



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:33 AM UTC

PDB ID : 8XGY / pdb_00008xgy
Title : Crystal structure of human Golgi resident glutaminyl cyclase in complex with (R,Z)-3-((1H-benzo[d]imidazol-5-yl)methylene)-4-((1-acetylpyrrolidin-3-yl)oxy)indolin-2-one
Authors : Li, G.-B.; Wang, X.-Y.
Deposited on : 2023-12-16
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

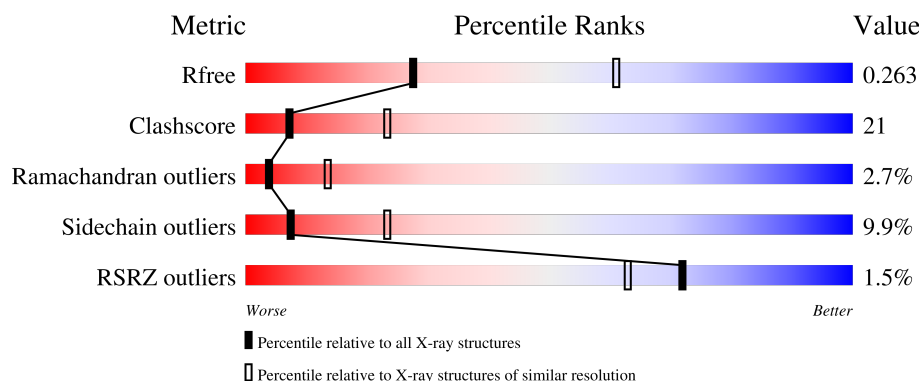
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	2% 56% 36% 5% ..
1	B	329	2% 50% 39% 8% ..
1	C	329	% 59% 32% 6% ..
1	D	329	% 60% 33% 5% .

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Mol	Chain	Length	Quality of chain
1	E	329	
1	F	329	
1	G	329	
1	H	329	
1	I	329	
1	J	329	
1	K	329	
1	L	329	

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
2	ZN	L	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31701 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	A	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	C	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	D	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	E	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	F	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	G	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	H	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	I	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	J	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	K	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	L	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

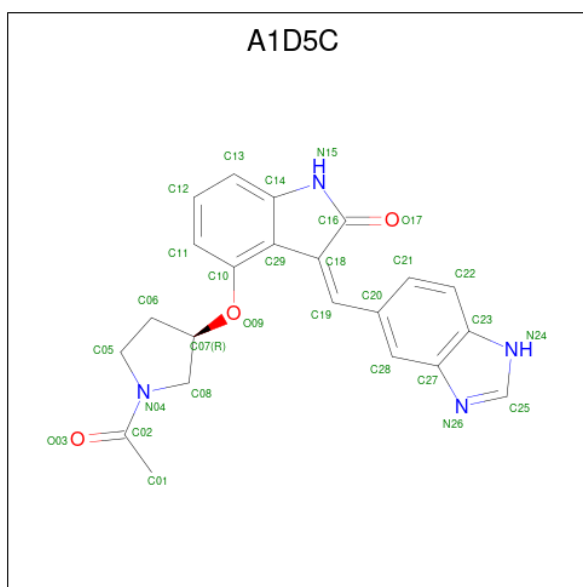
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	I	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	L	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (3 {Z})-3-(1 {H}-benzimidazol-5-ylmethylidene)-4-[(3 {R})-1-ethanoylpyrrolidin-3-yl]oxy-1 {H}-indol-2-one (CCD ID: A1D5C) (formula: C₂₂H₂₀N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 29 22 4 3	0	0
3	A	1	Total C N O 29 22 4 3	0	0
3	C	1	Total C N O 29 22 4 3	0	0
3	D	1	Total C N O 29 22 4 3	0	0
3	E	1	Total C N O 29 22 4 3	0	0
3	F	1	Total C N O 29 22 4 3	0	0
3	G	1	Total C N O 29 22 4 3	0	0
3	H	1	Total C N O 29 22 4 3	0	0
3	I	1	Total C N O 29 22 4 3	0	0
3	J	1	Total C N O 29 22 4 3	0	0
3	K	1	Total C N O 29 22 4 3	0	0
3	L	1	Total C N O 29 22 4 3	0	0

- Molecule 4 is water.

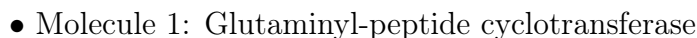
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total O 5 5	0	0
4	A	1	Total O 1 1	0	0
4	C	3	Total O 3 3	0	0
4	D	1	Total O 1 1	0	0
4	E	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0

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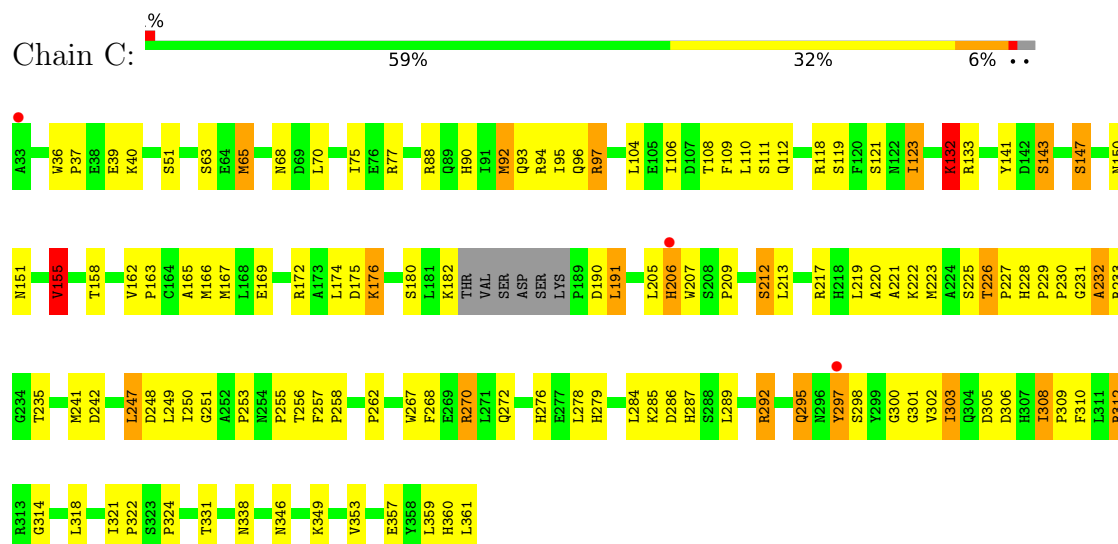
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	3	Total 3	O 3	0	0
4	L	1	Total 1	O 1	0	0

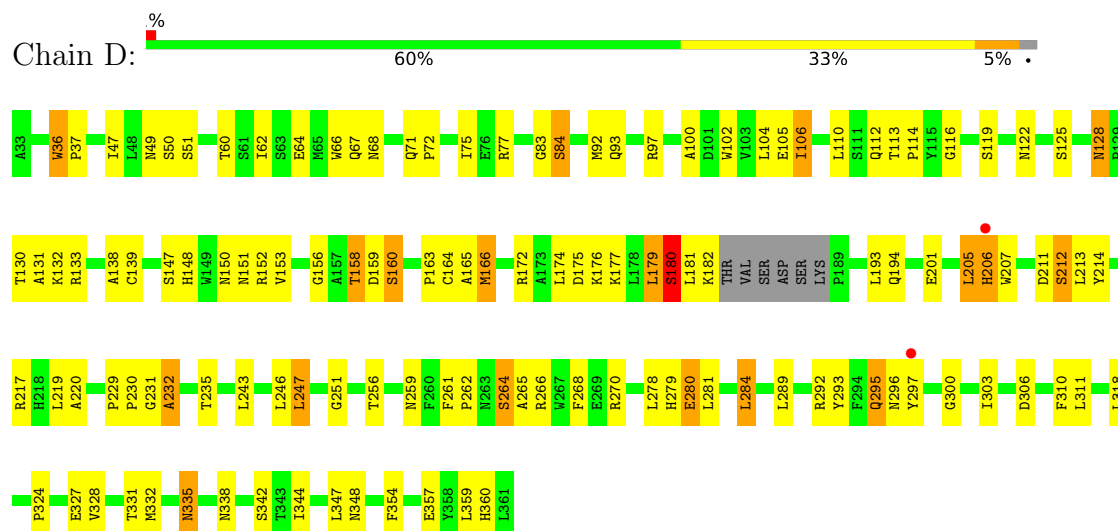
- Molecule 1: Glutaminyl-peptide cyclotransferase



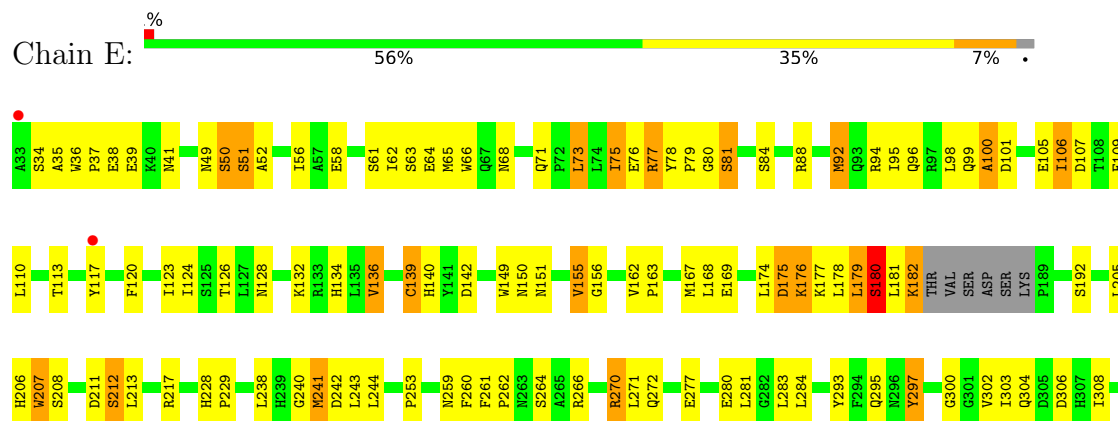
• Molecule 1: Glutaminyl-peptide cyclotransferase

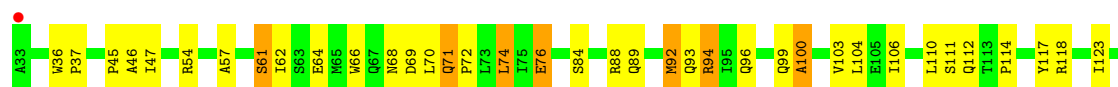


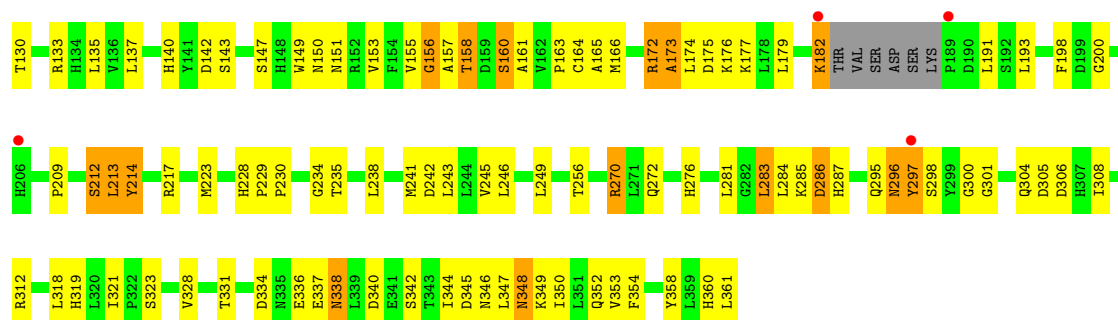
• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase

