



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:22 PM UTC

PDB ID : 9YC0 / pdb_00009yc0
Title : Plasmodium falciparum M17 aminopeptidase (PfA-M17) bound to inhibitor 3ab (MIPS3413)
Authors : Mansouri, M.; McGowan, S.; Webb, C.T.
Deposited on : 2025-09-17
Resolution : 2.37 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

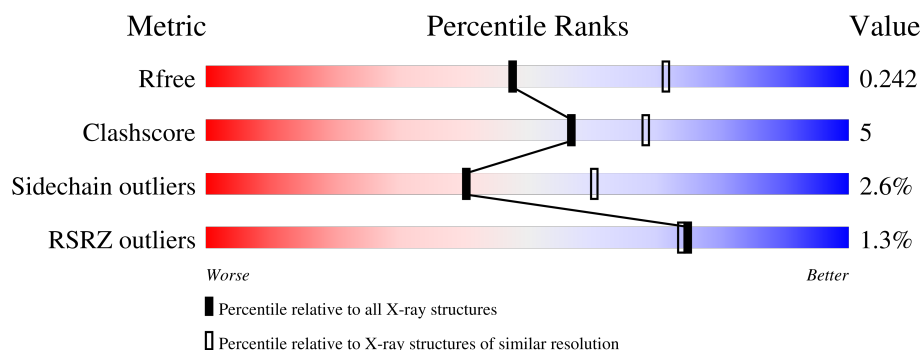
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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.



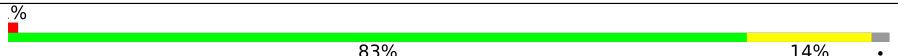
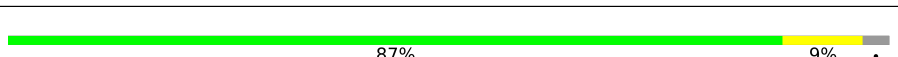
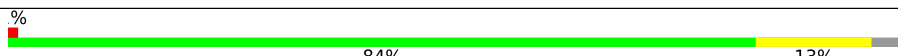
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	527	% 89% 9% .
1	B	527	3% 87% 10% .
1	C	527	% 88% 10% .
1	D	527	89% 8% .
1	E	527	85% 12% .
1	F	527	2% 86% 11% .

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Mol	Chain	Length	Quality of chain
1	G	527	
1	H	527	
1	I	527	
1	J	527	
1	K	527	
1	L	527	

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	CO3	L	703	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51849 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3994	2562	650	763	19			
1	B	512	Total	C	N	O	S	0	1	0
			3836	2459	624	734	19			
1	C	518	Total	C	N	O	S	0	0	0
			3951	2535	642	754	20			
1	D	515	Total	C	N	O	S	0	0	0
			3955	2539	643	753	20			
1	E	510	Total	C	N	O	S	0	0	0
			3931	2523	638	751	19			
1	F	511	Total	C	N	O	S	0	0	0
			3850	2472	624	735	19			
1	G	517	Total	C	N	O	S	0	0	0
			3960	2538	642	760	20			
1	H	512	Total	C	N	O	S	0	0	0
			3840	2465	625	731	19			
1	I	518	Total	C	N	O	S	0	0	0
			3957	2537	641	759	20			
1	J	514	Total	C	N	O	S	0	0	0
			3952	2537	644	751	20			
1	K	510	Total	C	N	O	S	0	0	0
			3922	2520	638	745	19			
1	L	511	Total	C	N	O	S	0	0	0
			3874	2486	626	743	19			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

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

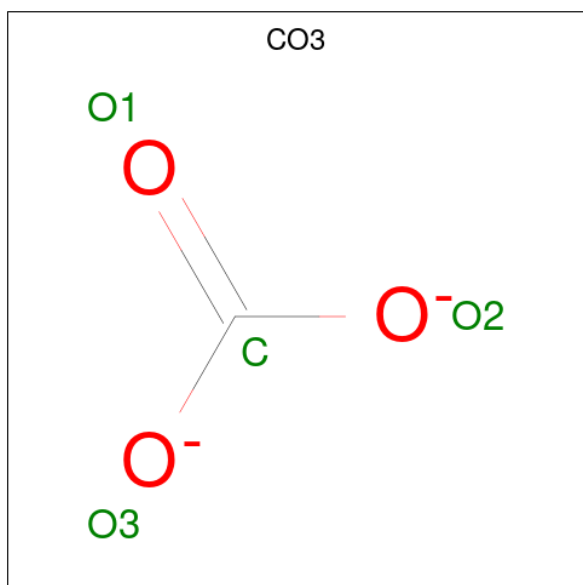
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	2	Total	Zn	0	0
			2	2		
2	L	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



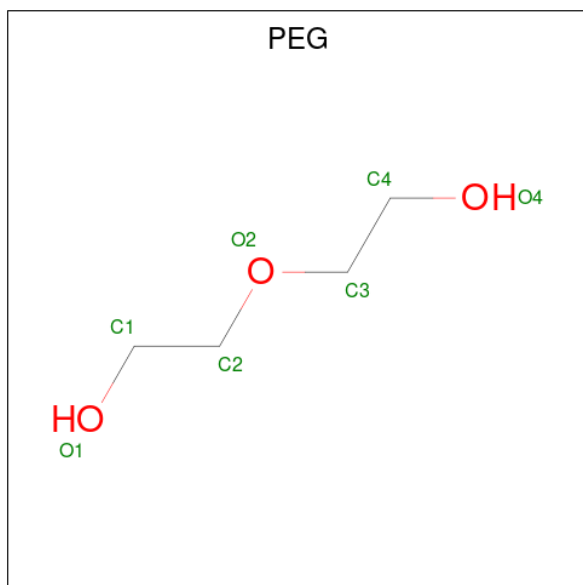
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

