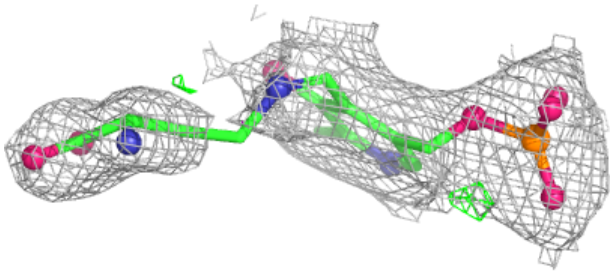


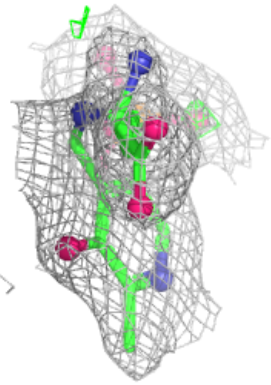


Electron density around Z98 A 767:

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

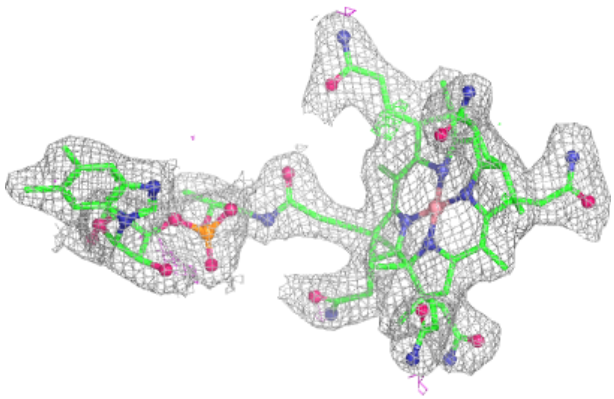


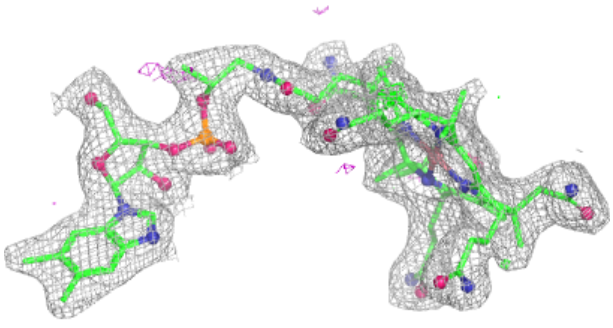


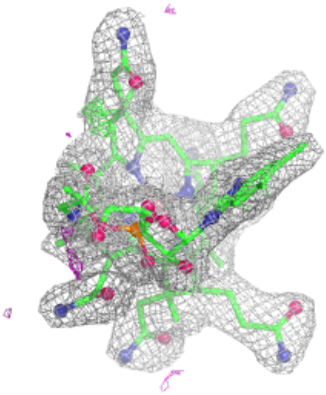


Electron density around B12 B 1801:

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

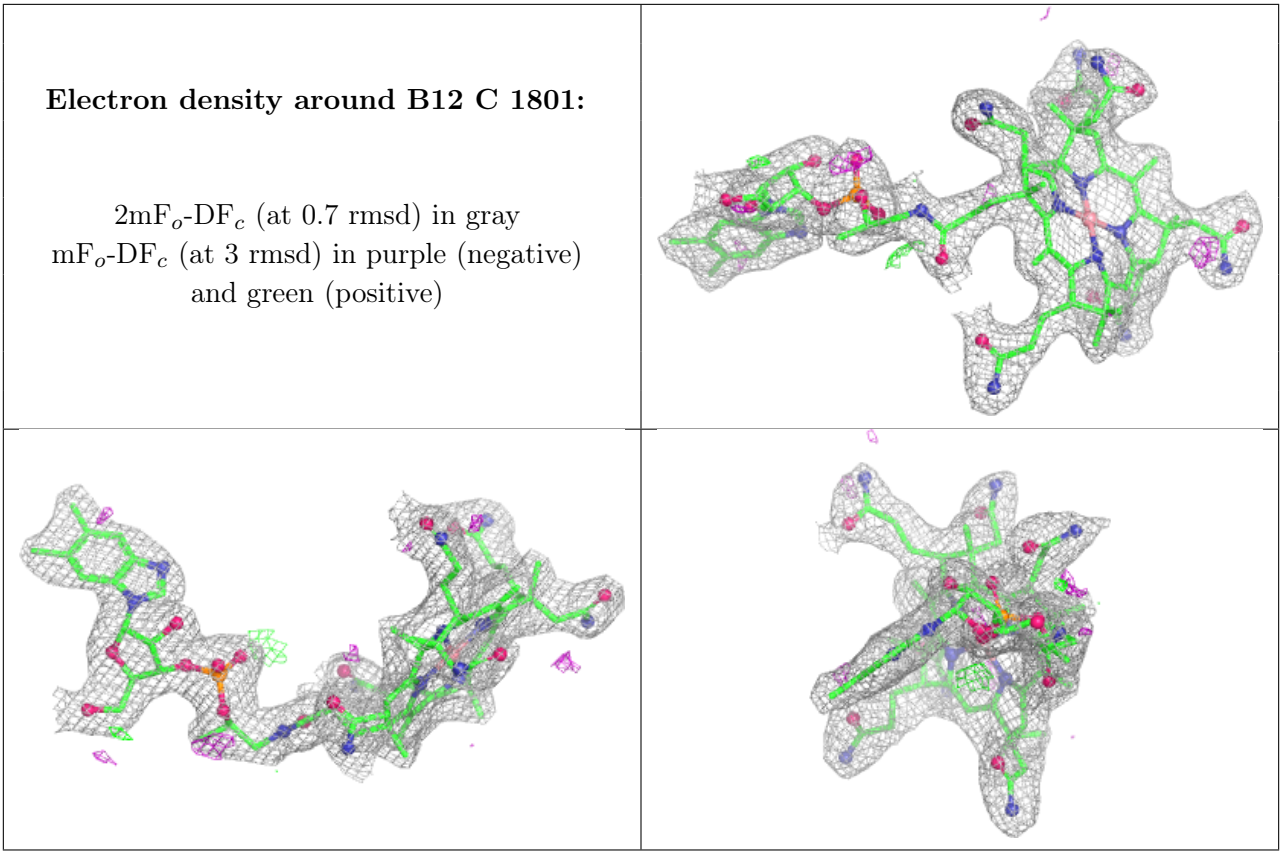






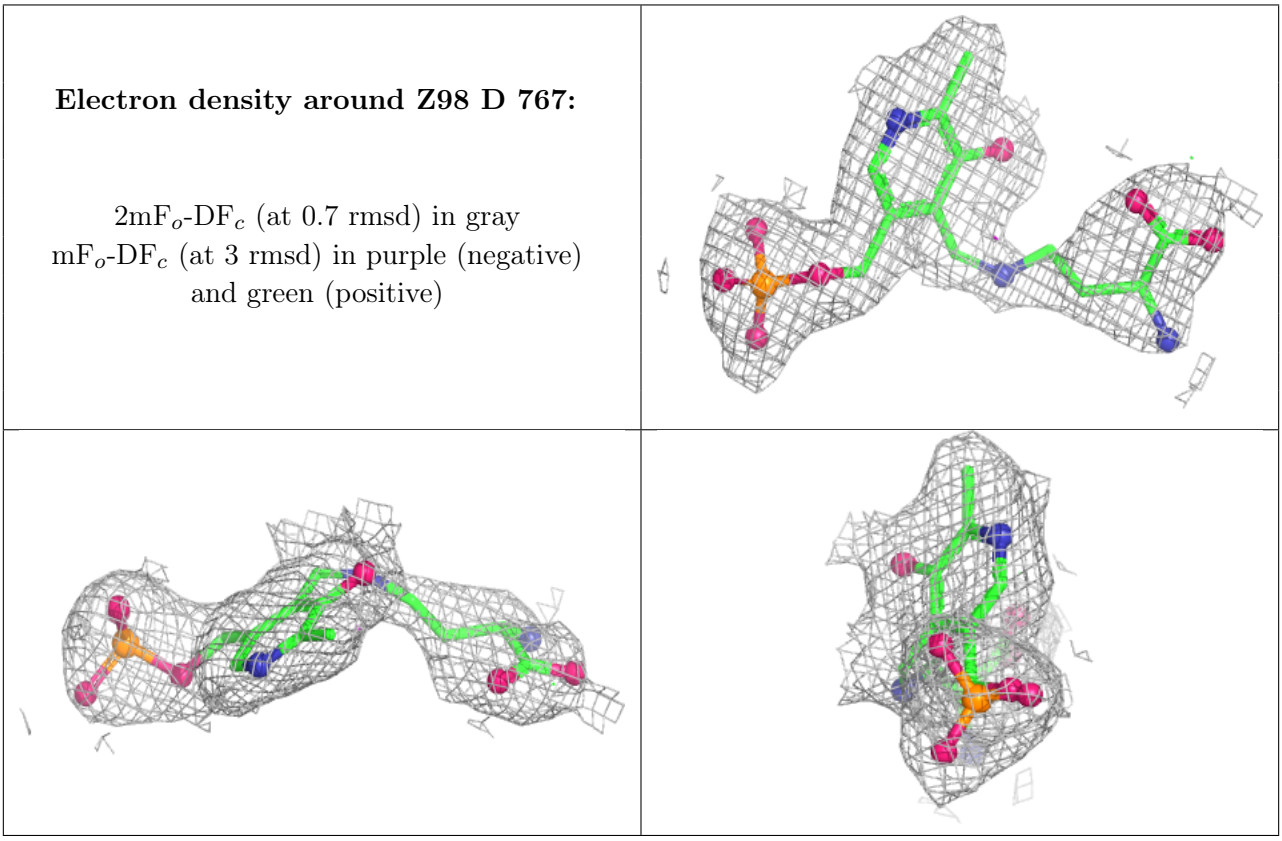
Electron density around B12 C 1801:

$2mF_o$-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.