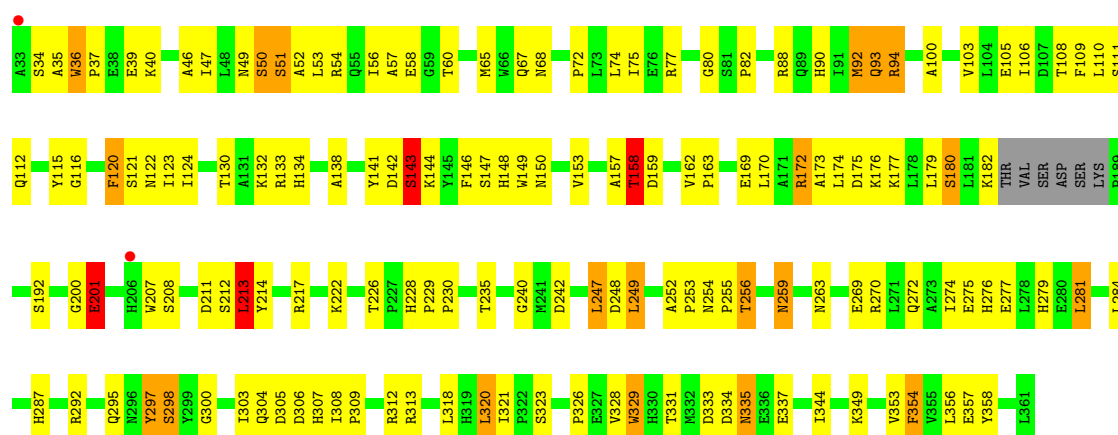






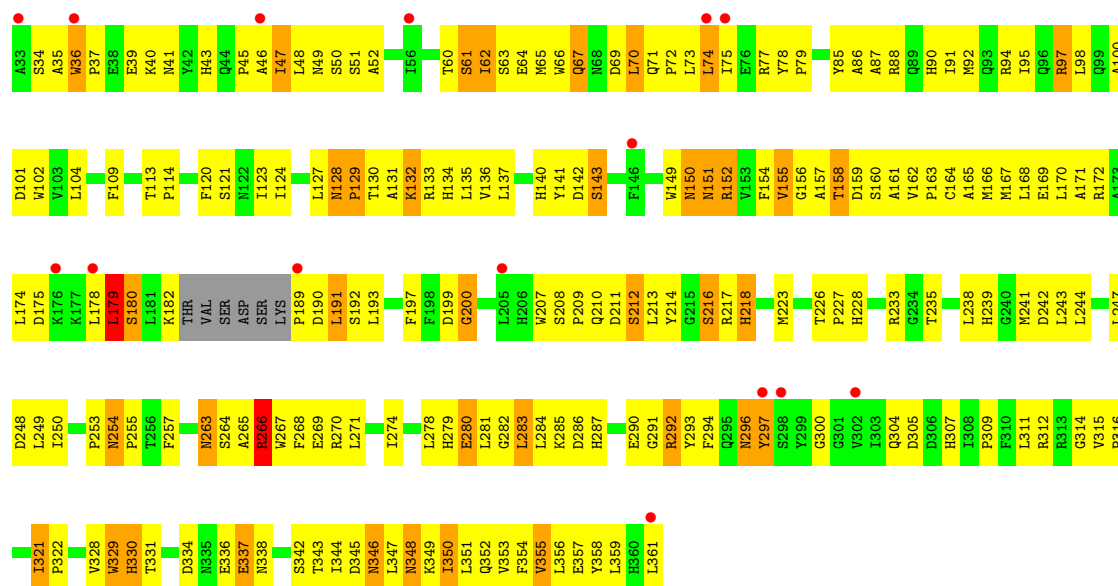
• Molecule 1: Glutaminyl-peptide cyclotransferase

Chain I: 52% 39% 6% ..

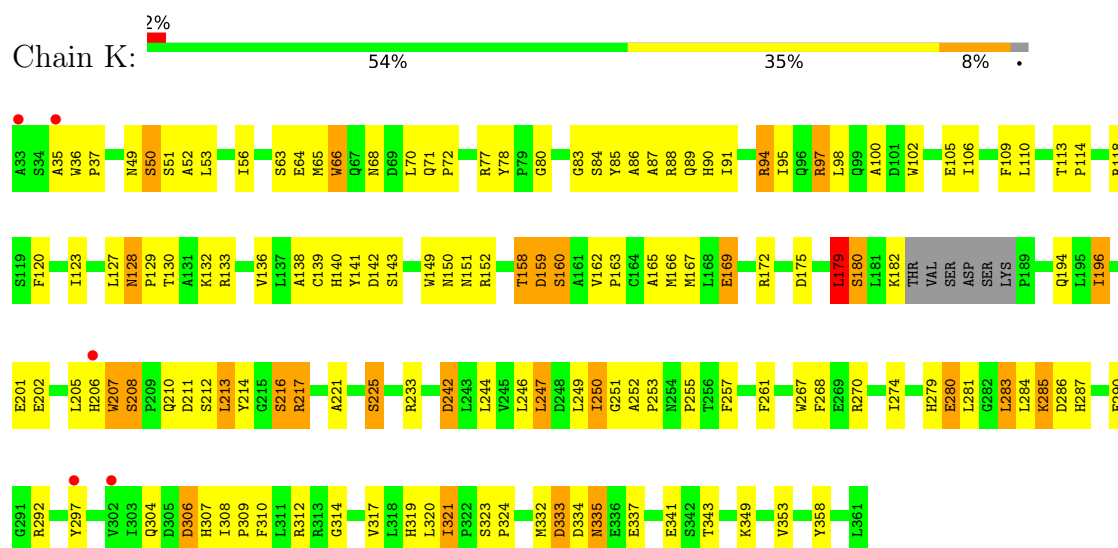


• Molecule 1: Glutaminyl-peptide cyclotransferase

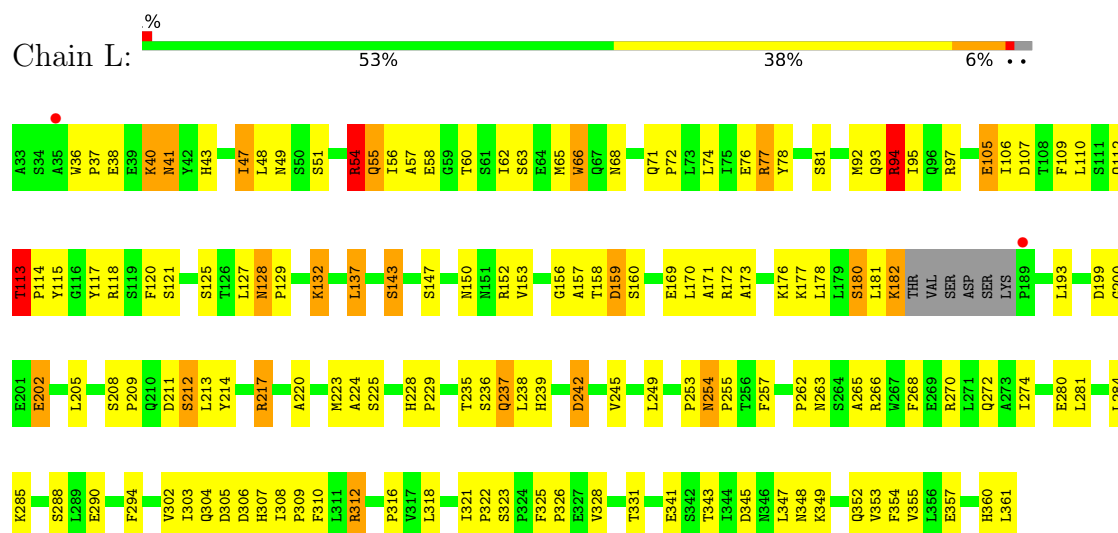
Chain J: 5% 36% 50% 12% ..



• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.72Å 217.25Å 242.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.12 – 2.81 78.12 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.12-2.81) 99.8 (78.12-2.81)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.188 , 0.258 0.200 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31701	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A1D5C

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	2.18	58/2687 (2.2%)	1.27	3/3656 (0.1%)
1	B	2.20	61/2687 (2.3%)	1.32	10/3656 (0.3%)
1	C	2.09	42/2687 (1.6%)	1.28	6/3656 (0.2%)
1	D	2.06	39/2687 (1.5%)	1.21	8/3656 (0.2%)
1	E	1.98	39/2687 (1.5%)	1.22	3/3656 (0.1%)
1	F	1.87	18/2687 (0.7%)	1.17	2/3656 (0.1%)
1	G	1.27	2/2687 (0.1%)	0.96	0/3656
1	H	1.49	5/2687 (0.2%)	1.08	0/3656
1	I	1.63	14/2687 (0.5%)	1.15	4/3656 (0.1%)
1	J	1.17	0/2687	1.01	0/3656
1	K	1.90	27/2687 (1.0%)	1.20	1/3656 (0.0%)
1	L	1.79	14/2687 (0.5%)	1.25	5/3656 (0.1%)
All	All	1.83	319/32244 (1.0%)	1.18	42/43872 (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

The worst 5 of 319 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	323	SER	CA-C	-11.80	1.42	1.52
1	B	312	ARG	C-O	-11.62	1.09	1.24
1	K	333	ASP	C-O	-10.39	1.10	1.24
1	L	323	SER	CA-C	-9.55	1.44	1.52
1	B	216	SER	CA-C	-9.44	1.41	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	333	ASP	O-C-N	-8.34	111.49	122.59
1	L	159	ASP	CB-CG-OD1	-7.49	101.19	118.40
1	B	218	HIS	N-CA-C	7.17	131.07	111.00
1	B	216	SER	N-CA-C	-7.07	97.68	109.07
1	L	159	ASP	CB-CG-OD2	6.57	133.51	118.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	GLY	Mainchain

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	2610	0	2529	68	0
1	B	2610	0	2529	98	0
1	C	2610	0	2529	68	0
1	D	2610	0	2529	63	0
1	E	2610	0	2529	78	0
1	F	2610	0	2529	113	0
1	G	2610	0	2529	157	0
1	H	2610	0	2529	105	0
1	I	2610	0	2529	106	0
1	J	2610	0	2529	238	0
1	K	2610	0	2529	92	0
1	L	2610	0	2529	130	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	2	0
3	A	29	0	0	2	0
3	B	29	0	0	3	0
3	C	29	0	0	1	0
3	D	29	0	0	2	0
3	E	29	0	0	0	0
3	F	29	0	0	0	0
3	G	29	0	0	4	0
3	H	29	0	0	1	0
3	I	29	0	0	2	0
3	J	29	0	0	2	0
3	K	29	0	0	5	0
3	L	29	0	0	5	0
4	A	1	0	0	2	0
4	B	5	0	0	1	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
4	K	3	0	0	1	0
4	L	1	0	0	0	0
All	All	31701	0	30348	1279	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 21.