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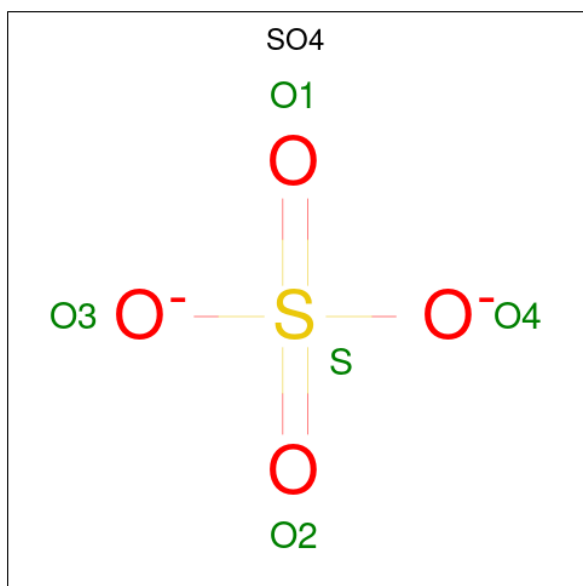
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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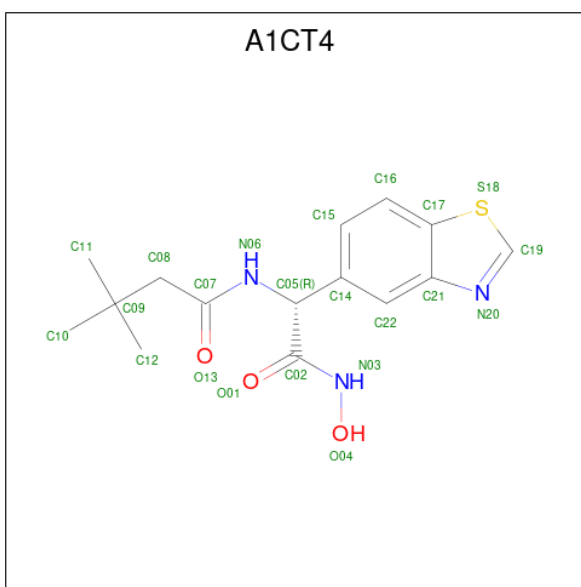
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		

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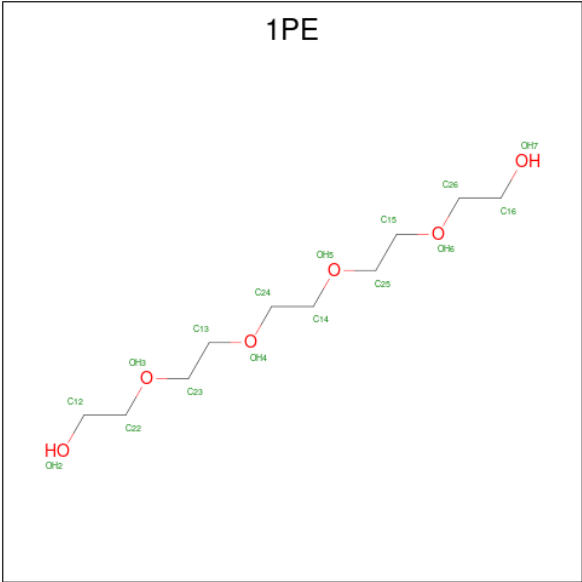
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is N-[(1R)-1-(1,3-benzothiazol-5-yl)-2-(hydroxyamino)-2-oxoethyl]-3,3-dimethylbutanamide (CCD ID: A1CT4) (formula: C₁₅H₁₉N₃O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	B	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	C	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	D	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	E	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	F	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	H	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	I	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	J	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	K	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
6	L	1	Total	C	N	O	S	0	0
			22	15	3	3	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			8	5	3		
7	D	1	Total	C	O	0	0
			11	8	3		
7	D	1	Total	C	O	0	0
			5	3	2		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			10	6	4		
7	E	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			16	10	6		

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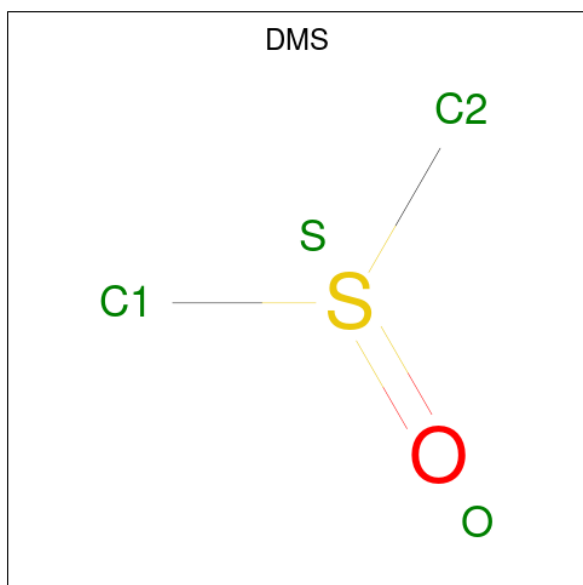
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			8	5	3		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			13	8	5		
7	I	1	Total	C	O	0	0
			13	8	5		
7	I	1	Total	C	O	0	0
			10	6	4		
7	I	1	Total	C	O	0	0
			9	6	3		
7	J	1	Total	C	O	0	0
			10	6	4		
7	J	1	Total	C	O	0	0
			10	6	4		
7	J	1	Total	C	O	0	0
			10	6	4		
7	J	1	Total	C	O	0	0
			11	8	3		
7	J	1	Total	C	O	0	0
			9	6	3		
7	K	1	Total	C	O	0	0
			8	5	3		
7	K	1	Total	C	O	0	0
			10	6	4		
7	K	1	Total	C	O	0	0
			11	7	4		
7	K	1	Total	C	O	0	0
			6	4	2		
7	L	1	Total	C	O	0	0
			10	6	4		
7	L	1	Total	C	O	0	0
			10	6	4		
7	L	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			7	4	3		
7	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



