wwPDB X-ray Structure Validation Summary Report (i)

Feb 14, 2024 – 04:31 AM EST

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

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

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

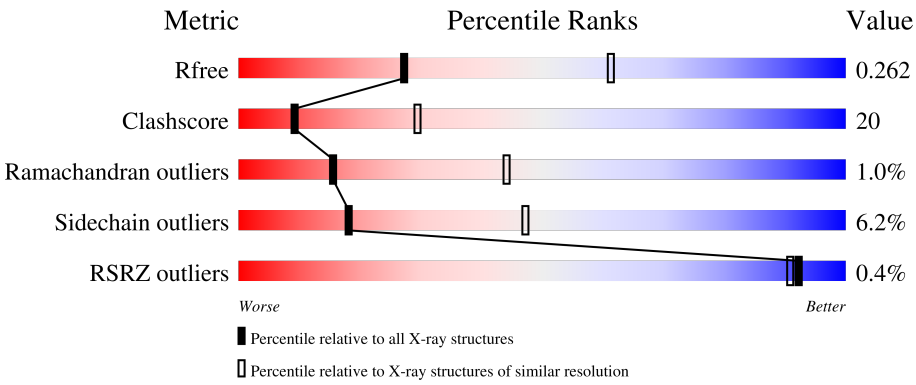
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	.% 61% 32% • 5%
1	B	763	58% 34% • 5%
1	C	763	59% 33% • 5%
1	D	763	.% 62% 31% • 5%
2	E	121	54% 36% • 9%

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Mol	Chain	Length	Quality of chain
2	F	121	61% 26% • 9%
2	G	121	55% 32% • 9%
2	H	121	60% 31% • 9%

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

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	5634	3550	976	1075	33	0	0	0
1	B	728	5665	3574	983	1074	34	0	0	0
1	C	728	5654	3570	981	1069	34	0	0	0
1	D	728	5664	3575	984	1071	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
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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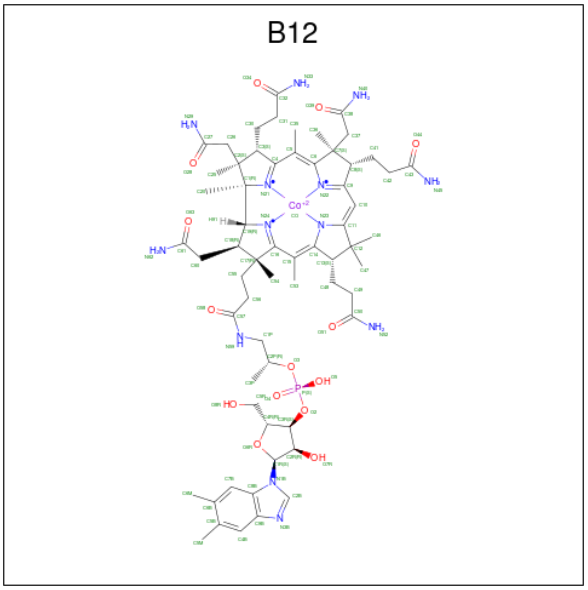
Chain	Residue	Modelled	Actual	Comment	Reference
C	752	VAL	-	expression tag	UNP Q8VPJ5
C	753	ASP	-	expression tag	UNP Q8VPJ5
C	754	LYS	-	expression tag	UNP Q8VPJ5
C	755	LEU	-	expression tag	UNP Q8VPJ5
C	756	ALA	-	expression tag	UNP Q8VPJ5
C	757	ALA	-	expression tag	UNP Q8VPJ5
C	758	ALA	-	expression tag	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.

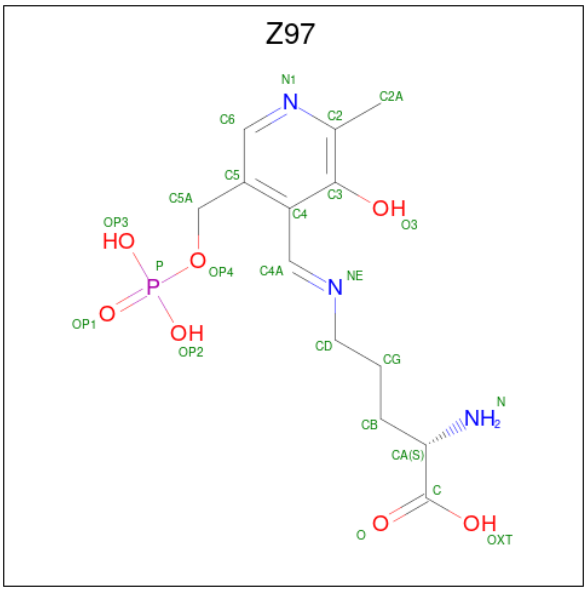
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	110	860	541	153	162	4	0	0	0
			Total	C	N	O	S			
2	F	110	863	542	153	164	4	0	0	0
			Total	C	N	O	S			
2	G	110	860	541	153	162	4	0	0	0
			Total	C	N	O	S			
2	H	110	860	541	153	162	4	0	0	0

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



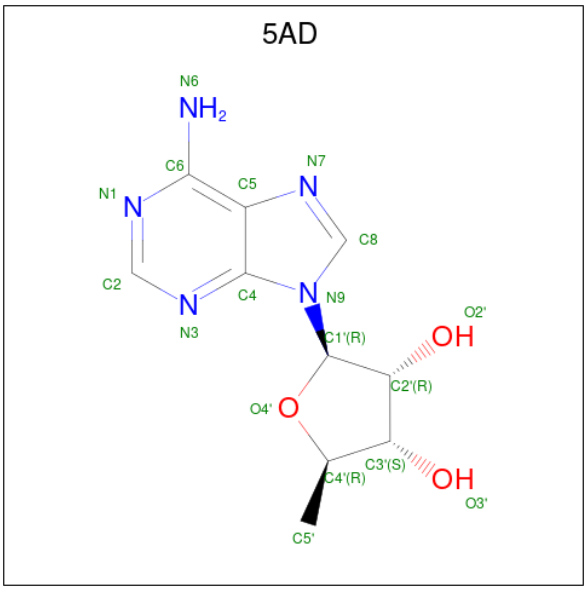
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	A	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	B	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	C	1	91	62	1	13	14	1	0	0
			Total	C	Co	N	O	P		
3	D	1	91	62	1	13	14	1	0	0

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



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

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



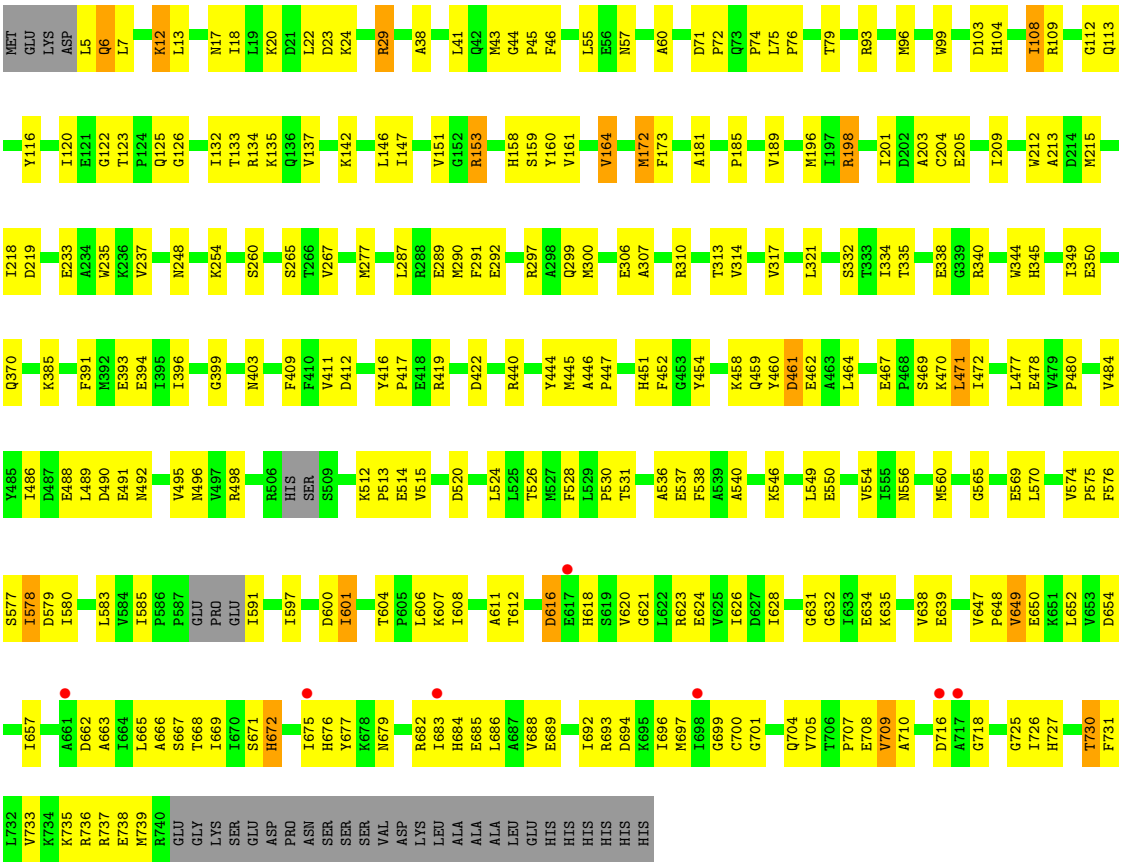
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	18	10	5	3	0	0
5	B	1	18	10	5	3	0	0
5	C	1	18	10	5	3	0	0
5	D	1	18	10	5	3	0	0

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.

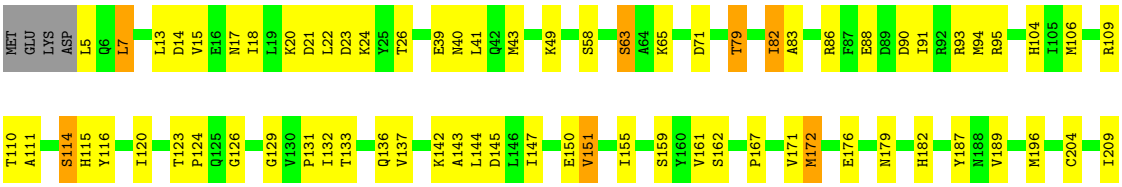
• Molecule 1: D-ornithine aminomutase E component