The worst 5 of 1279 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)
3:B:402:A1D5C:C07	3:B:402:A1D5C:C08	1.77	1.51
3:D:402:A1D5C:C07	3:D:402:A1D5C:C08	1.77	1.49
3:C:402:A1D5C:C08	3:C:402:A1D5C:C07	1.74	1.38
3:A:402:A1D5C:C07	3:A:402:A1D5C:C08	1.74	1.34
1:B:217:ARG:HB2	1:B:220:ALA:CB	1.67	1.24

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	319/329 (97%)	286 (90%)	30 (9%)	3 (1%)	14	38
1	B	319/329 (97%)	288 (90%)	26 (8%)	5 (2%)	7	24
1	C	319/329 (97%)	290 (91%)	24 (8%)	5 (2%)	7	24
1	D	319/329 (97%)	288 (90%)	24 (8%)	7 (2%)	5	17
1	E	319/329 (97%)	282 (88%)	28 (9%)	9 (3%)	4	13
1	F	319/329 (97%)	277 (87%)	36 (11%)	6 (2%)	6	20
1	G	319/329 (97%)	260 (82%)	45 (14%)	14 (4%)	2	6
1	H	319/329 (97%)	273 (86%)	35 (11%)	11 (3%)	3	10
1	I	319/329 (97%)	270 (85%)	42 (13%)	7 (2%)	5	17
1	J	319/329 (97%)	252 (79%)	47 (15%)	20 (6%)	1	3
1	K	319/329 (97%)	282 (88%)	29 (9%)	8 (2%)	4	15
1	L	319/329 (97%)	274 (86%)	38 (12%)	7 (2%)	5	17
All	All	3828/3948 (97%)	3322 (87%)	404 (11%)	102 (3%)	4	13

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	SER
1	B	218	HIS
1	B	232	ALA
1	A	232	ALA
1	A	301	GLY

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	284/290 (98%)	263 (93%)	21 (7%)	13	36
1	B	284/290 (98%)	256 (90%)	28 (10%)	7	23
1	C	284/290 (98%)	258 (91%)	26 (9%)	8	26
1	D	284/290 (98%)	256 (90%)	28 (10%)	7	23
1	E	284/290 (98%)	258 (91%)	26 (9%)	8	26
1	F	284/290 (98%)	255 (90%)	29 (10%)	7	22
1	G	284/290 (98%)	253 (89%)	31 (11%)	6	19
1	H	284/290 (98%)	259 (91%)	25 (9%)	9	28
1	I	284/290 (98%)	253 (89%)	31 (11%)	6	19
1	J	284/290 (98%)	255 (90%)	29 (10%)	7	22
1	K	284/290 (98%)	253 (89%)	31 (11%)	6	19
1	L	284/290 (98%)	252 (89%)	32 (11%)	5	18
All	All	3408/3480 (98%)	3071 (90%)	337 (10%)	7	23

5 of 337 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	182	LYS
1	K	158	THR
1	I	281	LEU
1	J	179	LEU
1	K	290	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	93	GLN
1	I	41	ASN
1	L	352	GLN
1	G	99	GLN
1	H	134	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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	A1D5C	E	402	2	33,33,33	3.73	14 (42%)	44,48,48	2.84	16 (36%)
3	A1D5C	H	402	-	33,33,33	3.82	16 (48%)	44,48,48	3.15	16 (36%)
3	A1D5C	I	402	2	33,33,33	4.02	16 (48%)	44,48,48	3.45	14 (31%)
3	A1D5C	F	402	2	33,33,33	3.84	16 (48%)	44,48,48	3.38	20 (45%)
3	A1D5C	A	402	2	33,33,33	4.20	18 (54%)	44,48,48	3.87	20 (45%)
3	A1D5C	D	402	2	33,33,33	4.21	17 (51%)	44,48,48	4.30	25 (56%)
3	A1D5C	L	402	-	33,33,33	3.86	16 (48%)	44,48,48	2.99	17 (38%)
3	A1D5C	B	402	2	33,33,33	4.27	17 (51%)	44,48,48	3.54	19 (43%)
3	A1D5C	G	402	2	33,33,33	3.97	17 (51%)	44,48,48	2.80	20 (45%)
3	A1D5C	K	402	-	33,33,33	3.63	18 (54%)	44,48,48	3.77	22 (50%)
3	A1D5C	C	402	-	33,33,33	4.40	18 (54%)	44,48,48	4.30	22 (50%)
3	A1D5C	J	402	-	33,33,33	3.77	15 (45%)	44,48,48	2.81	14 (31%)

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	A1D5C	E	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	H	402	-	-	4/12/39/39	0/5/5/5
3	A1D5C	I	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	F	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	A	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	D	402	2	-	6/12/39/39	0/5/5/5
3	A1D5C	L	402	-	-	2/12/39/39	0/5/5/5
3	A1D5C	B	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	G	402	2	-	1/12/39/39	0/5/5/5
3	A1D5C	K	402	-	-	3/12/39/39	0/5/5/5
3	A1D5C	C	402	-	-	4/12/39/39	0/5/5/5
3	A1D5C	J	402	-	-	2/12/39/39	0/5/5/5

The worst 5 of 198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1D5C	C08-C07	15.88	1.77	1.52
3	B	402	A1D5C	C08-C07	15.75	1.77	1.52
3	C	402	A1D5C	C08-C07	13.96	1.74	1.52
3	A	402	A1D5C	C08-C07	13.91	1.74	1.52
3	I	402	A1D5C	C08-C07	13.57	1.74	1.52

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1D5C	C05-N04-C08	-17.59	91.83	112.38
3	B	402	A1D5C	C05-N04-C08	-16.11	93.56	112.38
3	D	402	A1D5C	C05-N04-C08	-13.94	96.10	112.38
3	A	402	A1D5C	C05-N04-C08	-13.57	96.53	112.38
3	K	402	A1D5C	C14-N15-C16	-12.80	103.45	111.35

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1D5C	C16-C18-C19-C20
3	C	402	A1D5C	C29-C18-C19-C20
3	C	402	A1D5C	C16-C18-C19-C20
3	D	402	A1D5C	C06-C07-O09-C10
3	D	402	A1D5C	C08-C07-O09-C10

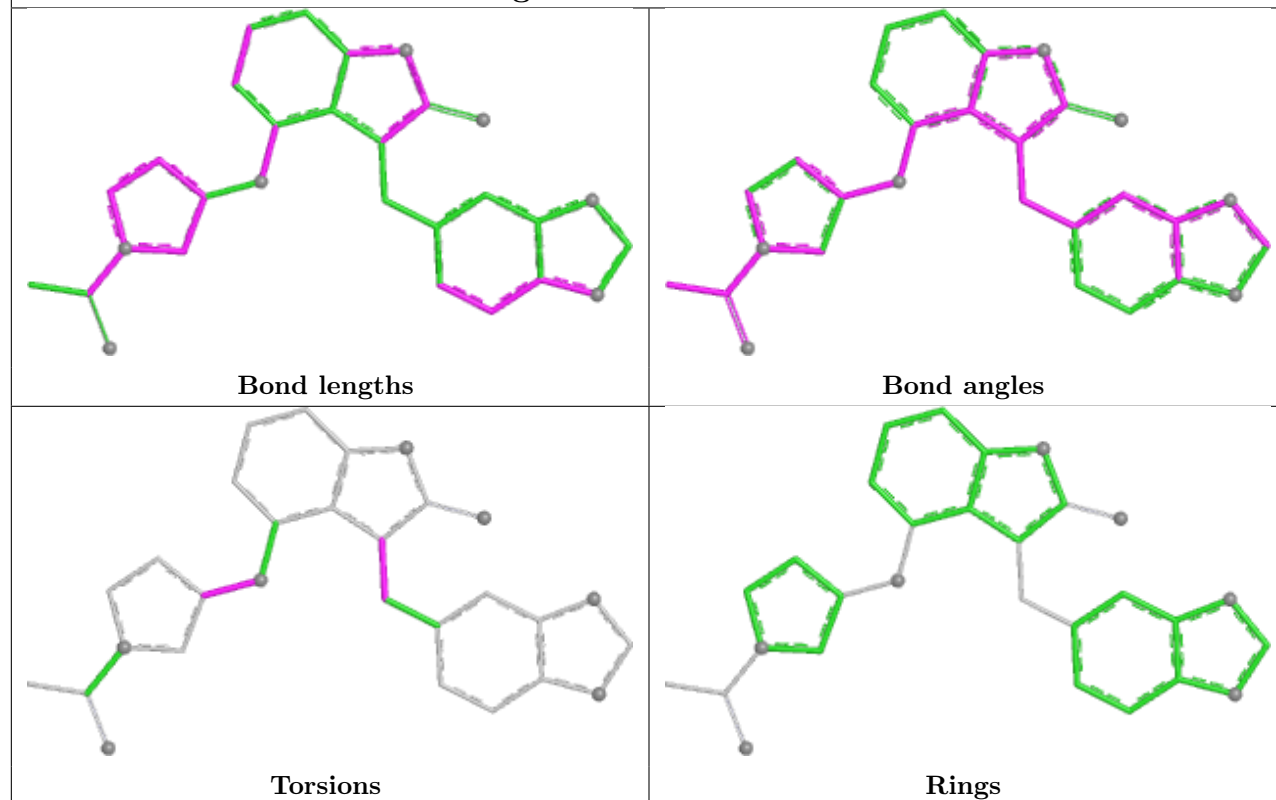
There are no ring outliers.

10 monomers are involved in 27 short contacts:

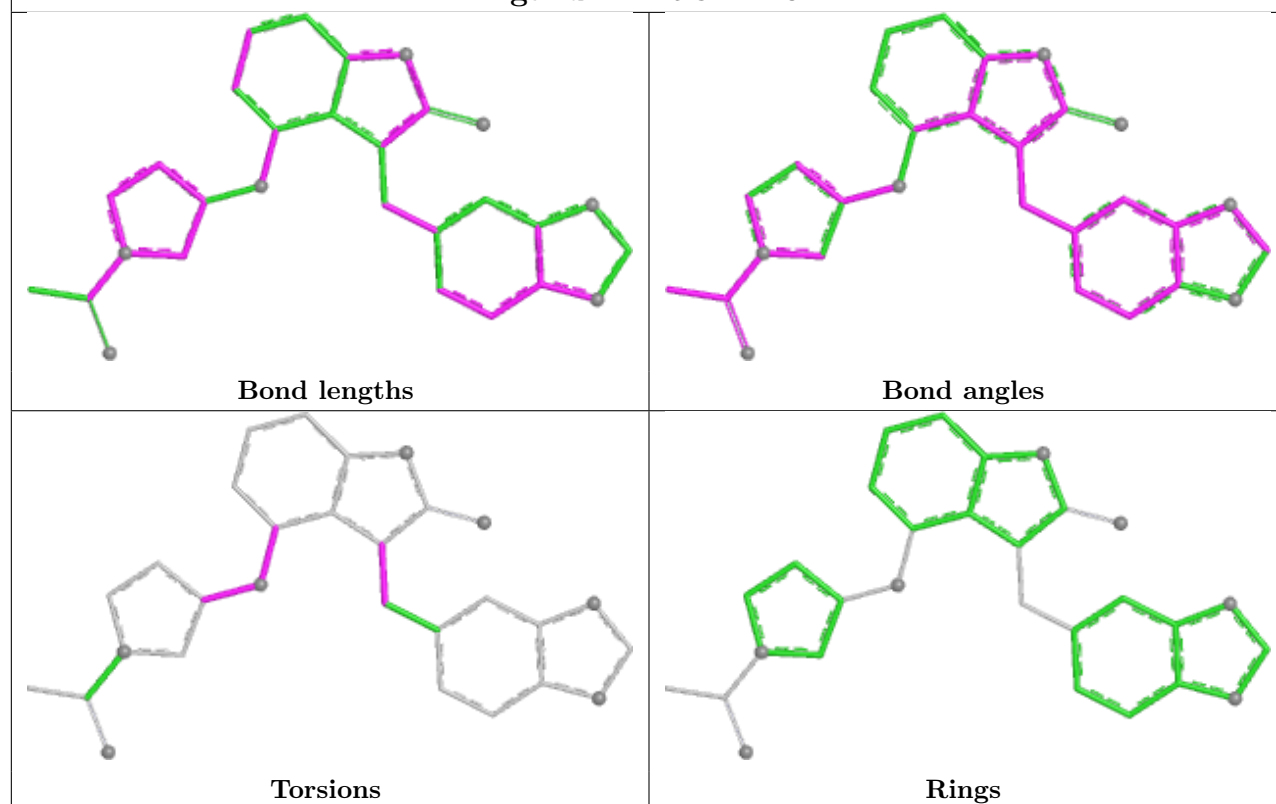
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	402	A1D5C	1	0
3	I	402	A1D5C	2	0
3	A	402	A1D5C	2	0
3	D	402	A1D5C	2	0
3	L	402	A1D5C	5	0
3	B	402	A1D5C	3	0
3	G	402	A1D5C	4	0
3	K	402	A1D5C	5	0
3	C	402	A1D5C	1	0
3	J	402	A1D5C	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