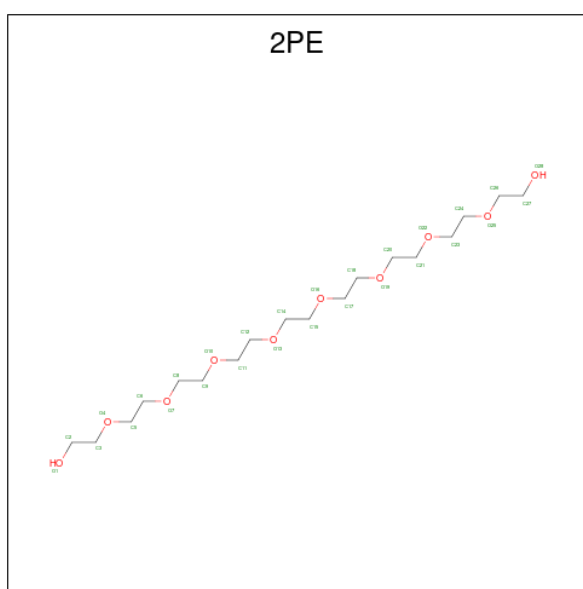
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	D	1	Total	C	O	S	0	0
			4	2	1	1		
8	G	1	Total	C	O	S	0	0
			4	2	1	1		
8	H	1	Total	C	O	S	0	0
			4	2	1	1		

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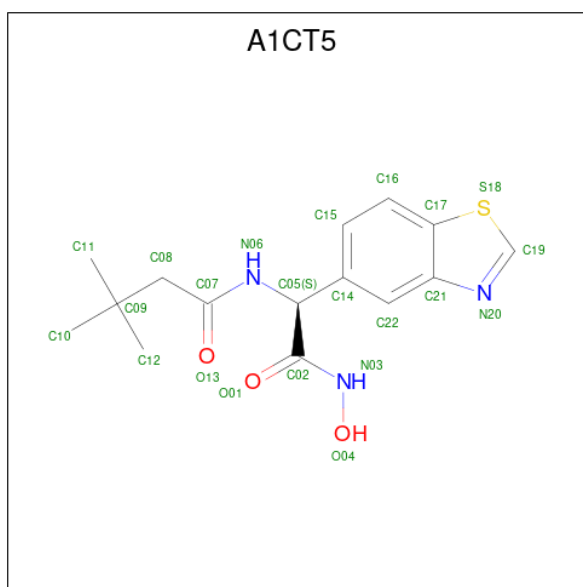
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	I	1	Total	C	O	S	0	0
			4	2	1	1		
8	J	1	Total	C	O	S	0	0
			4	2	1	1		
8	J	1	Total	C	O	S	0	0
			4	2	1	1		
8	L	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 9 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			26	17	9		
9	H	1	Total	C	O	0	0
			25	16	9		

- Molecule 10 is N-[(1S)-1-(1,3-benzothiazol-5-yl)-2-(hydroxyamino)-2-oxoethyl]-3,3-dimethyl butanamide (CCD ID: A1CT5) (formula: $C_{15}H_{19}N_3O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	G	1	Total	C	N	O	S	0	0
			22	15	3	3	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	320	Total	O	0	0
			320	320		
11	B	224	Total	O	0	0
			224	224		
11	C	286	Total	O	0	0
			286	286		
11	D	308	Total	O	0	0
			308	308		
11	E	337	Total	O	0	0
			337	337		
11	F	252	Total	O	0	0
			252	252		
11	G	299	Total	O	0	0
			299	299		
11	H	262	Total	O	0	0
			262	262		
11	I	295	Total	O	0	0
			295	295		
11	J	323	Total	O	0	0
			323	323		
11	K	310	Total	O	0	0
			310	310		

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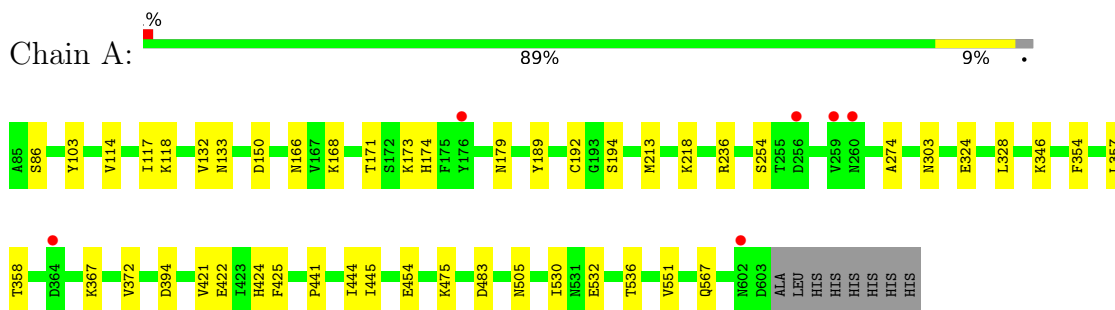
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	276	Total	O	0	0
			276	276		