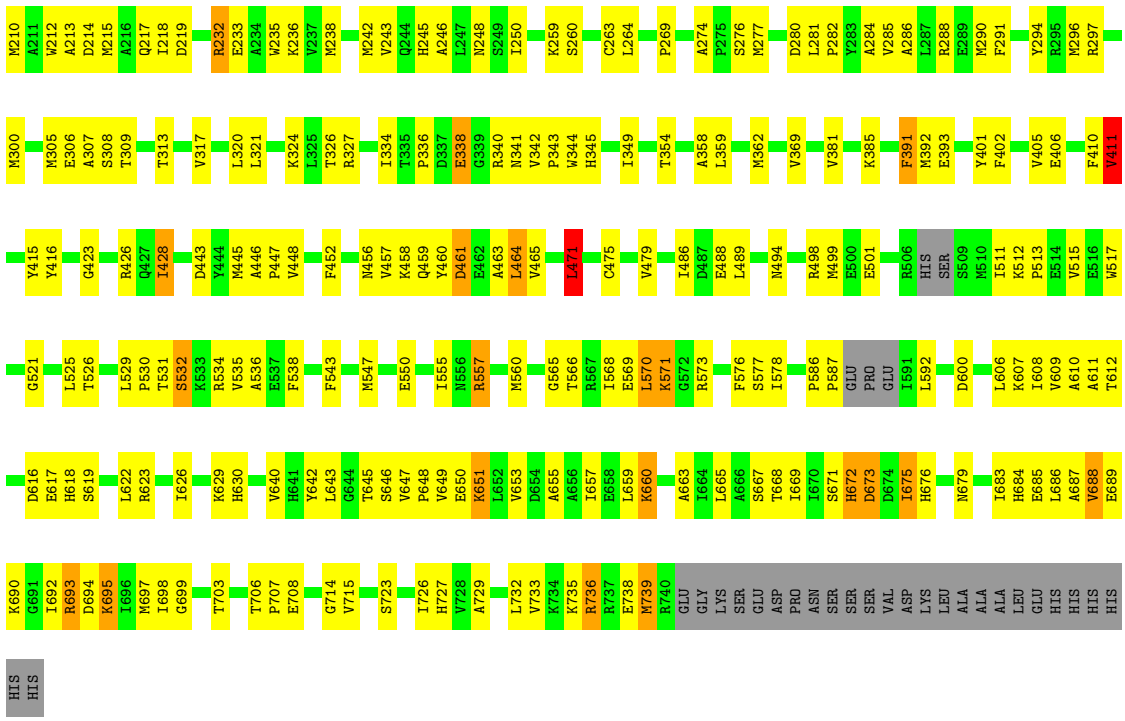
Chain A:



• Molecule 1: D-ornithine aminomutase E component

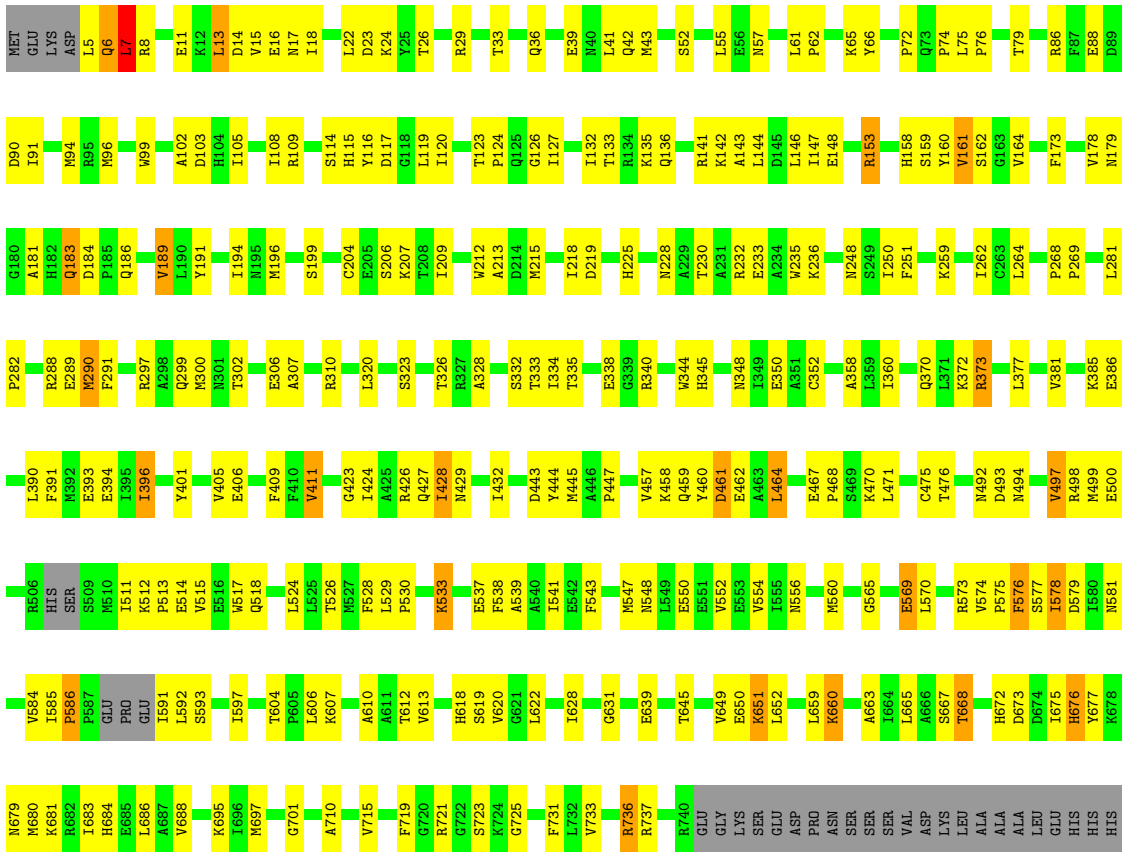
Chain B:





- Molecule 1: D-ornithine aminomutase E component

Chain C:



HIS HIS HIS

• Molecule 1: D-ornithine aminomutase E component

Chain D:

MET GLU LYS ASP L5 Q6 L7 R8 V9 N10 E11 K12 L13 D14 V15 L19 K20 D21 L22 Y25 T26 P27 K28 R29 R30 G31 L41 Q42 M43 F46 I47 D50 N57 P72 T79 T80 E81 I82 R86 F87 E88 W99 H104 V107 I108 R109 T110

H115 Y116 I120 T123 P124 I127 G128 P131 I132 T133 R134 K135 R138 E150 R153 V161 V164 M172 N179 Y187 N188 V189 I194 N195 M196 I197 C204 E205 W212 A213 D214 M215 D219 G223 A224 H225 R232 E233 A234 W235 K236 V237 M238

L241 M242 V243 Q244 H245 A246 L247 N248 S249 I250 M257 I262 C263 L264 S265 T266 M277 Y278 L281 P282 V285 R288 E289 M290 F291 N301 M305 E306 R310 E311 H316 L320 L321 P336 V342 P343 W344 Y347 A358 L359 I360 G361 M362

V369 R373 G378 R387 L390 F391 E394 E397 F402 E406 F409 F410 V411 Y416 P417 Q427 I428 N429 F438 D441 E442 M445 A446 P447 H451 F452 G453 Y454 Q459 Y460 D461 E462 A463 L464 E467 P468 S469 K470 L471 L477 E478 V479

P480 Y485 N494 R498 M499 T502 F505 R506 HIS SER S509 M510 I511 K512 P513 E514 V515 L524 L525 T526 M527 F528 L529 P530 R534 E537 F538 A539 A540 I541 K545 K546 E553 V554 I555 N556 R557 M560 Q561 E562 A563 E564 E569 L570 V574 P575 F576

S577 I578 D579 I580 N581 S582 I585 P586 P587 GLU PRO GLU I591 R598 K607 I608 A611 T612 V613 D616 E617 H618 S619 V620 G621 L622 R623 I626 D627 I628 K629 H630 G631 G632 I633 E634 K635 Y642 L643 G644 T645 S646 V647 P648 V649 E650 K651 L652 V653 I657 A663

I664 L665 A666 S667 T668 I669 I670 S671 D674 I675 H676 N679 M680 K681 R682 I683 H684 E685 L686 A687 V688 E689 K690 R693 D694 K695 I696 M697 C700 T703 Q704 V705 T706 V709 A710 V711 G714 V715 G718 F719 S723 K724 G725 I726 F731 R736 R737 E738 M739

R740 GLU GLY LYS SER GLU ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS HIS

• Molecule 2: D-ornithine aminomutase S component

Chain E:

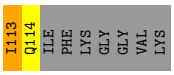
MET LYS ARG ALA D5 D6 F7 Q8 Q9 E21 L22 Q23 T24 R25 F26 M29 A30 E31 P36 D39 L40 G41 K42 P47 S48 I49 E50 R51 S52 V53 L54 M57 G58 F59 S60 S61 L62 E63 A64 V68 D69 K70 T71 M72 D73 R74 G75 L76 M77 A81 V85

I88 N93 G100 L101 K107 Y108 W109 D110 D111 A112 I113 Q114 ILE PHE LYS GLY GLY VAL LYS

• Molecule 2: D-ornithine aminomutase S component

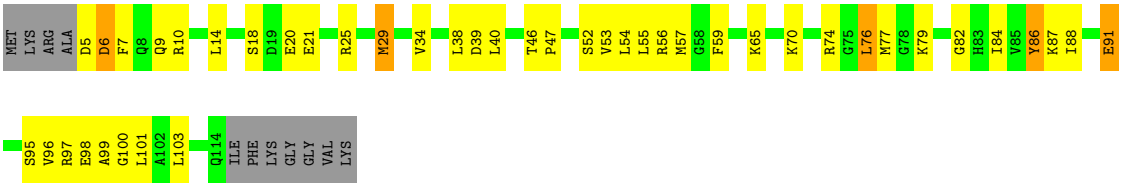
Chain F:

MET LYS ARG ALA D5 D6 F7 R10 R11 E20 Q23 T24 R25 M29 S48 I49 V53 L54 L55 R56 M57 G58 F59 E63 A64 K65 A66 I67 K70 R74 G75 L76 G82 I88 K92 N93 R97 G100 L101 A102 L103 Y108 W109 A112



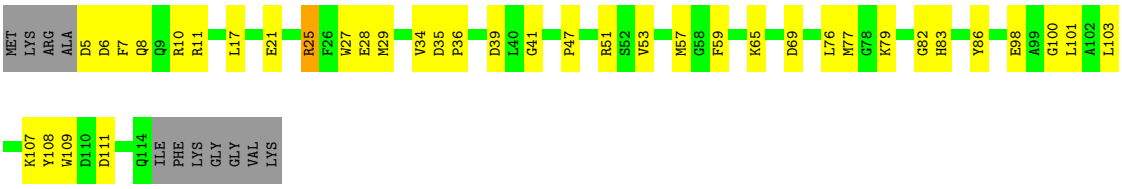
• Molecule 2: D-ornithine aminomutase S component

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	66.52Å 233.22Å 124.14Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	60.37 – 2.80 64.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (60.37-2.80) 93.8 (64.70-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5_2, REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.263 0.183 , 0.262	Depositor DCC
R_{free} test set	4265 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26592	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: Z97, B12, 5AD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.43	0/5739	0.61	0/7776
1	B	0.44	0/5770	0.61	0/7809
1	C	0.43	0/5759	0.60	0/7796
1	D	0.44	0/5769	0.61	0/7808
2	E	0.44	0/872	0.59	0/1170
2	F	0.44	0/875	0.63	0/1174
2	G	0.42	0/872	0.58	0/1170
2	H	0.46	0/872	0.57	0/1170
All	All	0.43	0/26528	0.61	0/35873

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5634	0	5544	217	0
1	B	5665	0	5629	238	0
1	C	5654	0	5621	223	0
1	D	5664	0	5636	231	0
2	E	860	0	865	34	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1054 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:ASP:HA	2:E:7:PHE:N	1.53	1.22
2:F:5:ASP:HA	2:F:7:PHE:N	1.61	1.13
1:A:43:MET:HE1	1:A:72:PRO:HA	1.30	1.09
1:D:537:GLU:HG3	1:D:554:VAL:HG21	1.36	1.07
1:A:306:GLU:HG3	1:A:307:ALA:H	0.87	1.03

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

5 of 32 Ramachandran outliers are listed below:

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

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

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

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

Mol	Chain	Res	Type
1	C	736	ARG
1	D	397	GLU
2	G	65	LYS
1	D	79	THR
1	D	469	SER

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

Mol	Chain	Res	Type
1	D	115	HIS
1	D	245	HIS
1	D	248	ASN
1	B	630	HIS
2	E	23	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 monosaccharides 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	$\#\|Z\| > 2$
4	Z97	A	767	-	23,24,24	2.59	9 (39%)	29,33,33	1.74	8 (27%)
4	Z97	D	767	-	23,24,24	2.56	8 (34%)	29,33,33	1.87	6 (20%)
5	5AD	C	1500	3	17,20,20	2.25	5 (29%)	15,30,30	4.14	8 (53%)
5	5AD	D	1500	3	17,20,20	2.28	6 (35%)	15,30,30	4.13	8 (53%)
4	Z97	B	767	-	23,24,24	2.40	7 (30%)	29,33,33	1.58	4 (13%)
3	B12	A	1801	1,5	90,101,101	1.34	8 (8%)	137,166,166	2.31	35 (25%)
3	B12	B	1801	1,5	90,101,101	1.36	9 (10%)	137,166,166	2.25	30 (21%)
5	5AD	A	1500	3	17,20,20	2.09	4 (23%)	15,30,30	4.04	7 (46%)
3	B12	D	1801	1,5	90,101,101	1.39	10 (11%)	137,166,166	2.28	26 (18%)
5	5AD	B	1500	3	17,20,20	2.31	5 (29%)	15,30,30	4.57	7 (46%)
3	B12	C	1801	1,5	90,101,101	1.41	9 (10%)	137,166,166	2.40	29 (21%)
4	Z97	C	767	-	23,24,24	2.57	7 (30%)	29,33,33	1.65	6 (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
4	Z97	A	767	-	-	6/18/18/18	0/1/1/1
4	Z97	D	767	-	-	9/18/18/18	0/1/1/1
5	5AD	C	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
5	5AD	D	1500	3	3/3/4/4	0/0/20/20	0/3/3/3
4	Z97	B	767	-	-	10/18/18/18	0/1/1/1
3	B12	A	1801	1,5	1/1/36/38	23/52/223/223	0/3/11/11
3	B12	B	1801	1,5	1/1/36/38	16/52/223/223	0/3/11/11
5	5AD	A	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
3	B12	D	1801	1,5	1/1/36/38	16/52/223/223	0/3/11/11
5	5AD	B	1500	3	2/2/4/4	0/0/20/20	0/3/3/3
3	B12	C	1801	1,5	1/1/36/38	9/52/223/223	0/3/11/11
4	Z97	C	767	-	-	10/18/18/18	0/1/1/1

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	767	Z97	C4-C5	6.96	1.50	1.42
4	D	767	Z97	C4-C5	6.81	1.50	1.42
4	A	767	Z97	C4-C5	6.66	1.50	1.42
4	B	767	Z97	C4-C5	6.42	1.50	1.42
3	D	1801	B12	C14-N23	5.84	1.42	1.35

The worst 5 of 174 bond angle outliers are listed below:

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

5 of 14 chirality outliers are listed below:

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

5 of 99 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	B12	C14-C13-C48-C49
3	A	1801	B12	C16-C17-C55-C56
3	A	1801	B12	C54-C17-C55-C56
3	A	1801	B12	C18-C17-C55-C56
3	A	1801	B12	C56-C57-N59-C1P

There are no ring outliers.

11 monomers are involved in 114 short contacts:

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

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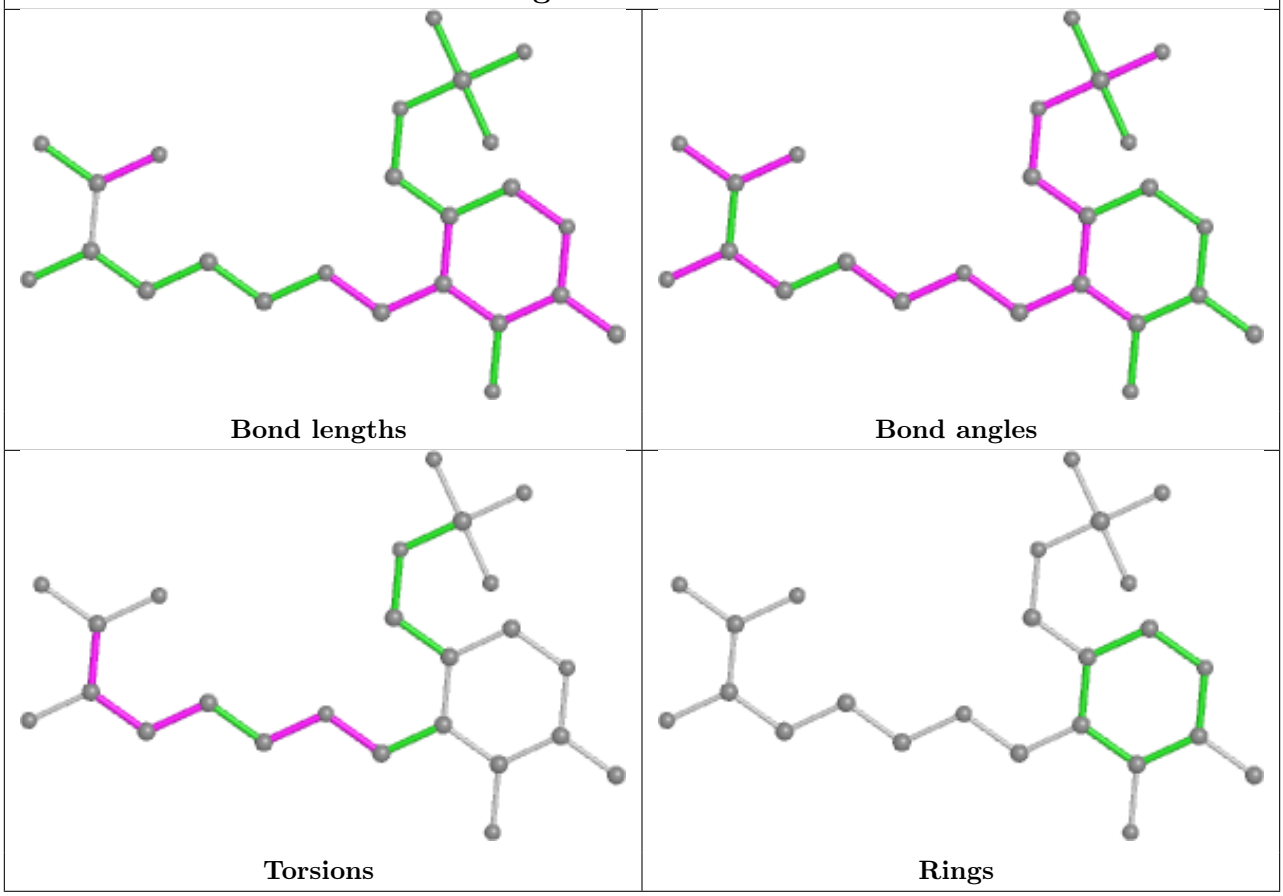
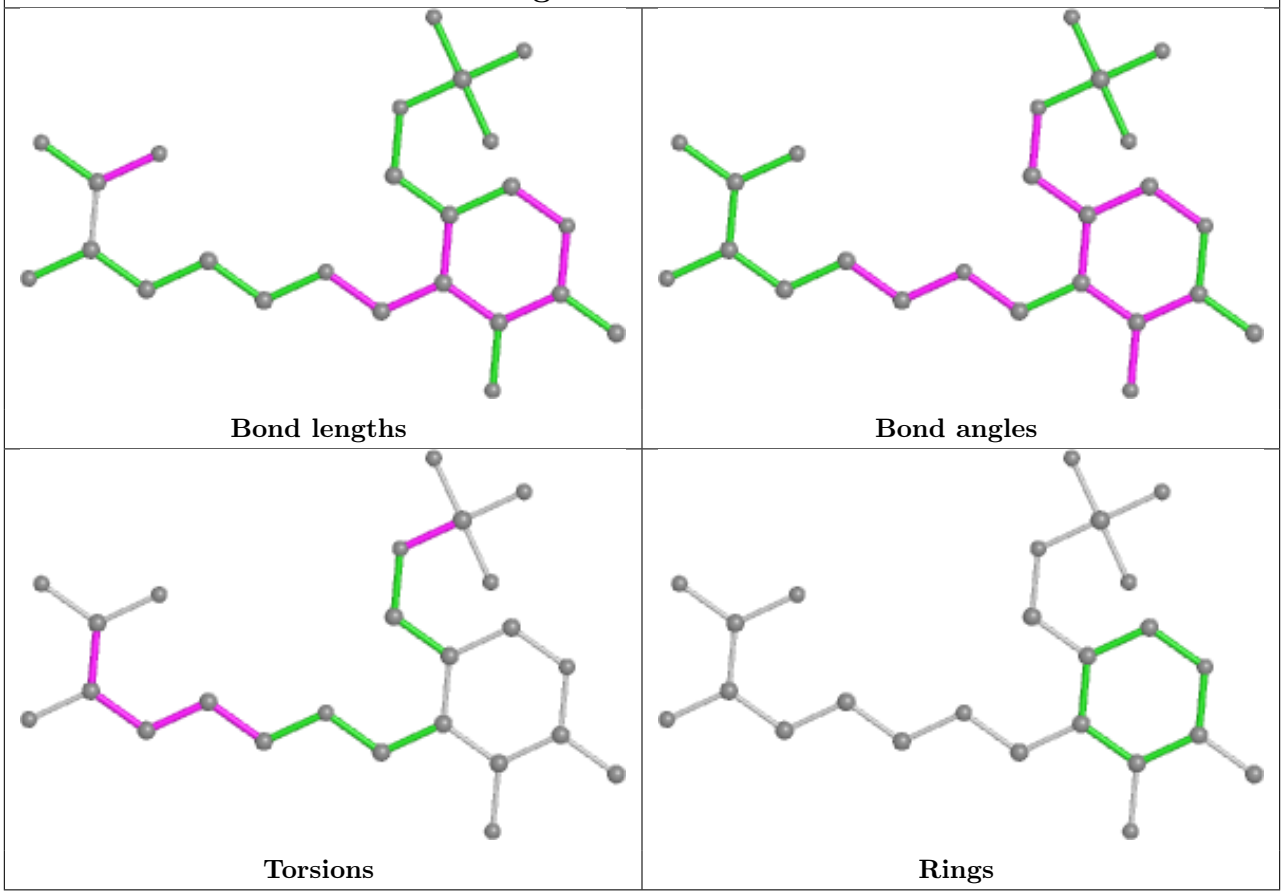
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	B12	24	0
3	B	1801	B12	22	0
5	A	1500	5AD	3	0
3	D	1801	B12	33	0
5	B	1500	5AD	4	0
3	C	1801	B12	26	0
4	C	767	Z97	2	0

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.