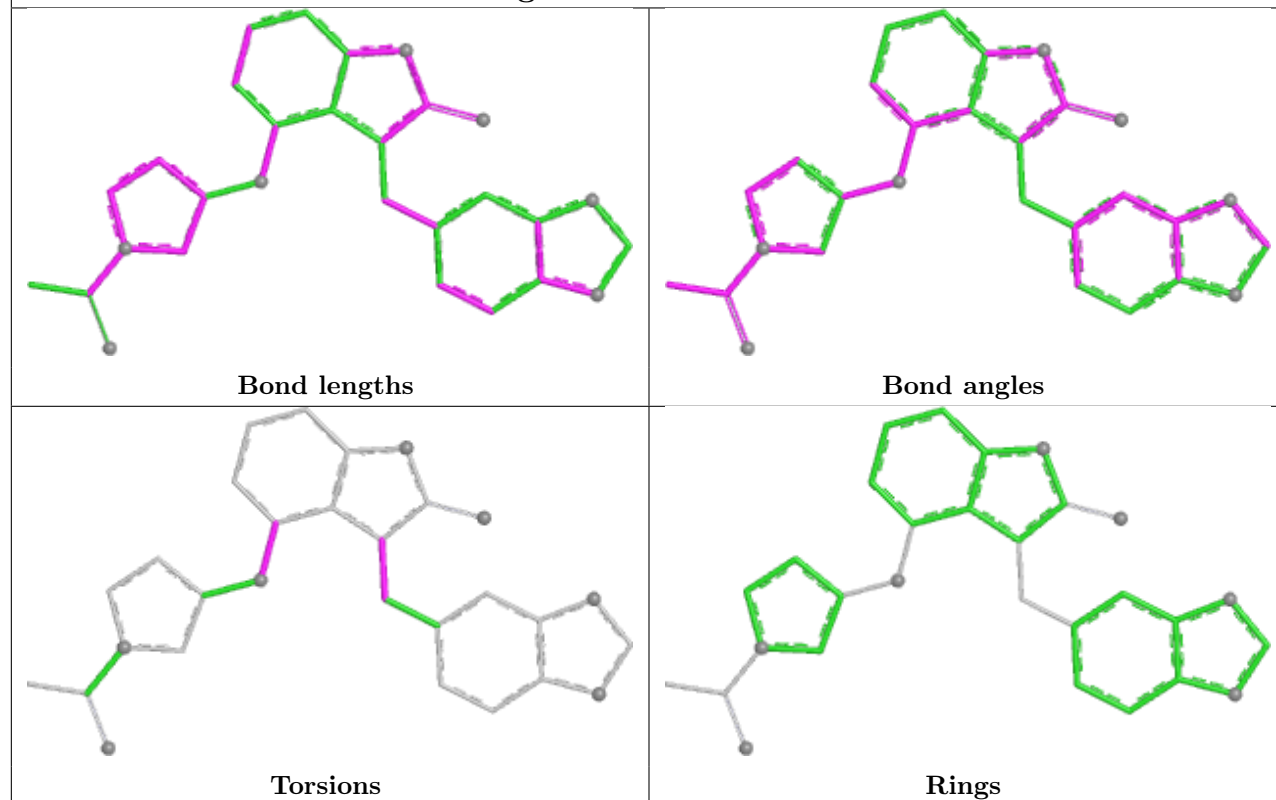
Ligand A1D5C E 402



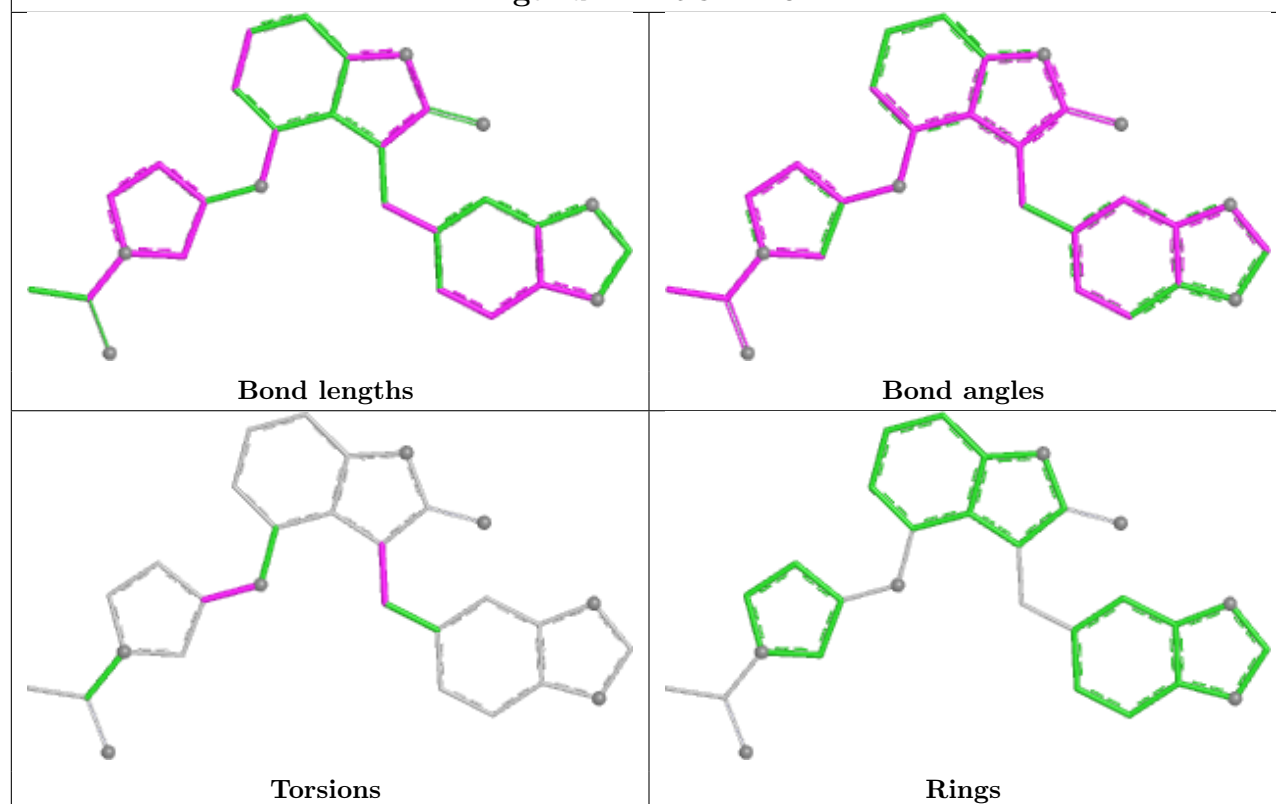
Ligand A1D5C H 402



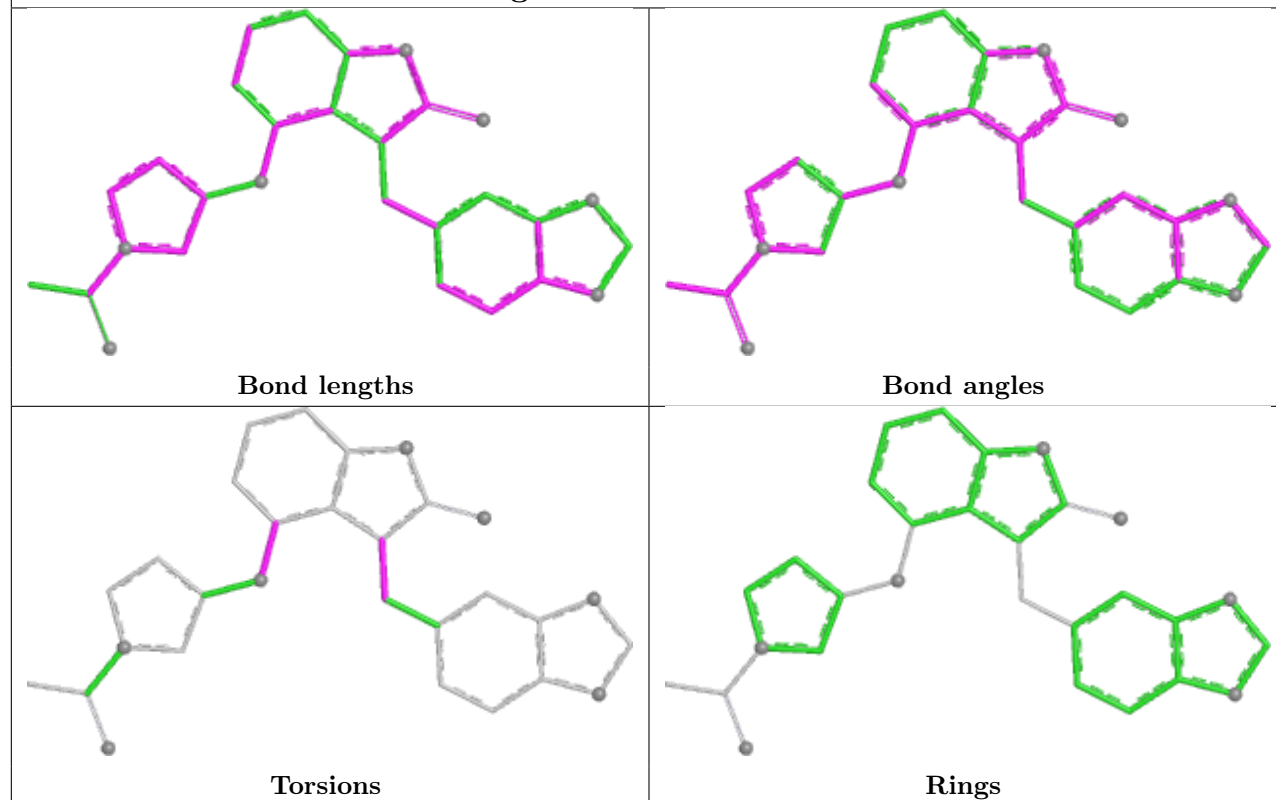
Ligand A1D5C I 402