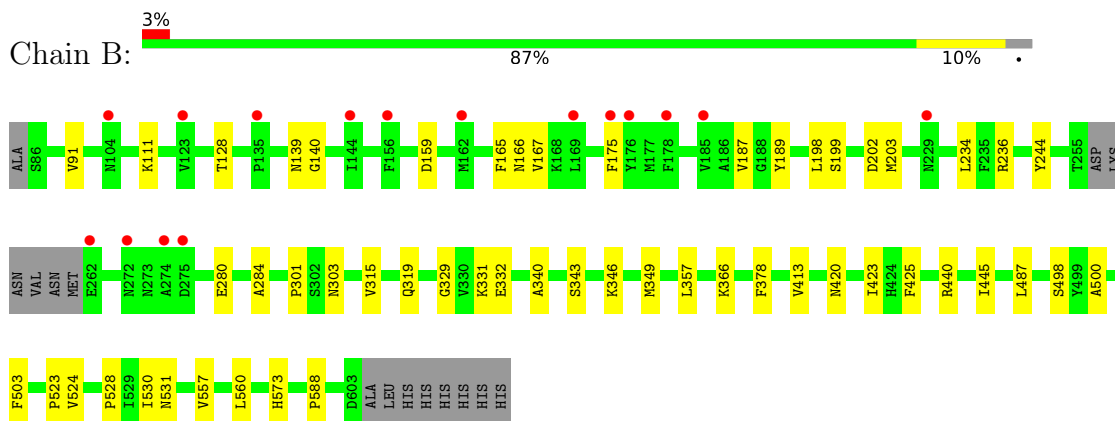
3 Residue-property plots

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.