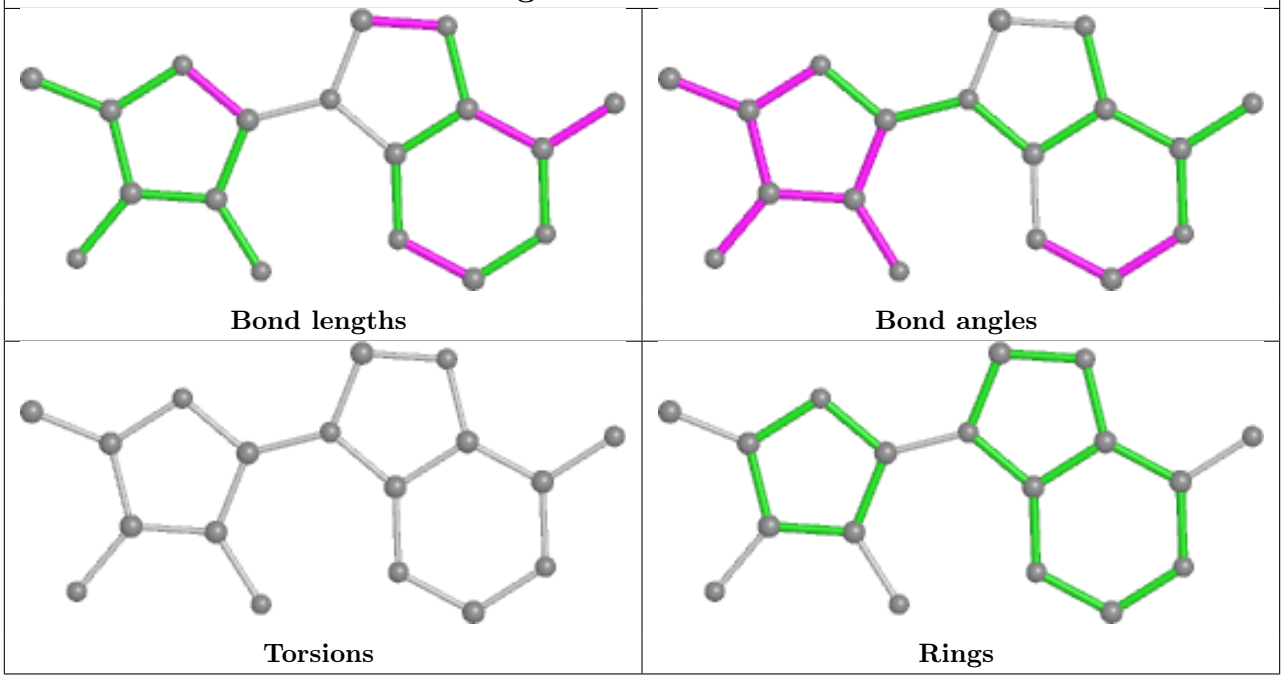
Ligand Z97 A 767



Ligand Z97 D 767



Ligand 5AD C 1500



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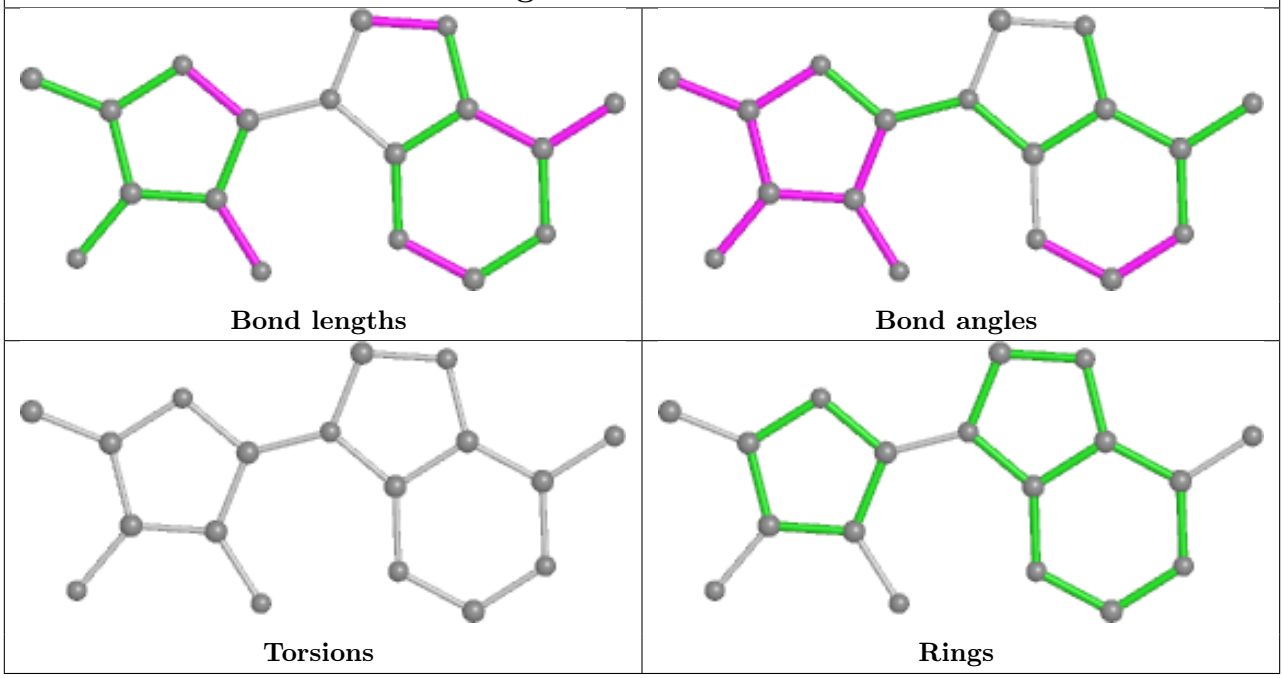
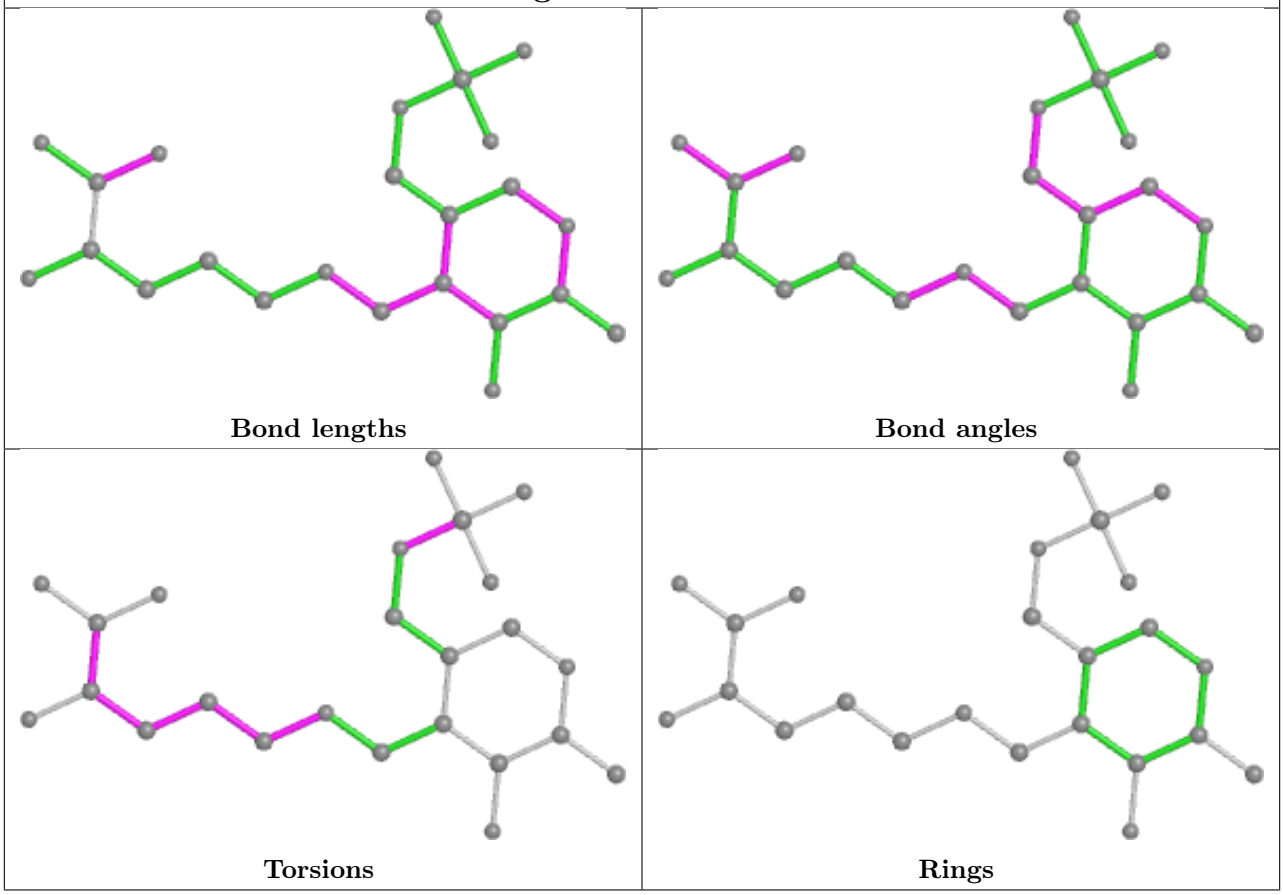
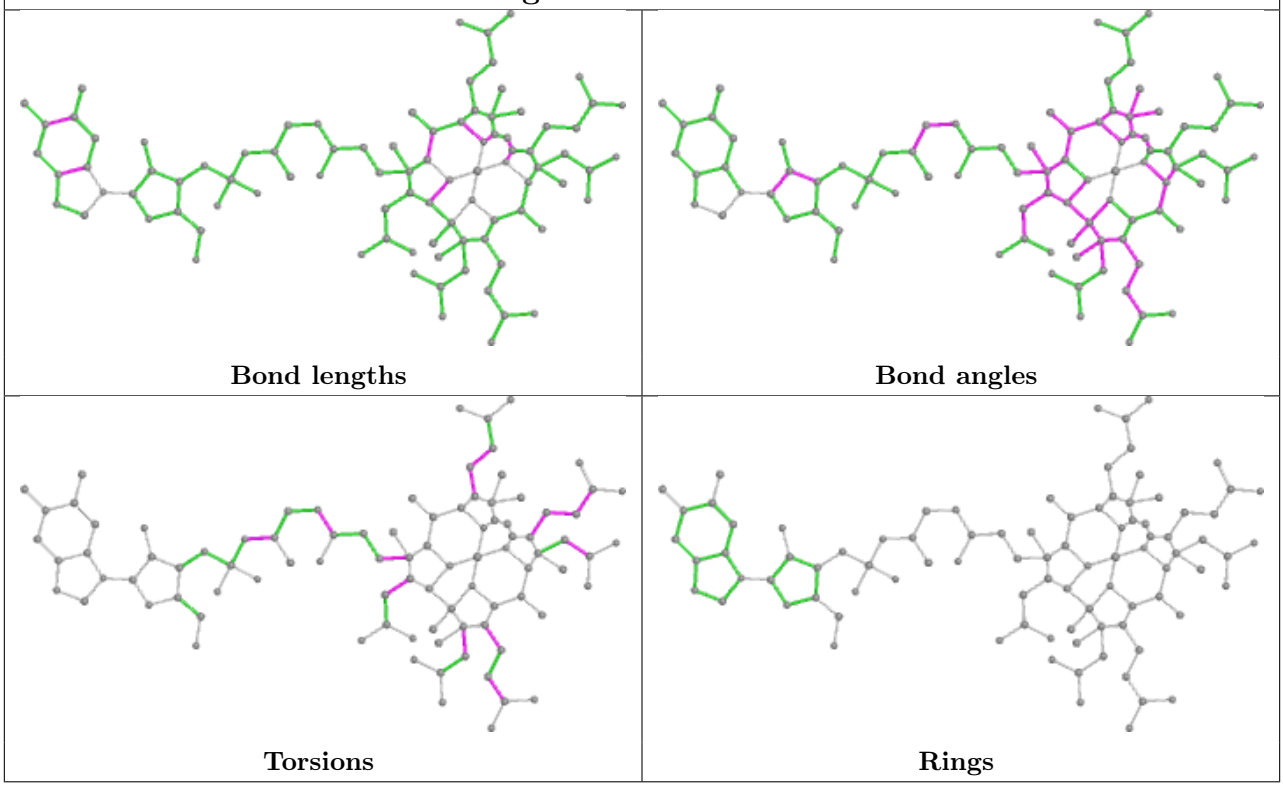