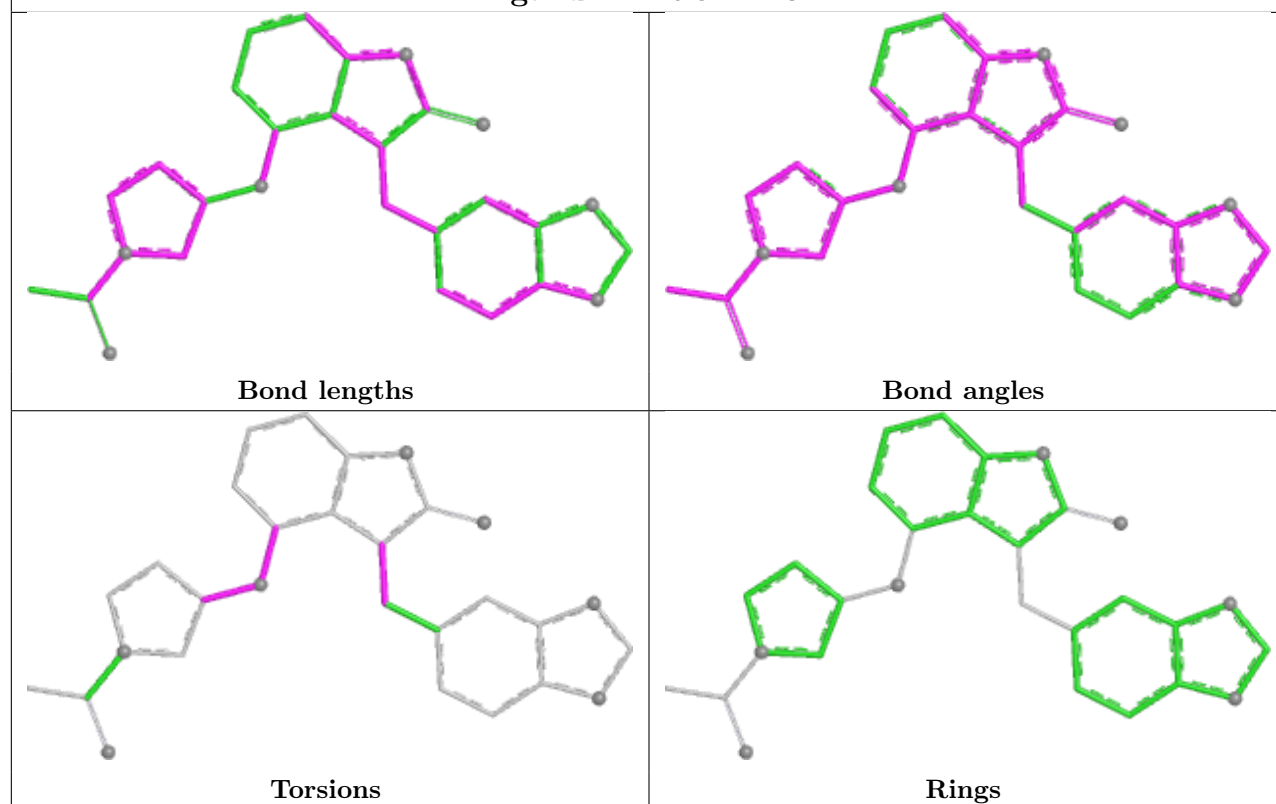
Ligand A1D5C F 402



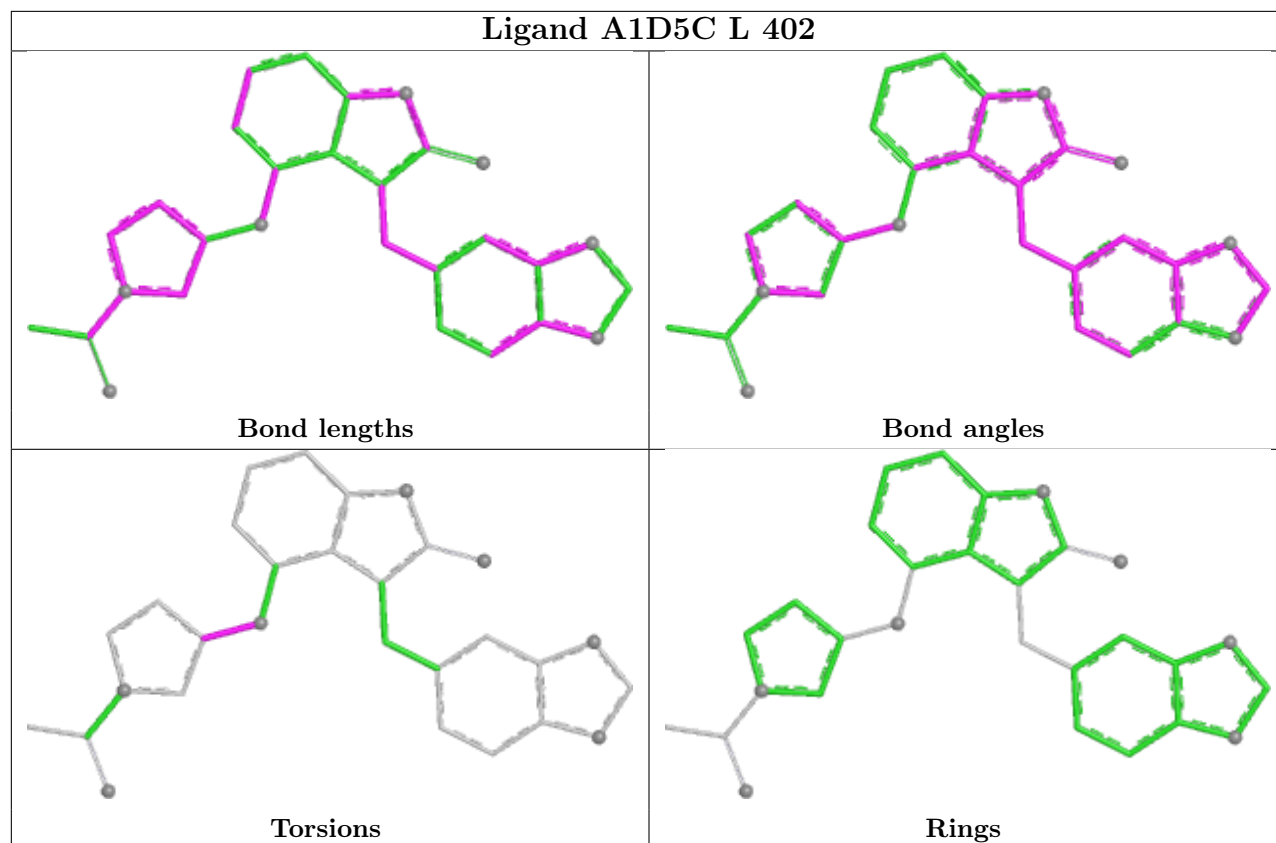
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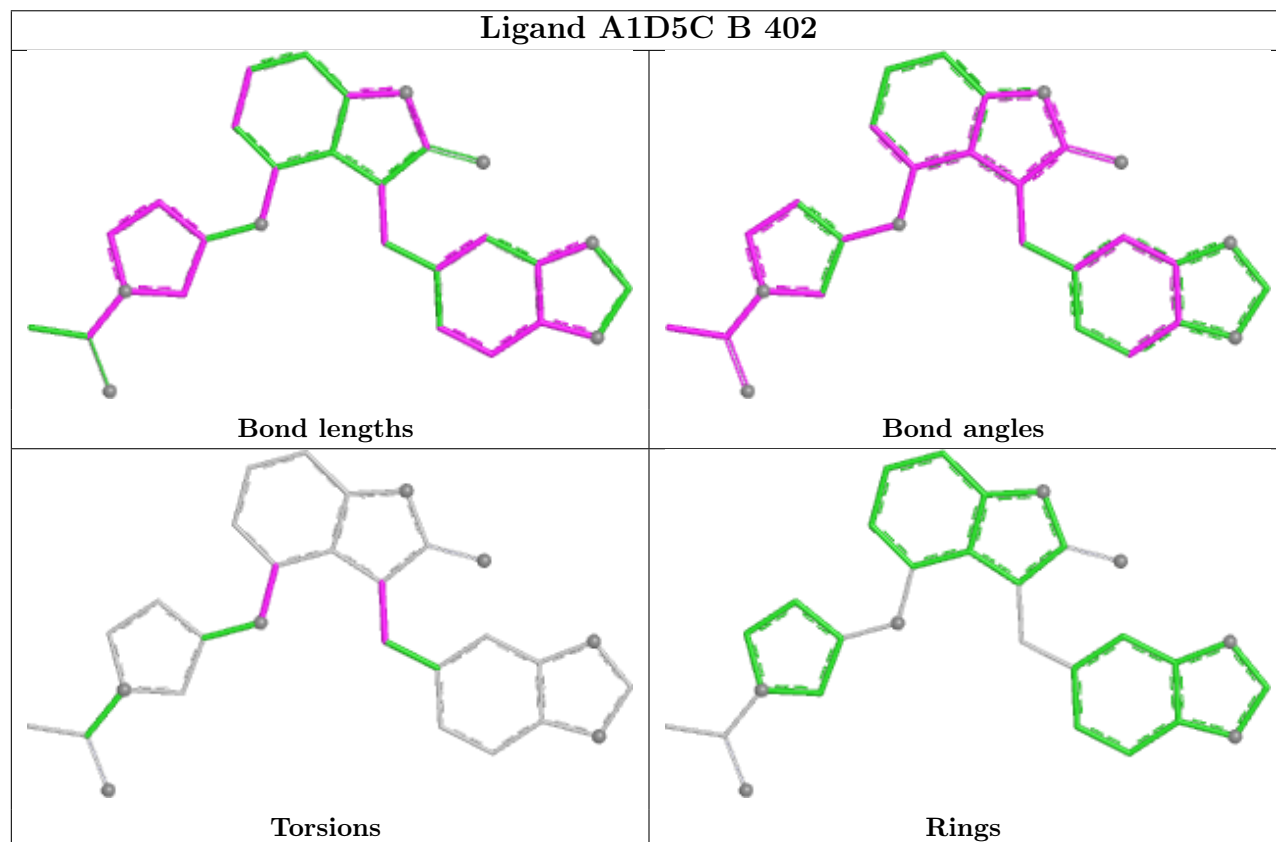
Ligand A1D5C D 402