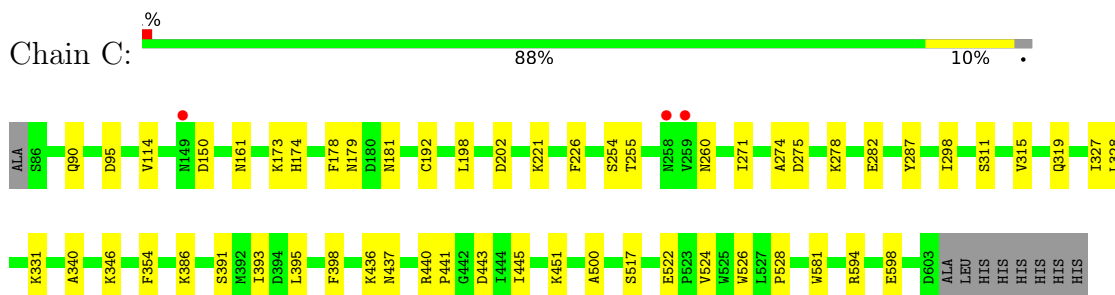
• Molecule 1: M17 leucyl aminopeptidase



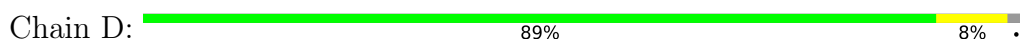
• Molecule 1: M17 leucyl aminopeptidase

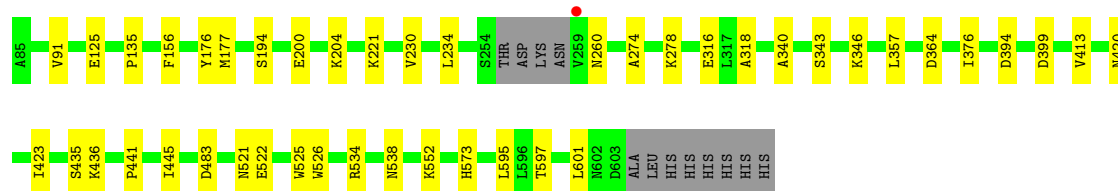


• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase





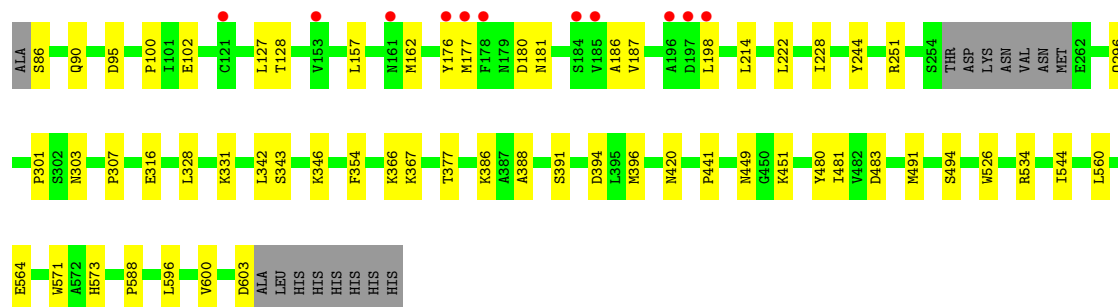
• Molecule 1: M17 leucyl aminopeptidase

Chain E: 85% 12%



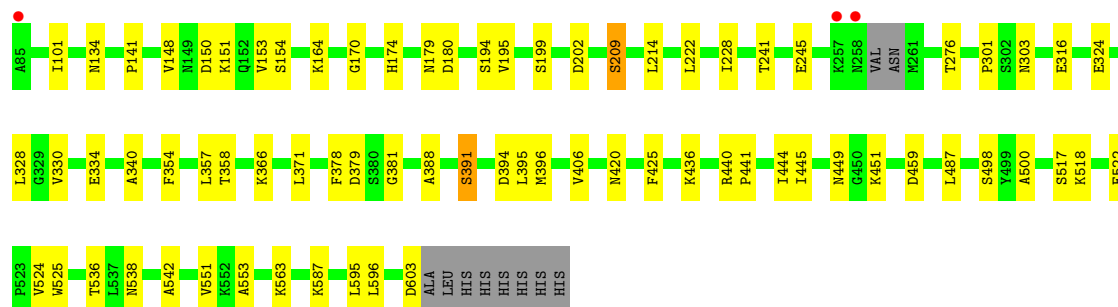
• Molecule 1: M17 leucyl aminopeptidase

Chain F: 86% 11%

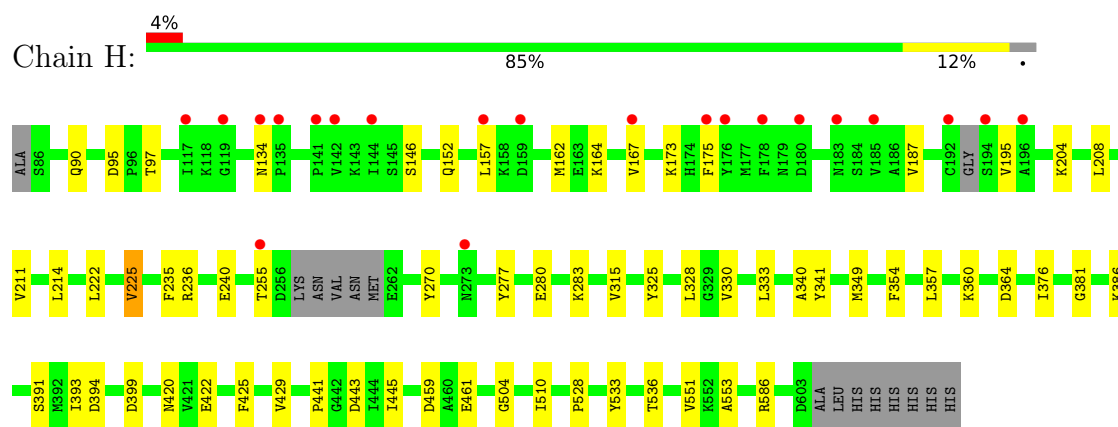


• Molecule 1: M17 leucyl aminopeptidase

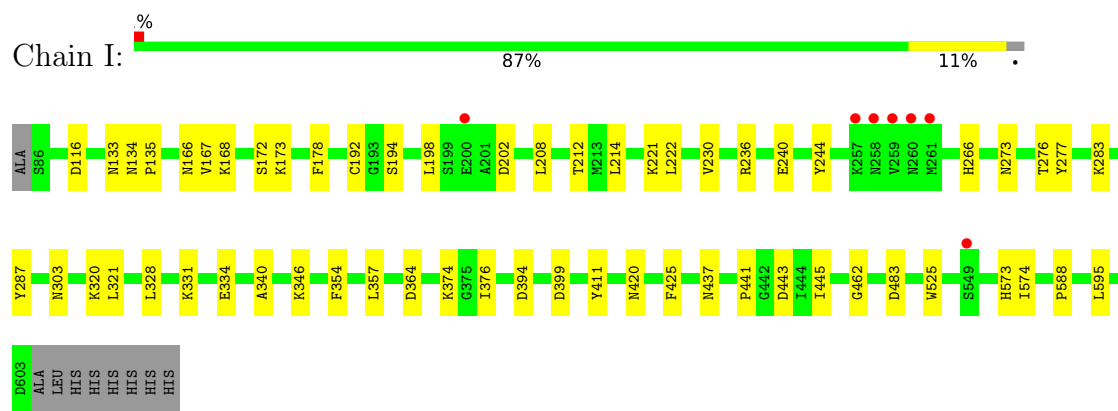
Chain G: 84% 14%



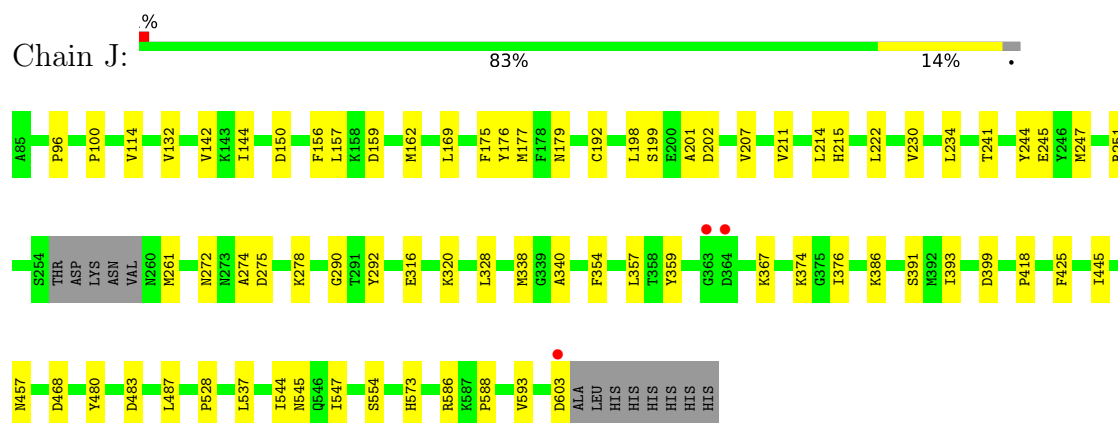
• Molecule 1: M17 leucyl aminopeptidase



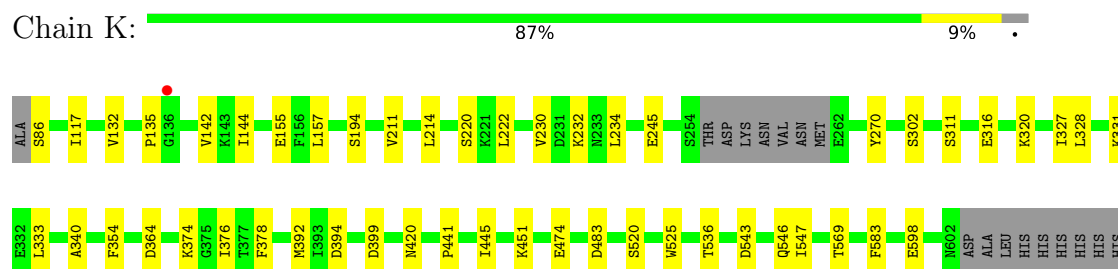
• Molecule 1: M17 leucyl aminopeptidase



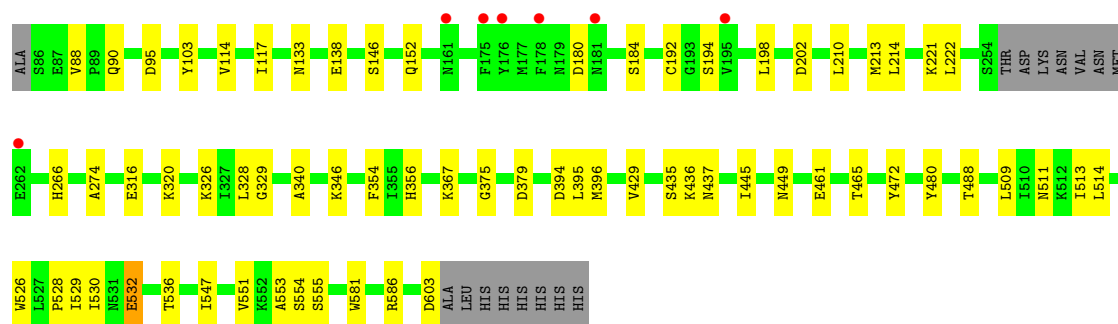
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



Chain L: 84% 13% 3%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.73Å 176.51Å 231.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.37 48.42 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.8 (48.42-2.37) 93.1 (48.42-2.37)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.218 , 0.271 (Not available) , 0.242	Depositor DCC