Ligand Z97 B 767



Ligand B12 A 1801



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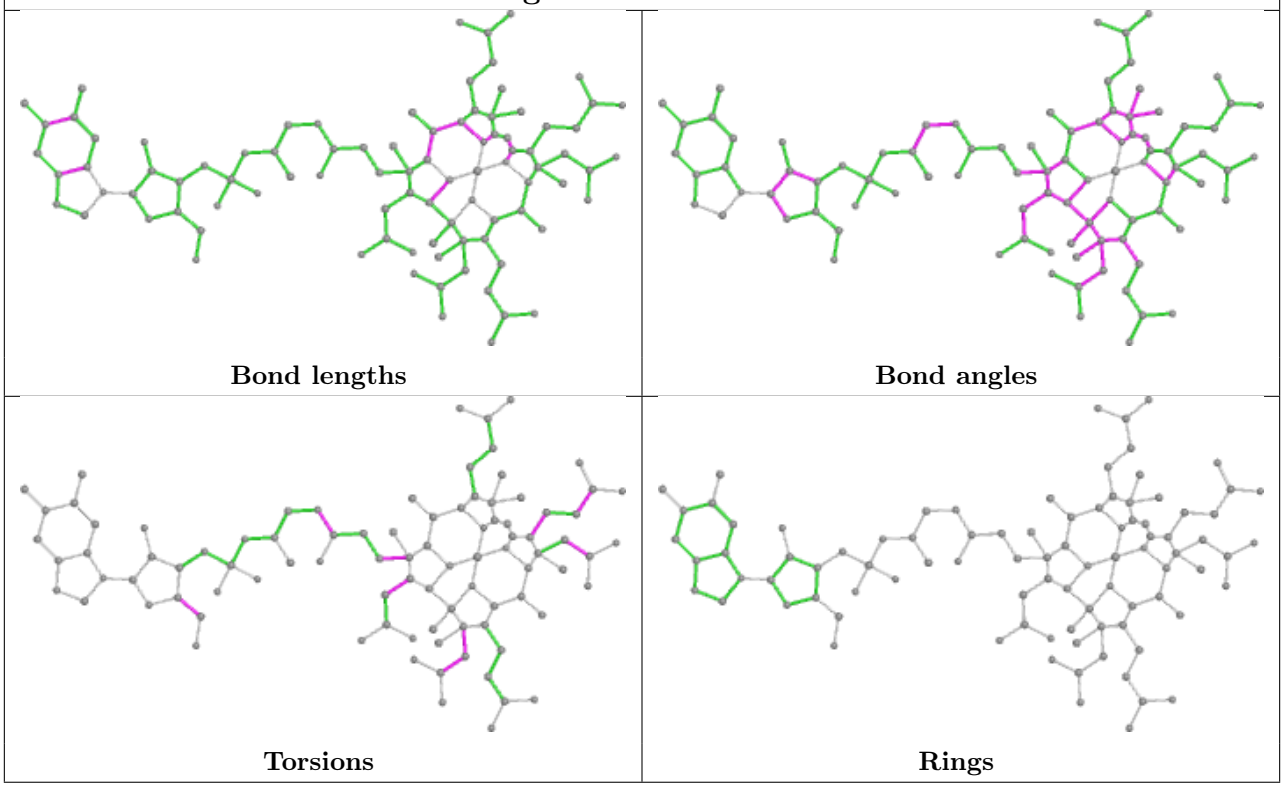

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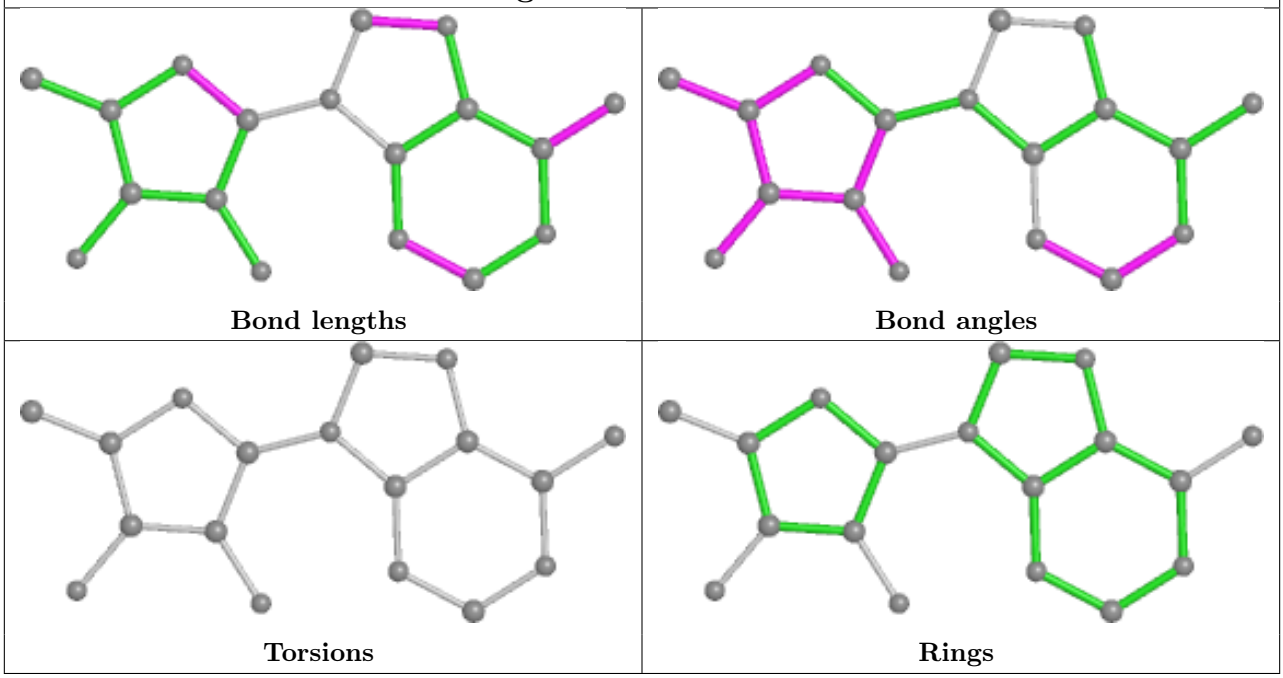

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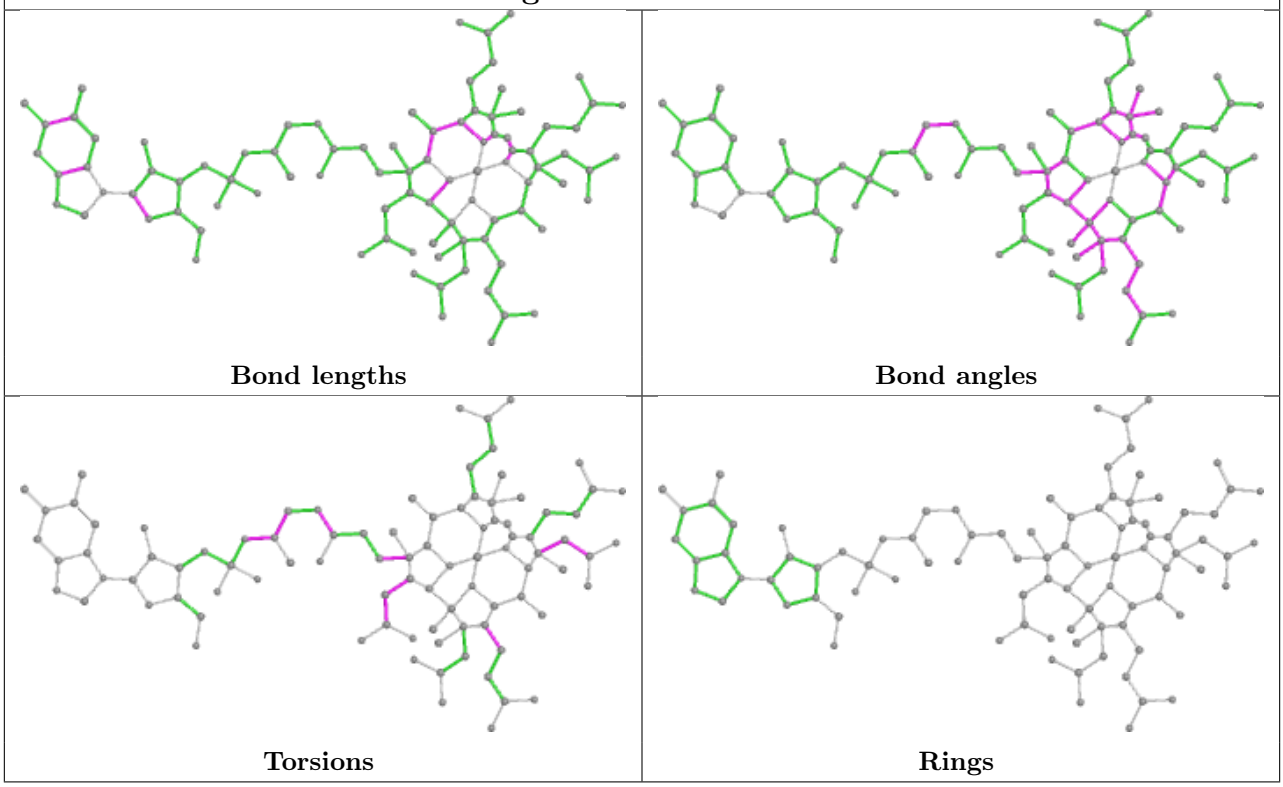