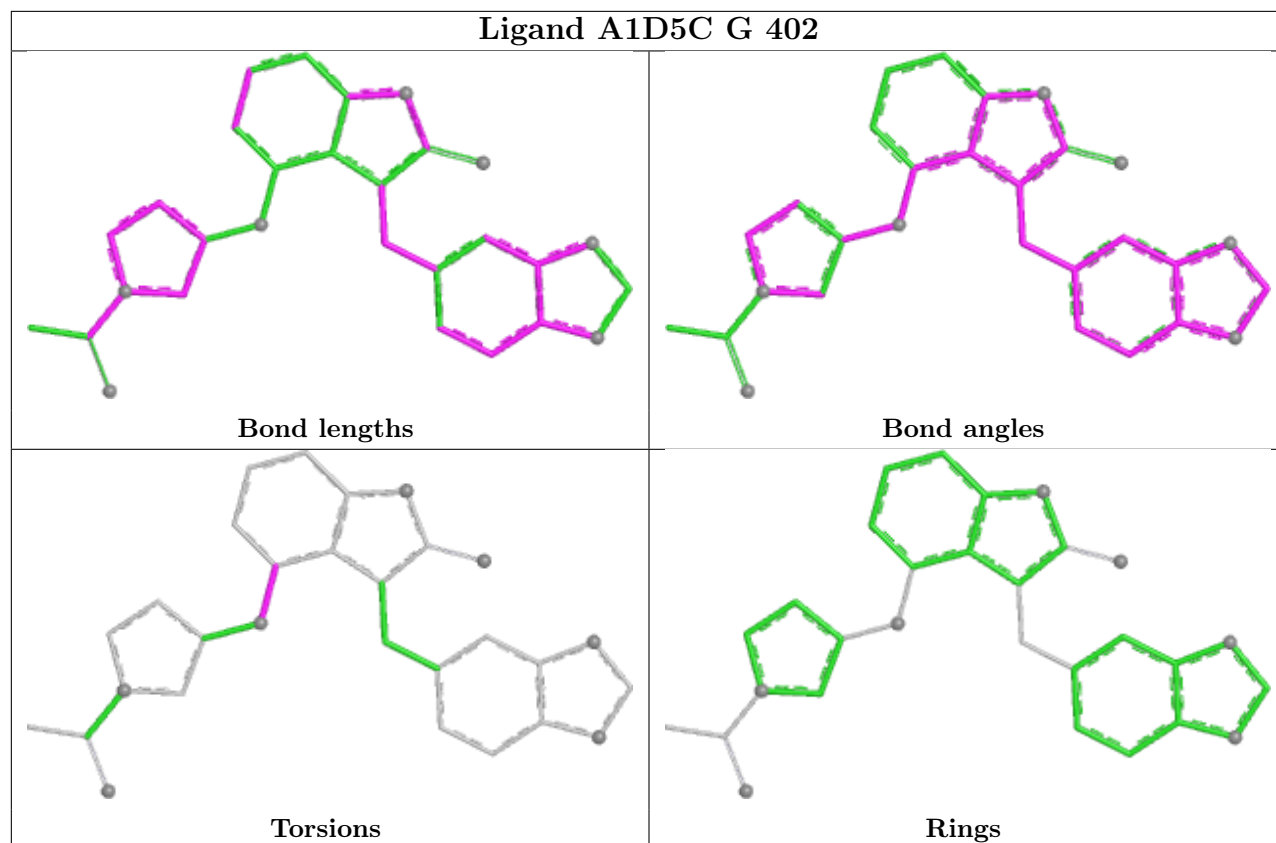
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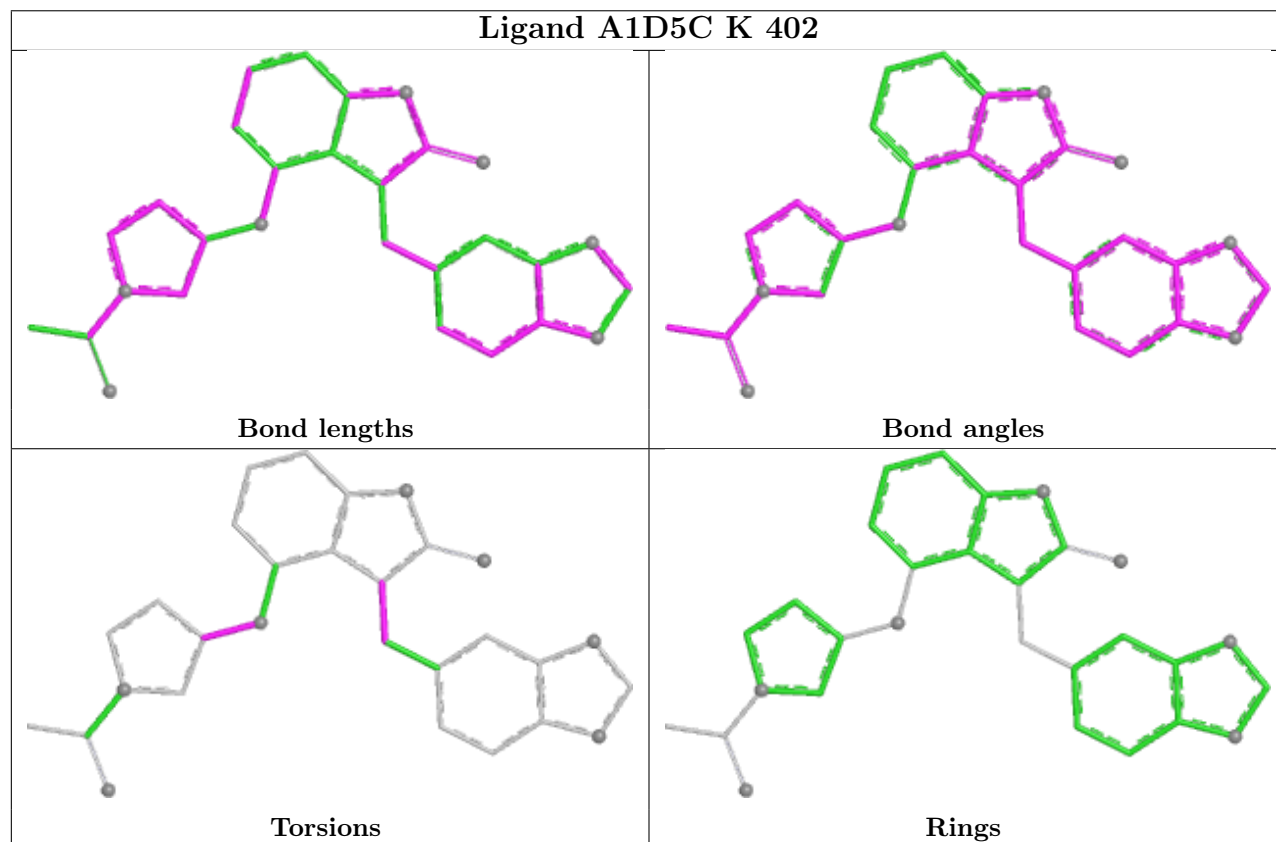
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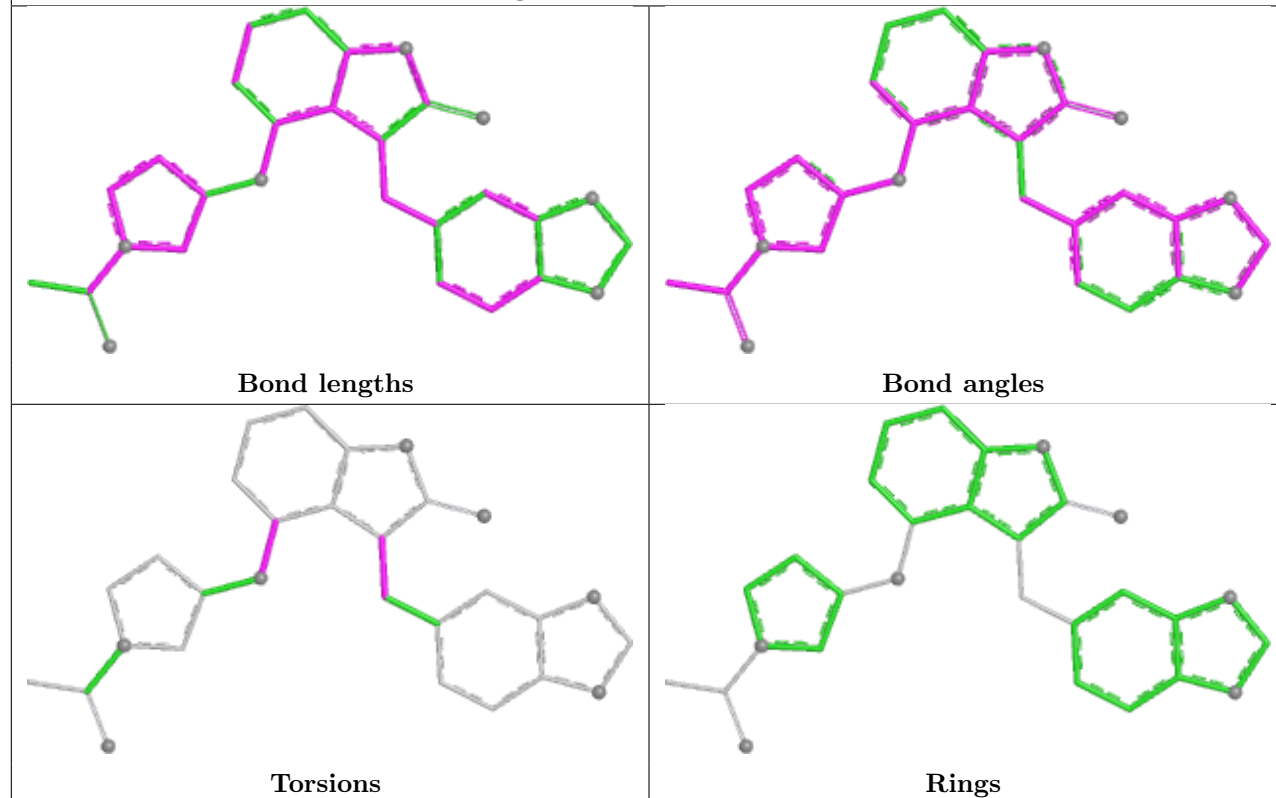
Ligand A1D5C G 402



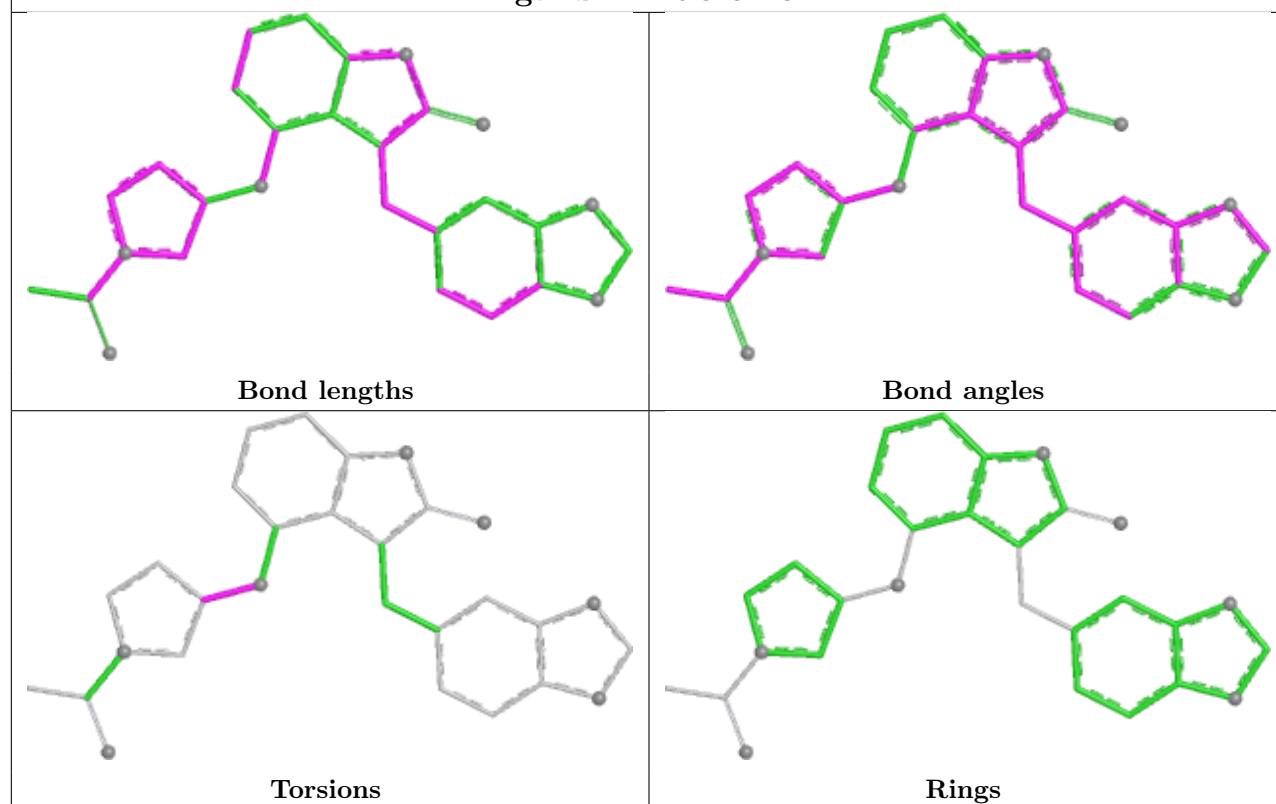
Ligand A1D5C K 402



Ligand A1D5C C 402



Ligand A1D5C J 402



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	322/329 (97%)	-0.47	5 (1%) 70 61	19, 35, 70, 125	0
1	B	322/329 (97%)	-0.46	6 (1%) 66 57	16, 36, 66, 105	0
1	C	322/329 (97%)	-0.40	3 (0%) 81 74	18, 39, 72, 136	0
1	D	322/329 (97%)	-0.44	2 (0%) 85 80	22, 39, 69, 122	0
1	E	322/329 (97%)	-0.33	2 (0%) 85 80	19, 42, 73, 110	0
1	F	322/329 (97%)	-0.32	3 (0%) 81 74	25, 45, 75, 98	0
1	G	322/329 (97%)	0.44	7 (2%) 62 52	40, 75, 110, 135	0
1	H	322/329 (97%)	0.07	5 (1%) 70 61	34, 61, 94, 135	0
1	I	322/329 (97%)	-0.06	2 (0%) 85 80	29, 54, 90, 116	0
1	J	322/329 (97%)	0.76	15 (4%) 36 28	48, 87, 116, 150	0
1	K	322/329 (97%)	-0.23	5 (1%) 70 61	24, 47, 74, 136	0
1	L	322/329 (97%)	-0.23	2 (0%) 85 80	27, 45, 84, 130	0
All	All	3864/3948 (97%)	-0.14	57 (1%) 72 63	16, 48, 97, 150	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ARG	4.5
1	L	35	ALA	3.3
1	A	33	ALA	3.1
1	F	33	ALA	3.0
1	G	33	ALA	3.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