R_{free} test set	14294 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51849	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1082e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1CT5, PEG, 2PE, CO3, ZN, SO4, 1PE, A1CT4, DMS

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	0.08	0/4072	0.24	0/5519
1	B	0.10	0/3914	0.27	0/5321
1	C	0.08	0/4029	0.24	0/5469
1	D	0.08	0/4032	0.24	0/5466
1	E	0.08	0/4008	0.25	0/5431
1	F	0.08	0/3926	0.26	0/5336
1	G	0.08	0/4037	0.24	0/5477
1	H	0.08	0/3915	0.24	0/5322
1	I	0.07	0/4035	0.23	0/5477
1	J	0.08	0/4029	0.24	0/5460
1	K	0.08	0/3999	0.25	0/5420
1	L	0.08	0/3950	0.24	0/5368
All	All	0.08	0/47946	0.24	0/65066

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

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	3994	0	3958	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3836	0	3686	37	0
1	C	3951	0	3879	39	0
1	D	3955	0	3918	30	0
1	E	3931	0	3897	39	0
1	F	3850	0	3718	42	0
1	G	3960	0	3893	42	0
1	H	3840	0	3703	38	0
1	I	3957	0	3881	36	0
1	J	3952	0	3922	46	0
1	K	3922	0	3894	35	0
1	L	3874	0	3759	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	1	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	2	0
4	A	35	0	50	6	0
4	B	14	0	20	3	0