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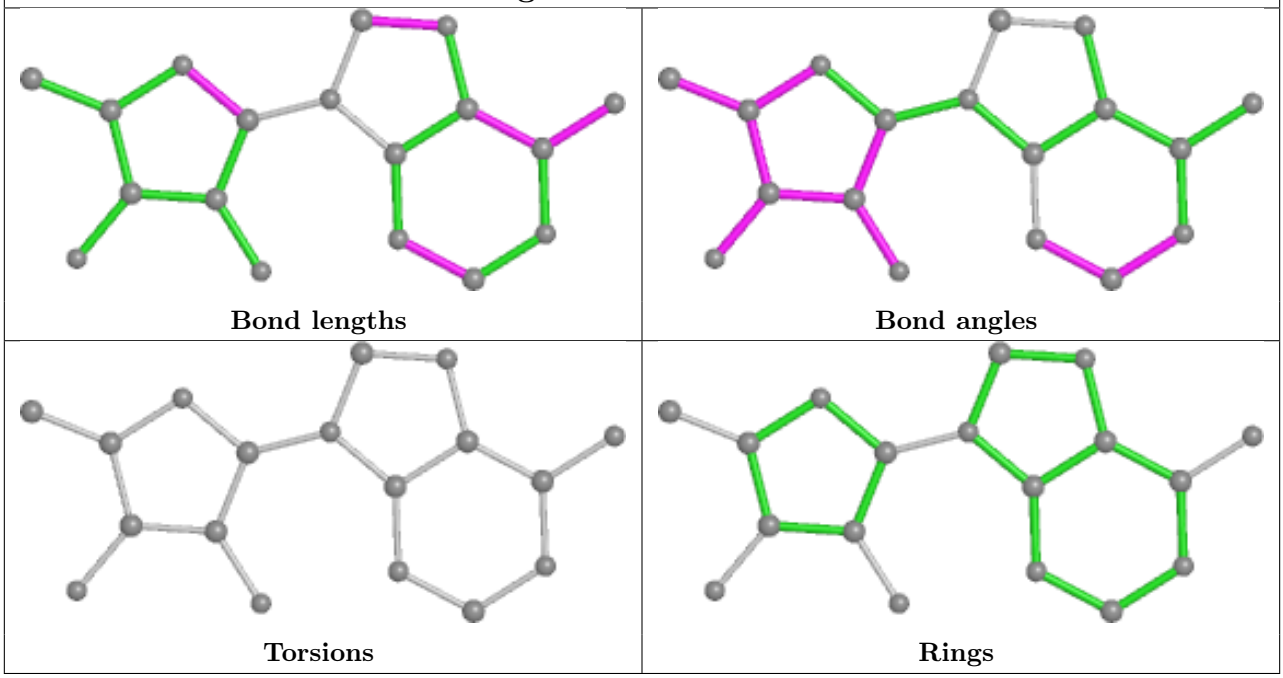

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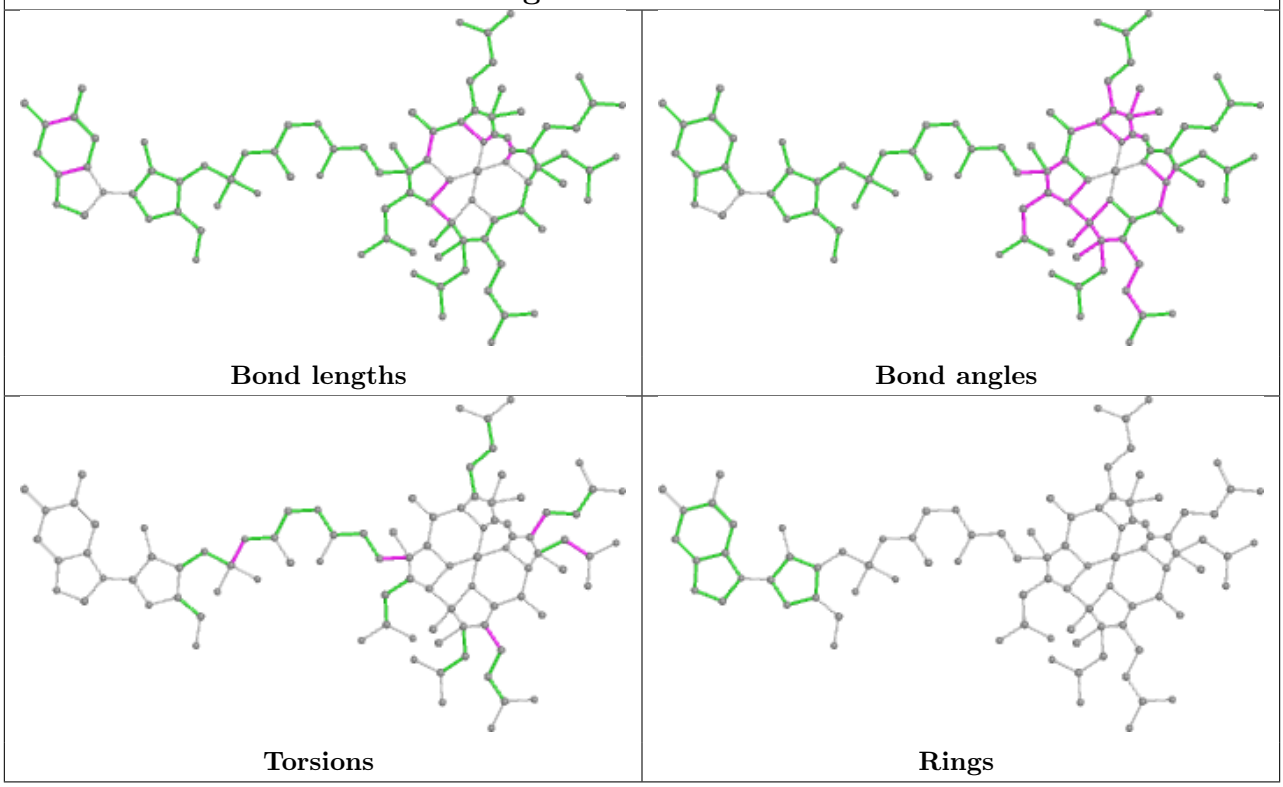
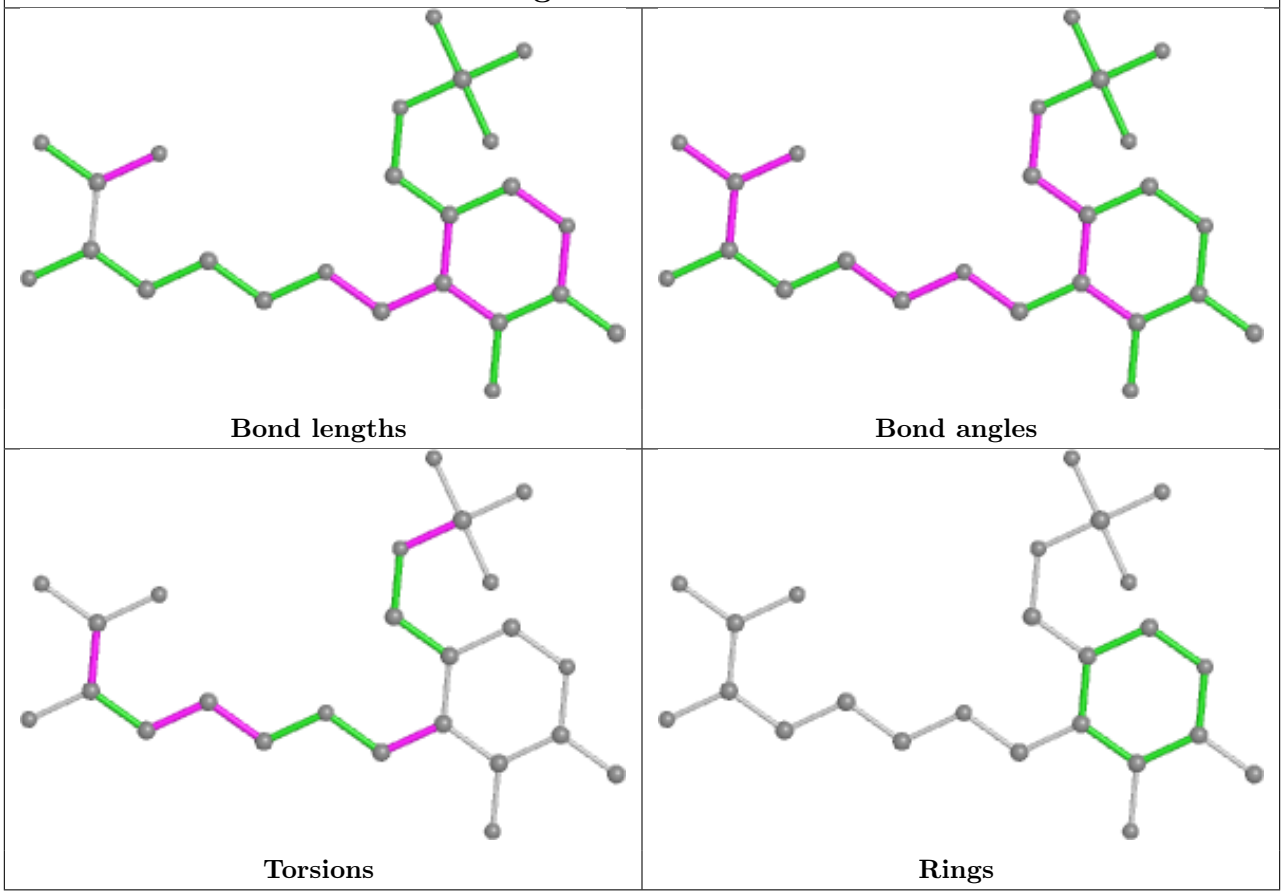


Ligand Z97 C 767



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

The worst 5 of 15 RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

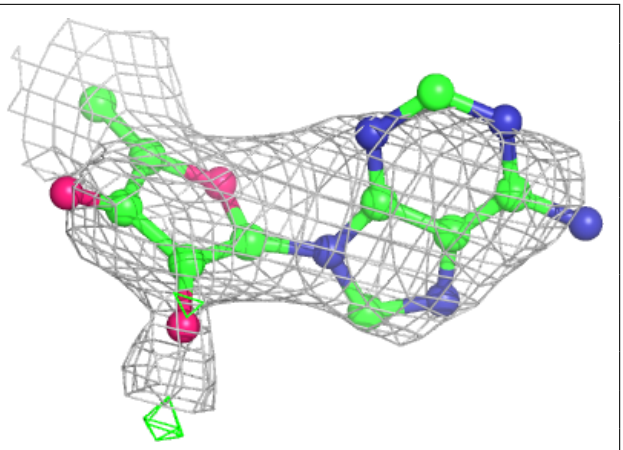
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

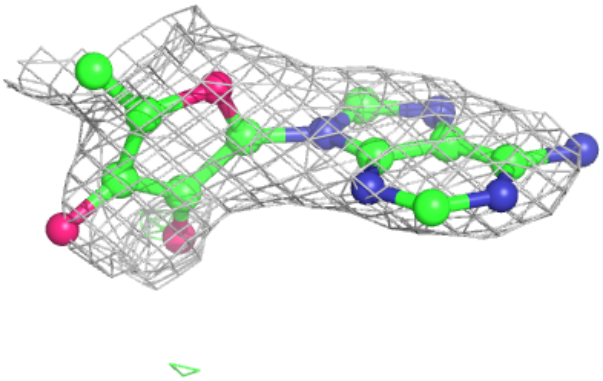
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	5AD	C	1500	18/18	0.86	0.24	78,87,94,97	0
5	5AD	B	1500	18/18	0.88	0.33	64,76,83,84	0
5	5AD	D	1500	18/18	0.92	0.22	48,60,65,66	0
5	5AD	A	1500	18/18	0.93	0.21	37,46,54,55	0
3	B12	A	1801	91/91	0.93	0.27	57,87,98,99	0
3	B12	D	1801	91/91	0.94	0.19	40,73,84,86	0
4	Z97	C	767	24/24	0.97	0.18	35,40,50,56	0
4	Z97	D	767	24/24	0.97	0.17	25,36,41,44	0
3	B12	C	1801	91/91	0.97	0.16	20,34,46,51	0
3	B12	B	1801	91/91	0.97	0.18	35,55,67,70	0
4	Z97	A	767	24/24	0.97	0.18	22,29,36,38	0
4	Z97	B	767	24/24	0.97	0.15	22,32,46,50	0