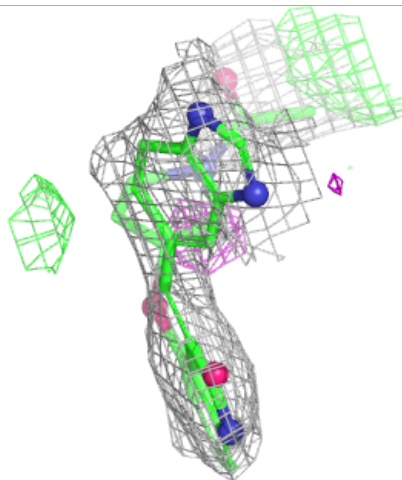
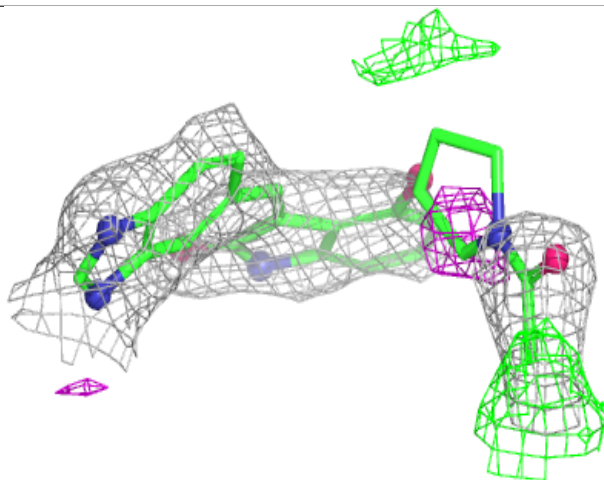
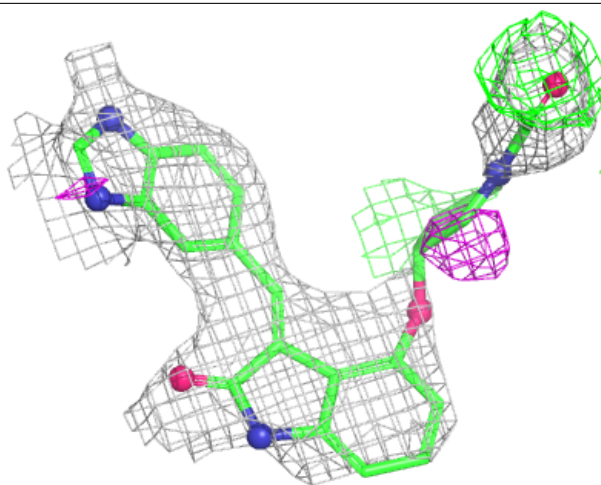
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1D5C	A	402	29/29	0.82	0.15	32,59,85,89	0
3	A1D5C	H	402	29/29	0.82	0.14	54,67,94,100	0
3	A1D5C	J	402	29/29	0.82	0.15	64,81,113,115	0
3	A1D5C	E	402	29/29	0.84	0.14	36,63,93,96	0
3	A1D5C	F	402	29/29	0.84	0.15	42,70,101,111	0
3	A1D5C	L	402	29/29	0.84	0.16	43,79,115,120	0
3	A1D5C	G	402	29/29	0.85	0.16	50,98,120,128	0
3	A1D5C	I	402	29/29	0.85	0.17	43,71,107,119	0
3	A1D5C	B	402	29/29	0.88	0.12	30,44,78,88	0
3	A1D5C	D	402	29/29	0.91	0.12	32,51,89,98	0
3	A1D5C	K	402	29/29	0.91	0.11	38,53,84,93	0
3	A1D5C	C	402	29/29	0.91	0.12	33,59,93,96	0
2	ZN	G	401	1/1	0.99	0.04	52,52,52,52	0
2	ZN	J	401	1/1	0.99	0.04	53,53,53,53	0
2	ZN	L	401	1/1	0.99	0.04	78,78,78,78	0
2	ZN	B	401	1/1	1.00	0.03	31,31,31,31	0
2	ZN	H	401	1/1	1.00	0.01	52,52,52,52	0
2	ZN	I	401	1/1	1.00	0.02	40,40,40,40	0
2	ZN	A	401	1/1	1.00	0.04	28,28,28,28	0
2	ZN	K	401	1/1	1.00	0.03	34,34,34,34	0
2	ZN	C	401	1/1	1.00	0.03	29,29,29,29	0
2	ZN	D	401	1/1	1.00	0.01	36,36,36,36	0
2	ZN	E	401	1/1	1.00	0.03	33,33,33,33	0
2	ZN	F	401	1/1	1.00	0.03	35,35,35,35	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.

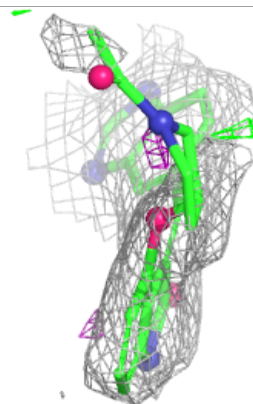
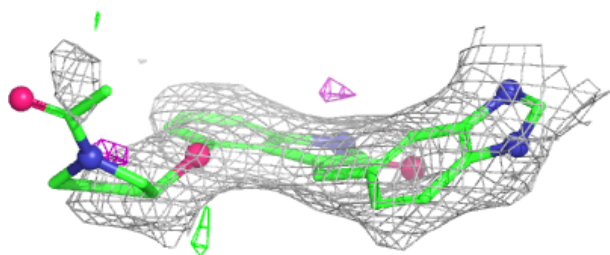
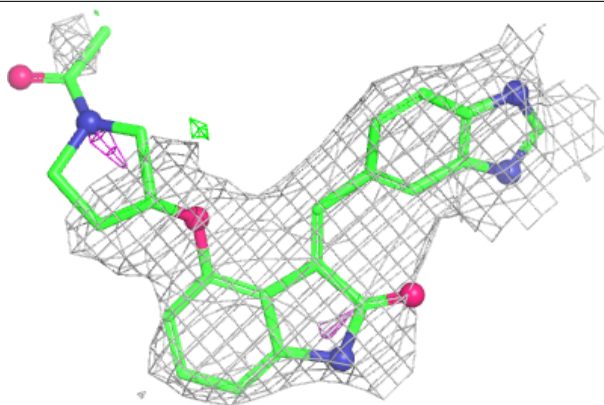
Electron density around A1D5C A 402:

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

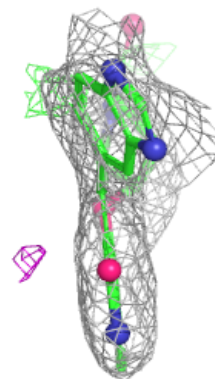
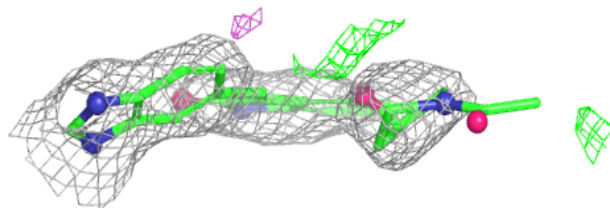
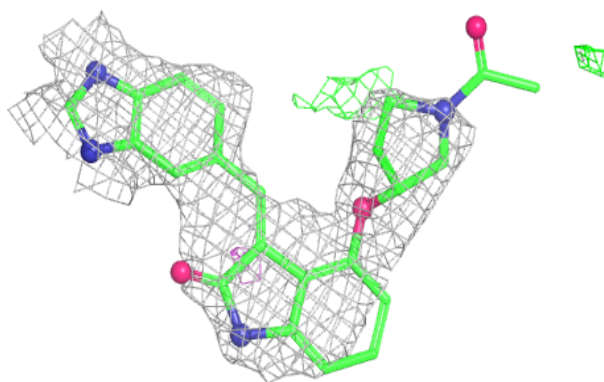


Electron density around A1D5C H 402:

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

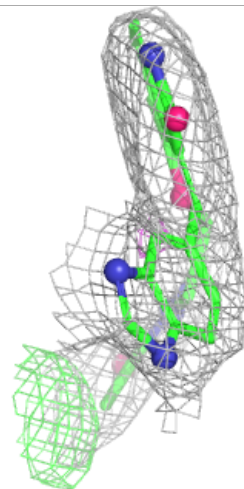
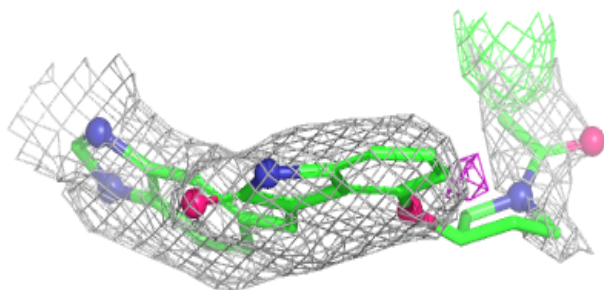
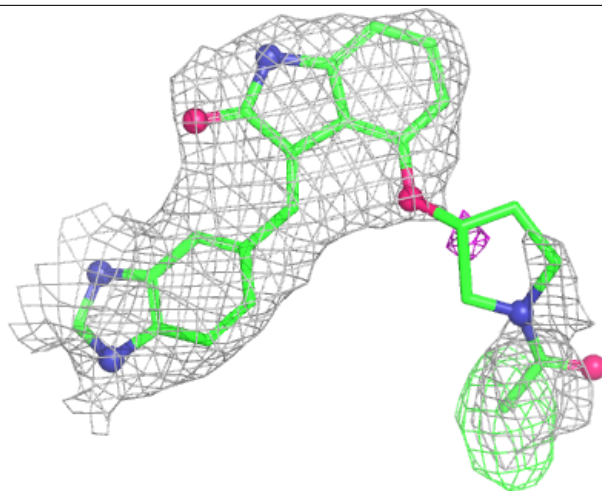
**Electron density around A1D5C J 402:**

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and green (positive)



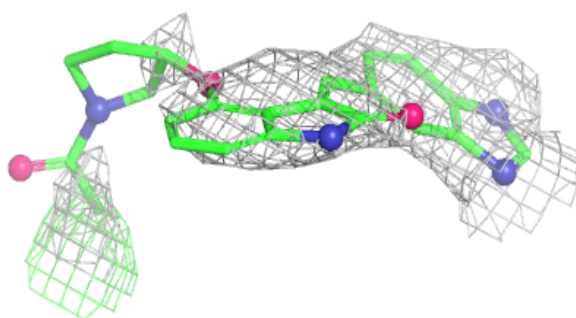
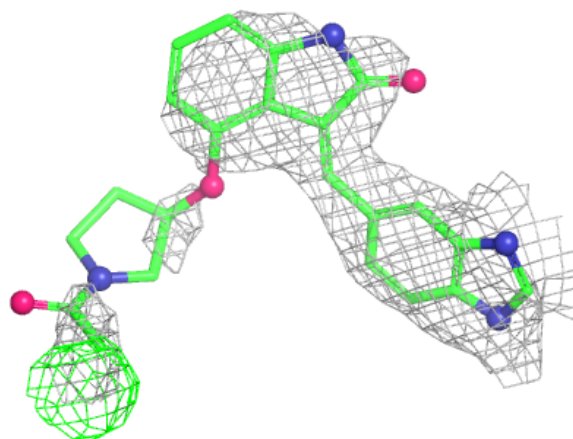
Electron density around A1D5C E 402:

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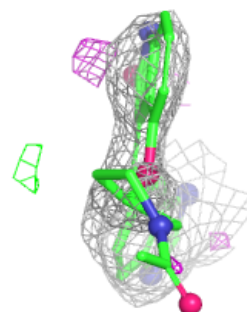
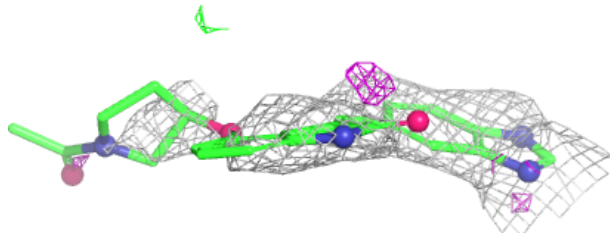
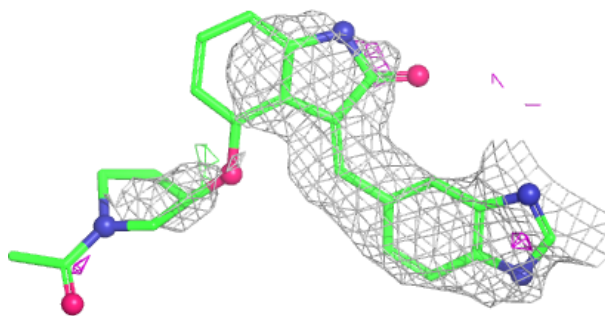


Electron density around A1D5C F 402:

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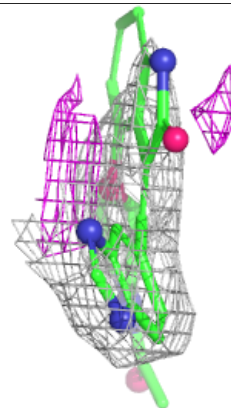
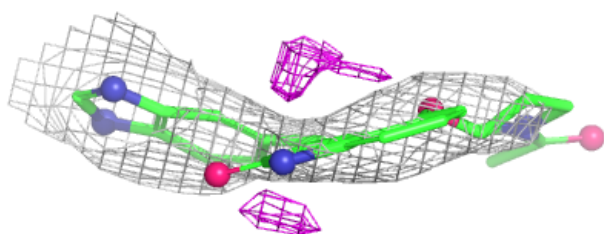
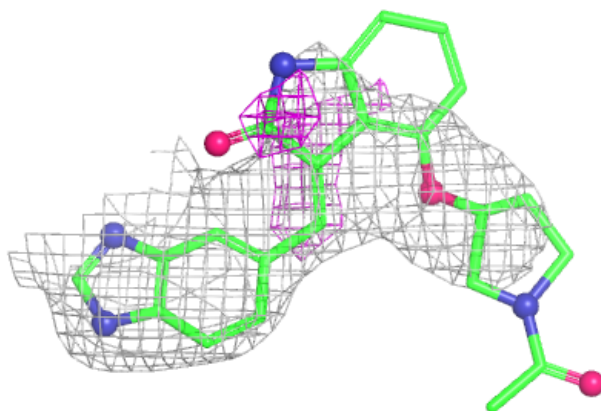
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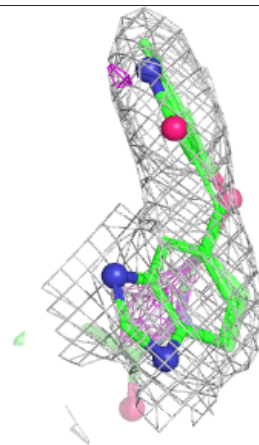
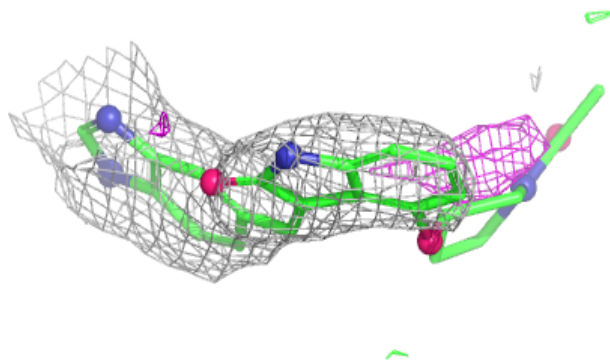
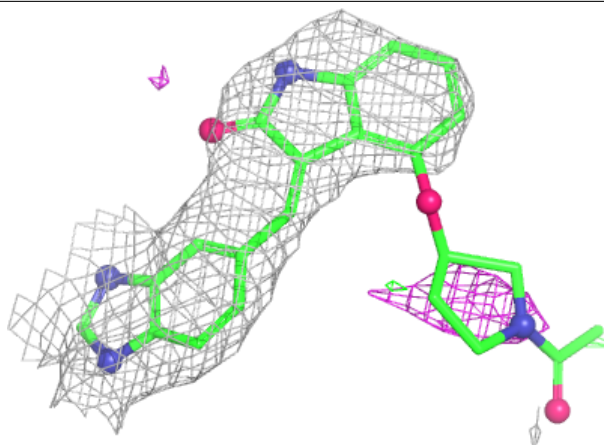
Electron density around A1D5C G 402:

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and green (positive)



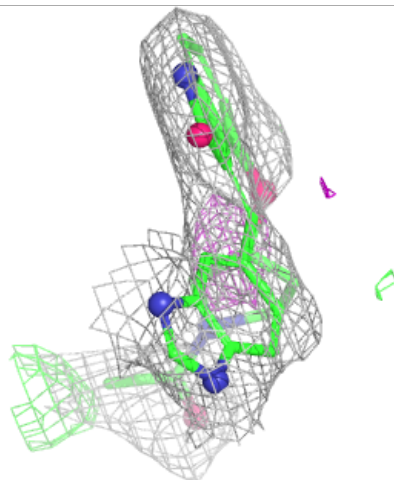
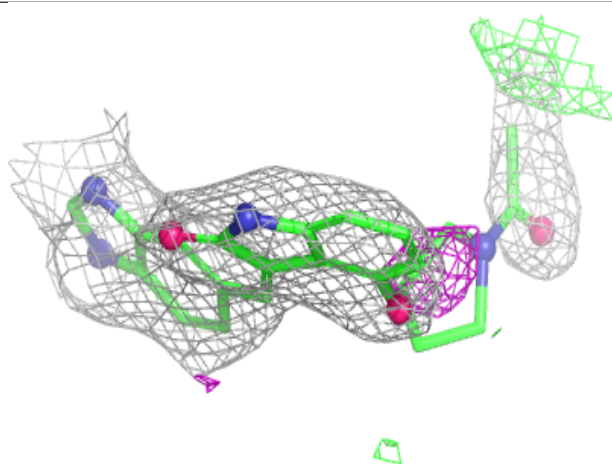
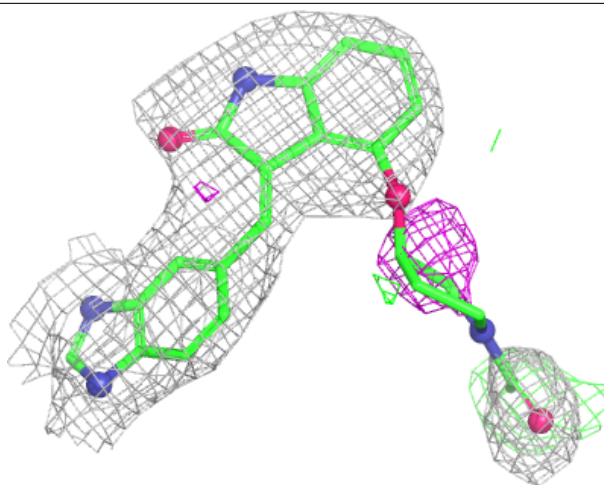
Electron density around A1D5C I 402:

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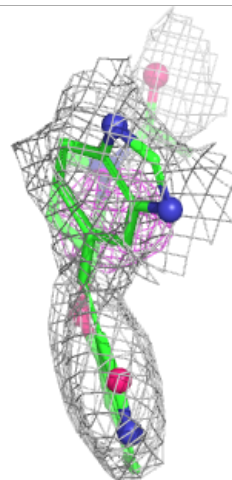
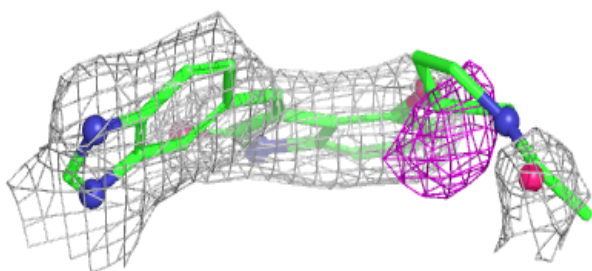
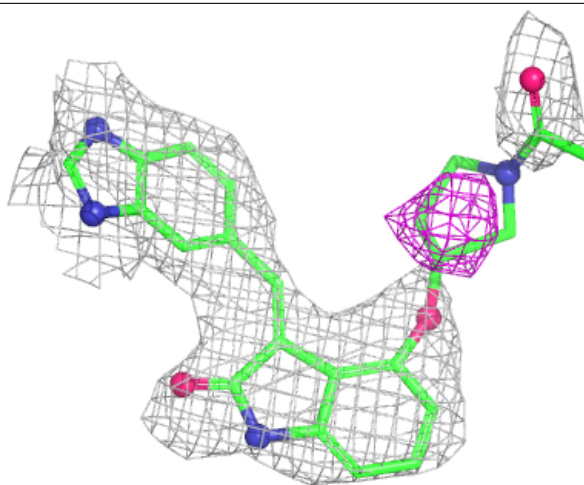
Electron density around A1D5C B 402:

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



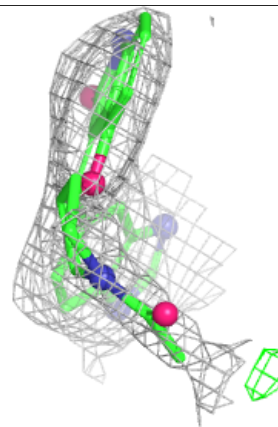
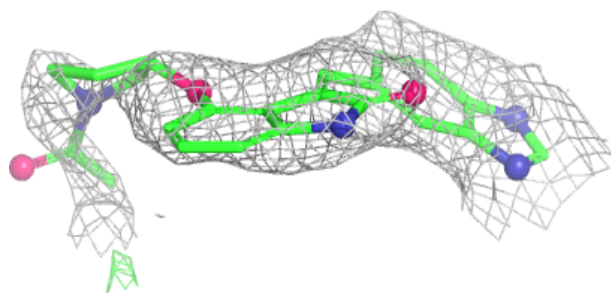
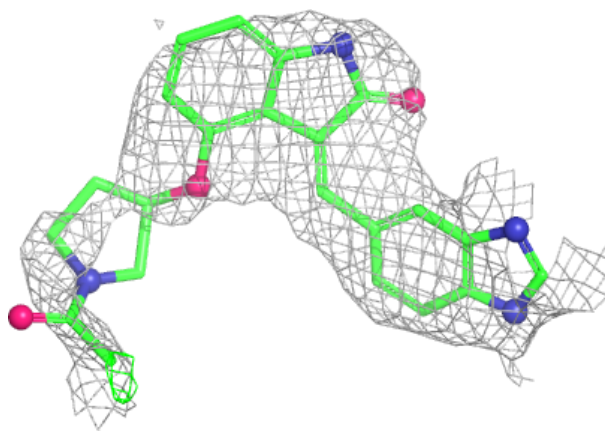
Electron density around A1D5C D 402:

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



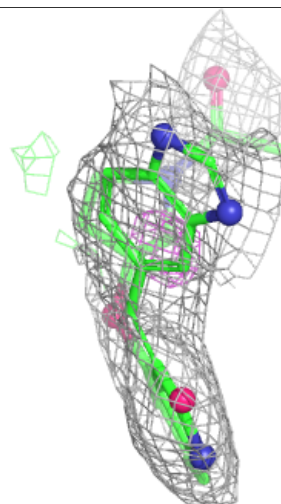
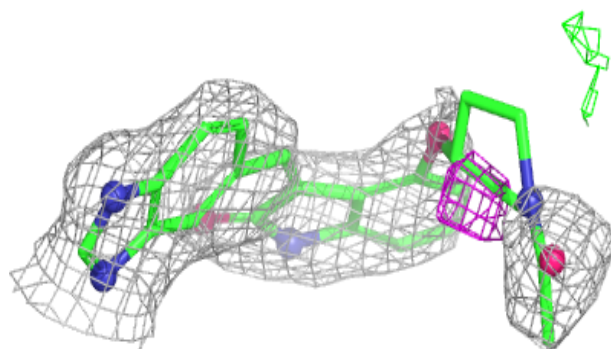
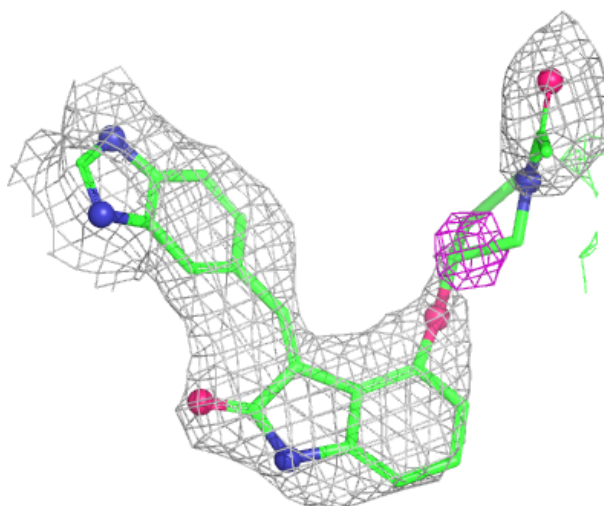
Electron density around A1D5C K 402:

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



Electron density around A1D5C C 402:

$2mF_o-DF_c$ (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.