4	C	42	0	60	2	0
4	D	21	0	30	3	0
4	E	21	0	30	1	0
4	F	7	0	10	0	0
4	G	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	7	0	10	0	0
4	I	28	0	40	2	0
4	J	21	0	30	4	0
4	K	14	0	20	0	0
4	L	35	0	50	6	0
5	A	30	0	0	0	0
5	B	15	0	0	1	0
5	C	20	0	0	0	0
5	D	25	0	0	0	0
5	E	35	0	0	0	0
5	F	20	0	0	0	0
5	G	30	0	0	0	0
5	H	25	0	0	1	0
5	I	20	0	0	0	0
5	J	35	0	0	2	0
5	K	35	0	0	1	0
5	L	5	0	0	0	0
6	A	22	0	0	0	0
6	B	22	0	0	2	0
6	C	22	0	0	0	0
6	D	22	0	0	0	0
6	E	22	0	0	1	0
6	F	22	0	0	0	0
6	H	22	0	0	0	0
6	I	22	0	0	0	0
6	J	22	0	0	0	0
6	K	22	0	0	1	0
6	L	22	0	0	2	0
7	A	14	0	16	1	0
7	B	7	0	9	0	0
7	C	17	0	20	0	0
7	D	44	0	50	3	0
7	E	33	0	41	2	0
7	F	36	0	48	1	0
7	G	33	0	37	1	0
7	I	32	0	39	1	0
7	J	50	0	61	2	0
7	K	35	0	36	5	0
7	L	48	0	59	6	0
8	B	12	0	18	1	0
8	C	12	0	18	3	0
8	D	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	4	0	6	0	0
8	H	4	0	6	1	0
8	I	4	0	6	0	0
8	J	8	0	12	4	0
8	L	4	0	6	0	0
9	B	26	0	33	0	0
9	H	25	0	33	0	0
10	G	22	0	0	1	0
11	A	320	0	0	4	0
11	B	224	0	0	1	0
11	C	286	0	0	2	0
11	D	308	0	0	1	0
11	E	337	0	0	0	0
11	F	252	0	0	2	0
11	G	299	0	0	4	0
11	H	262	0	0	0	0
11	I	295	0	0	2	0
11	J	323	0	0	0	0
11	K	310	0	0	1	0
11	L	276	0	0	1	0
All	All	51849	0	47028	434	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 5.