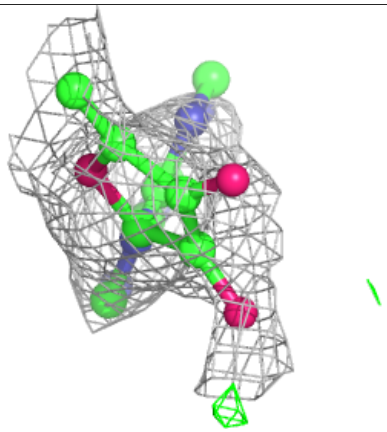
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD C 1500:

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

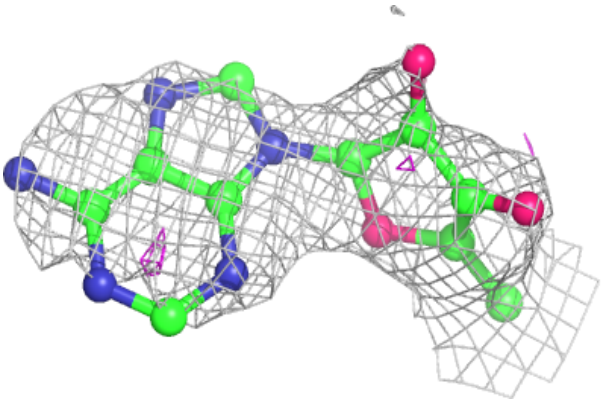


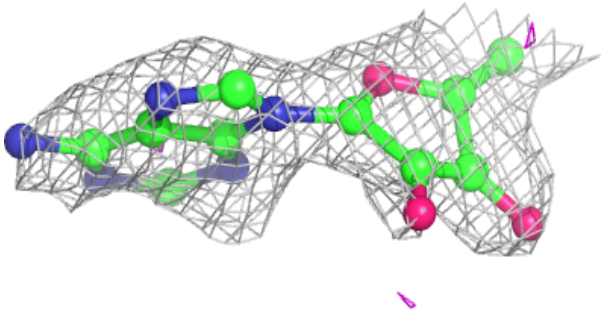


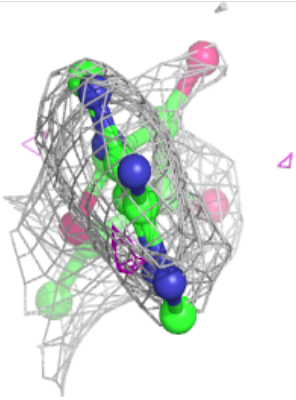


Electron density around 5AD B 1500:

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

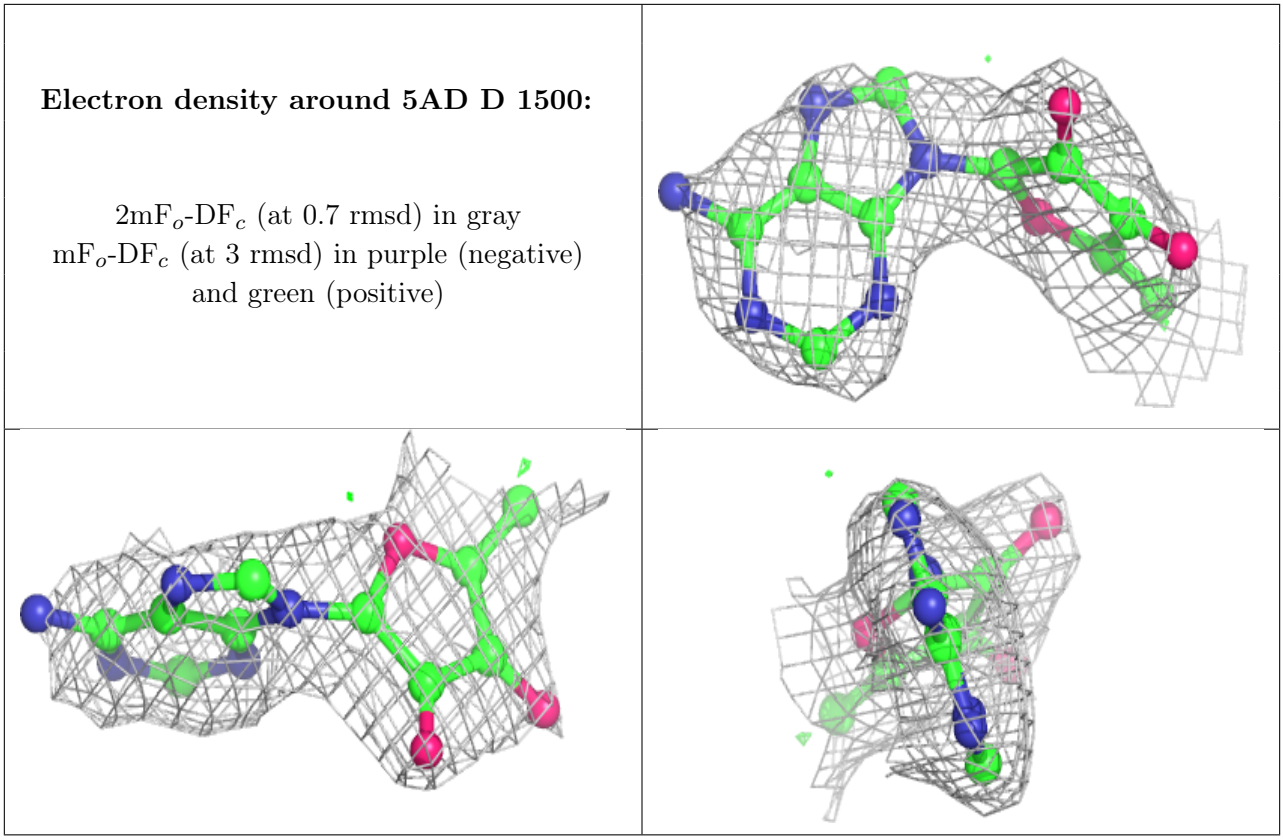






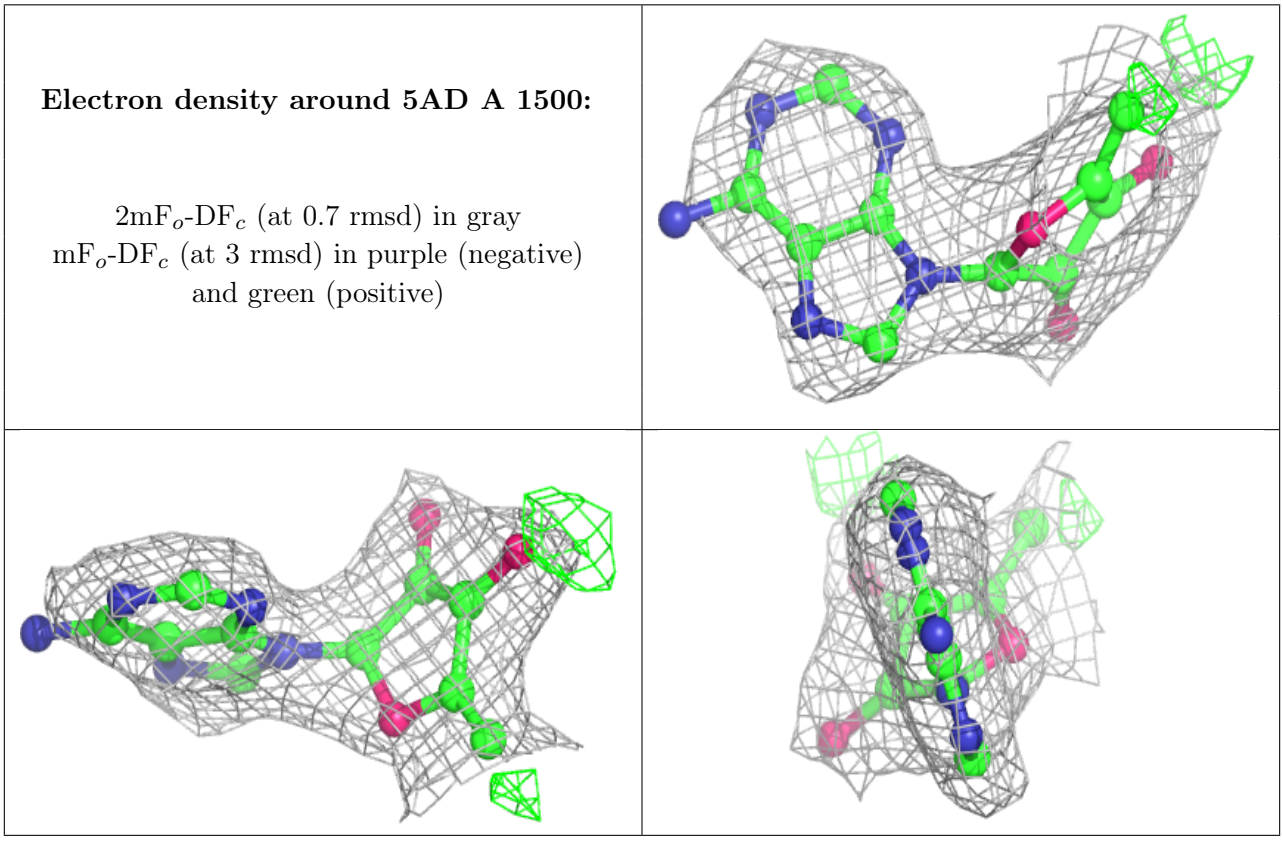
Electron density around 5AD D 1500:

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



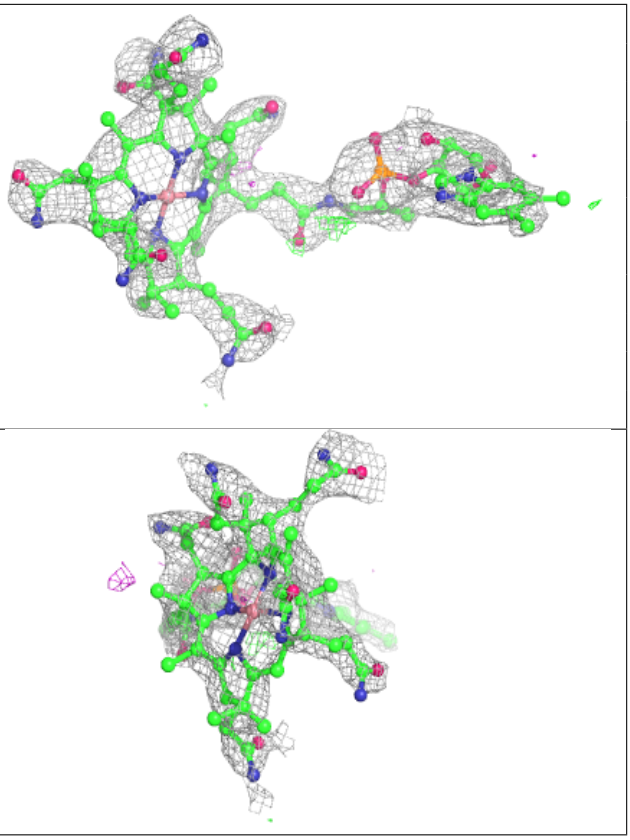
Electron density around 5AD A 1500:

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



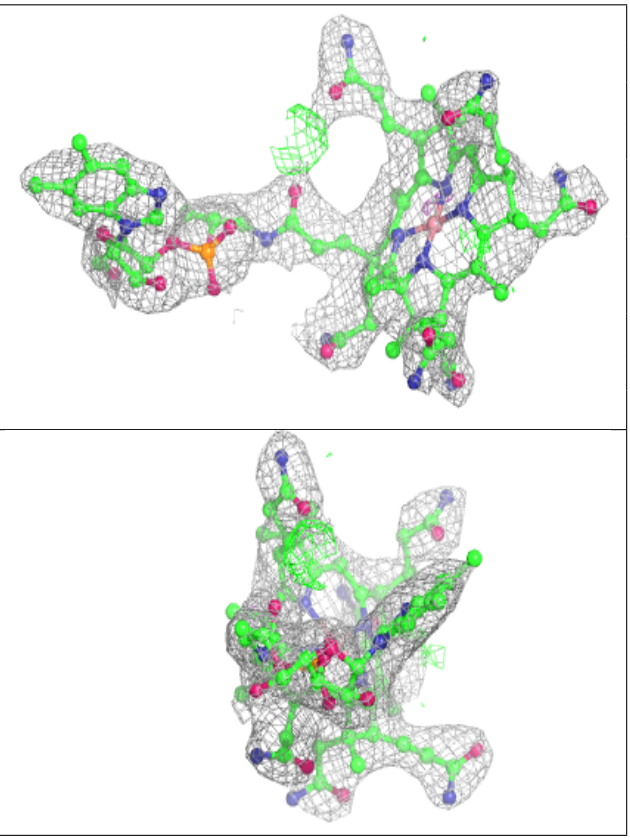
Electron density around B12 A 1801:

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



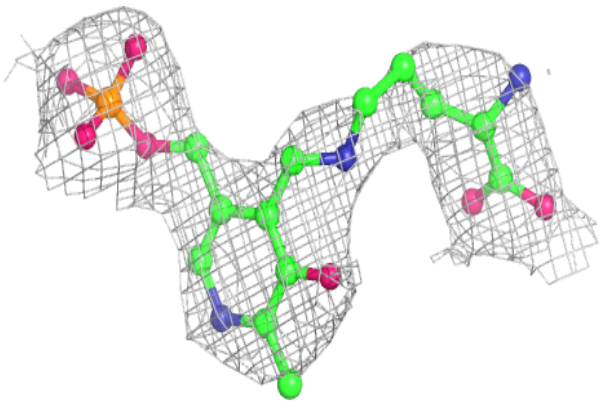
Electron density around B12 D 1801:

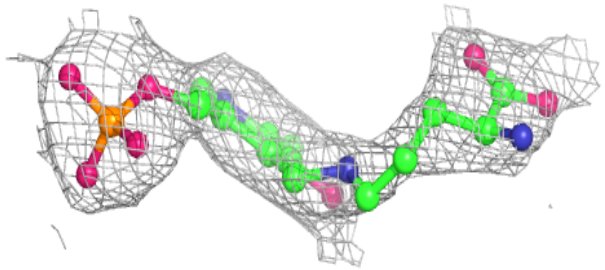
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

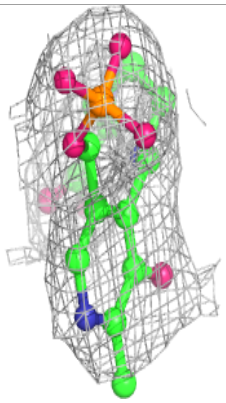


Electron density around Z97 C 767:

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

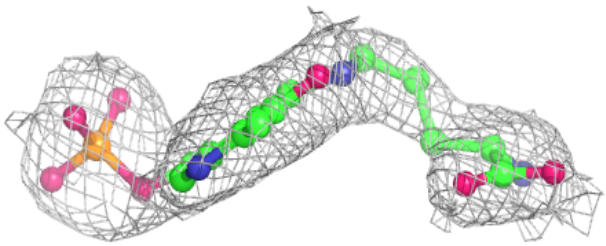


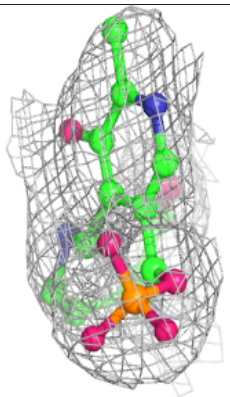




Electron density around Z97 D 767:

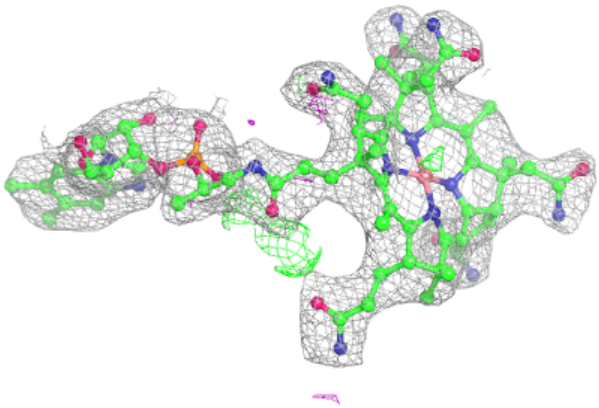
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

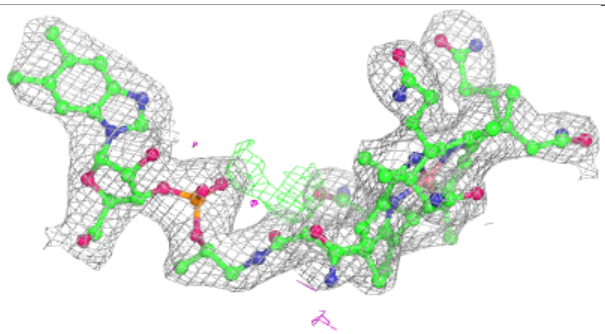


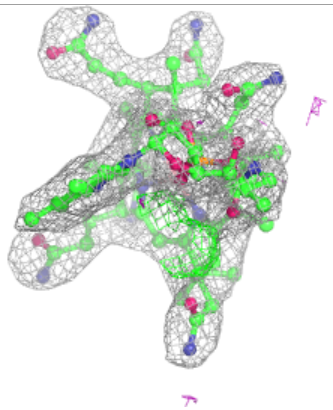


Electron density around B12 C 1801:

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

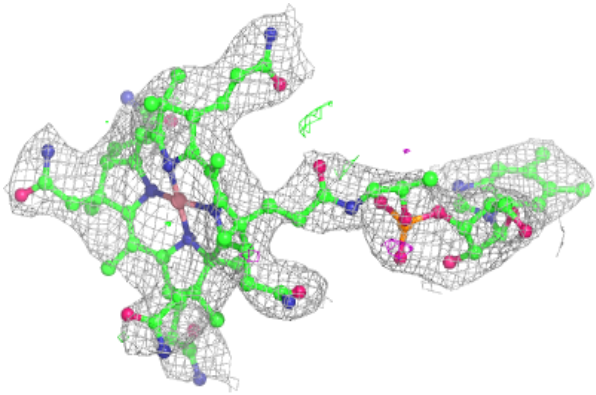


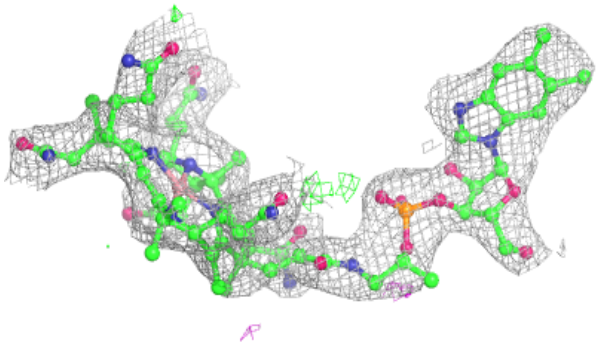


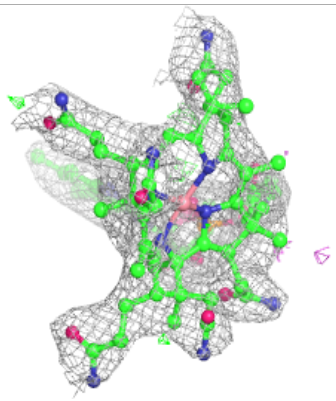


Electron density around B12 B 1801:

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

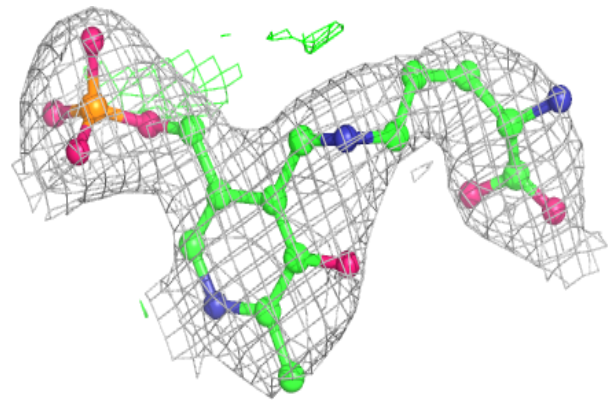


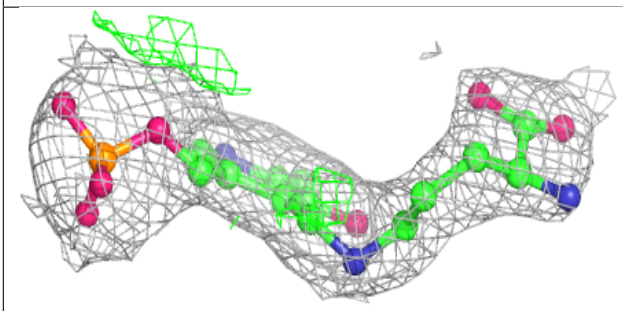




Electron density around Z97 A 767:

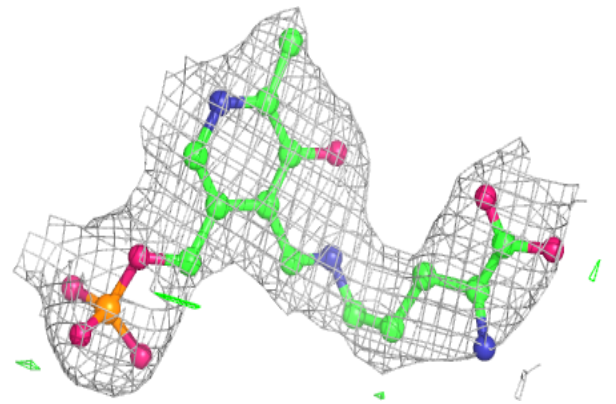
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

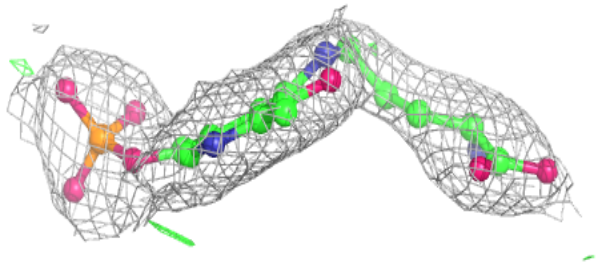


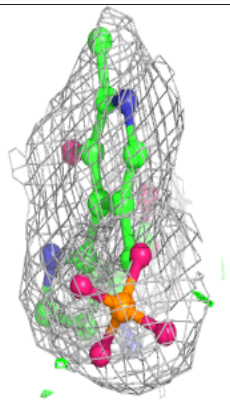


Electron density around Z97 B 767:

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







6.5 Other polymers (i)

There are no such residues in this entry.