The worst 5 of 434 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.63	0.79
1:E:232:LYS:H	1:E:232:LYS:HD2	1.53	0.73
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.69	0.73
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.70	0.72
1:L:586:ARG:HB3	4:L:706:PEG:H21	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/454 (92%)	410 (98%)	7 (2%)	53	72
1	F	70/454 (15%)	68 (97%)	2 (3%)	37	57
1	G	340/454 (75%)	328 (96%)	12 (4%)	32	50
1	H	177/454 (39%)	170 (96%)	7 (4%)	28	44
1	J	42/454 (9%)	39 (93%)	3 (7%)	13	21
1	K	268/454 (59%)	264 (98%)	4 (2%)	57	75
1	L	273/454 (60%)	267 (98%)	6 (2%)	45	65
All	All	1587/3178 (50%)	1546 (97%)	41 (3%)	40	60

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	544	ILE
1	L	88	VAL
1	J	554	SER
1	K	394	ASP
1	L	532	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	531	ASN
1	J	568	ASN
1	H	174	HIS
1	G	567	GLN

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Mol	Chain	Res	Type
1	H	322	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](#)

Of 195 ligands modelled in this entry, 24 are monoatomic - leaving 171 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	$\# Z > 2$
7	1PE	G	714	-	5,5,15	0.15	0	4,4,14	0.20	0
7	1PE	L	713	-	9,9,15	0.10	0	8,8,14	0.13	0
5	SO4	G	709	-	4,4,4	0.24	0	6,6,6	0.06	0
7	1PE	F	712	-	9,9,15	0.10	0	8,8,14	0.13	0
5	SO4	D	709	-	4,4,4	0.23	0	6,6,6	0.08	0
8	DMS	C	713	-	3,3,3	0.65	0	3,3,3	0.47	0
4	PEG	I	710	-	6,6,6	0.11	0	5,5,5	0.12	0
8	DMS	J	710	-	3,3,3	0.67	0	3,3,3	0.49	0
4	PEG	E	706	-	6,6,6	0.10	0	5,5,5	0.11	0
4	PEG	A	709	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	C	708	-	6,6,6	0.12	0	5,5,5	0.08	0
4	PEG	J	709	-	6,6,6	0.11	0	5,5,5	0.10	0
7	1PE	J	705	-	9,9,15	0.10	0	8,8,14	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	C	716	-	4,4,4	0.24	0	6,6,6	0.08	0
8	DMS	C	706	-	3,3,3	0.67	0	3,3,3	0.55	0
6	A1CT4	E	708	2	22,23,23	2.84	12 (54%)	26,33,33	2.84	5 (19%)
5	SO4	J	716	-	4,4,4	0.23	0	6,6,6	0.08	0
4	PEG	H	704	-	6,6,6	0.12	0	5,5,5	0.07	0
4	PEG	L	705	-	6,6,6	0.13	0	5,5,5	0.07	0
7	1PE	L	715	-	6,6,15	0.10	0	5,5,14	0.20	0
5	SO4	C	715	-	4,4,4	0.24	0	6,6,6	0.07	0
4	PEG	D	706	-	6,6,6	0.12	0	5,5,5	0.08	0
5	SO4	K	711	-	4,4,4	0.23	0	6,6,6	0.09	0
4	PEG	J	708	-	6,6,6	0.11	0	5,5,5	0.10	0
8	DMS	H	706	-	3,3,3	0.67	0	3,3,3	0.51	0
3	CO3	J	703	-	3,3,3	0.87	0	2,3,3	0.21	0
4	PEG	E	704	-	6,6,6	0.11	0	5,5,5	0.10	0
5	SO4	B	713	-	4,4,4	0.24	0	6,6,6	0.07	0
9	2PE	B	714	-	25,25,27	0.13	0	24,24,26	0.09	0
5	SO4	G	708	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	E	711	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	I	712	-	4,4,4	0.24	0	6,6,6	0.07	0
4	PEG	A	708	-	6,6,6	0.11	0	5,5,5	0.10	0
5	SO4	A	715	-	4,4,4	0.23	0	6,6,6	0.08	0
4	PEG	A	707	-	6,6,6	0.10	0	5,5,5	0.08	0
7	1PE	I	716	-	8,8,15	0.15	0	7,7,14	0.12	0
7	1PE	E	717	-	9,9,15	0.08	0	8,8,14	0.17	0
7	1PE	K	717	-	5,5,15	0.22	0	4,4,14	0.08	0
7	1PE	D	716	-	10,10,15	0.19	0	9,9,14	0.12	0
7	1PE	I	715	-	9,9,15	0.11	0	8,8,14	0.17	0
5	SO4	K	713	-	4,4,4	0.24	0	6,6,6	0.09	0
4	PEG	B	704	-	6,6,6	0.10	0	5,5,5	0.09	0
3	CO3	H	703	-	3,3,3	0.82	0	2,3,3	0.12	0
5	SO4	E	712	-	4,4,4	0.23	0	6,6,6	0.09	0
7	1PE	G	715	-	5,5,15	0.16	0	4,4,14	0.16	0
7	1PE	L	707	-	9,9,15	0.11	0	8,8,14	0.13	0
7	1PE	E	716	-	9,9,15	0.11	0	8,8,14	0.15	0
4	PEG	L	704	-	6,6,6	0.09	0	5,5,5	0.11	0
7	1PE	D	714	-	6,6,15	0.09	0	5,5,14	0.18	0
6	A1CT4	D	707	2	22,23,23	2.84	12 (54%)	26,33,33	2.79	5 (19%)
7	1PE	F	711	-	9,9,15	0.10	0	8,8,14	0.14	0
5	SO4	H	707	-	4,4,4	0.23	0	6,6,6	0.07	0
4	PEG	C	711	-	6,6,6	0.12	0	5,5,5	0.09	0
4	PEG	J	717	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	B	705	-	6,6,6	0.12	0	5,5,5	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	J	711	-	4,4,4	0.23	0	6,6,6	0.07	0
6	A1CT4	H	705	2	22,23,23	2.83	12 (54%)	26,33,33	2.84	5 (19%)
6	A1CT4	C	710	2	22,23,23	2.83	12 (54%)	26,33,33	2.85	6 (23%)
6	A1CT4	J	707	2	22,23,23	2.83	12 (54%)	26,33,33	2.82	4 (15%)
7	1PE	J	720	-	10,10,15	0.19	0	9,9,14	0.10	0
7	1PE	K	716	-	10,10,15	0.15	0	9,9,14	0.12	0
4	PEG	A	706	-	6,6,6	0.12	0	5,5,5	0.07	0
7	1PE	L	716	-	10,10,15	0.14	0	9,9,14	0.08	0
7	1PE	K	715	-	9,9,15	0.08	0	8,8,14	0.17	0
4	PEG	C	704	-	6,6,6	0.11	0	5,5,5	0.09	0
5	SO4	A	712	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	J	712	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	I	711	-	4,4,4	0.24	0	6,6,6	0.09	0
4	PEG	E	715	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	K	705	-	6,6,6	0.11	0	5,5,5	0.10	0
5	SO4	F	705	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	G	711	-	4,4,4	0.23	0	6,6,6	0.07	0
9	2PE	H	712	-	24,24,27	0.12	0	23,23,26	0.08	0
5	SO4	D	712	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	B	711	-	4,4,4	0.23	0	6,6,6	0.10	0
10	A1CT5	G	705	2	22,23,23	2.81	12 (54%)	26,33,33	2.88	6 (23%)
5	SO4	C	714	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	A	713	-	4,4,4	0.24	0	6,6,6	0.08	0
8	DMS	I	705	-	3,3,3	0.67	0	3,3,3	0.54	0
7	1PE	A	716	-	6,6,15	0.09	0	5,5,14	0.19	0
3	CO3	D	703	-	3,3,3	0.80	0	2,3,3	0.14	0
5	SO4	E	705	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	K	708	-	4,4,4	0.23	0	6,6,6	0.07	0
4	PEG	F	704	-	6,6,6	0.12	0	5,5,5	0.07	0
8	DMS	D	718	-	3,3,3	0.67	0	3,3,3	0.54	0
8	DMS	B	707	-	3,3,3	0.68	0	3,3,3	0.53	0
7	1PE	I	707	-	12,12,15	0.10	0	11,11,14	0.14	0
3	CO3	K	703	-	3,3,3	0.79	0	2,3,3	0.04	0
4	PEG	D	705	-	6,6,6	0.11	0	5,5,5	0.09	0
3	CO3	G	703	-	3,3,3	0.78	0	2,3,3	0.05	0
5	SO4	J	714	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	E	713	-	4,4,4	0.23	0	6,6,6	0.07	0
4	PEG	I	706	-	6,6,6	0.11	0	5,5,5	0.11	0
7	1PE	D	715	-	7,7,15	0.15	0	6,6,14	0.14	0
5	SO4	H	711	-	4,4,4	0.23	0	6,6,6	0.08	0
4	PEG	L	711	-	6,6,6	0.11	0	5,5,5	0.10	0
4	PEG	I	709	-	6,6,6	0.11	0	5,5,5	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CO3	C	703	-	3,3,3	0.84	0	2,3,3	0.20	0
7	1PE	F	706	-	15,15,15	0.12	0	14,14,14	0.07	0
5	SO4	H	708	-	4,4,4	0.24	0	6,6,6	0.08	0
4	PEG	L	706	-	6,6,6	0.12	0	5,5,5	0.04	0
5	SO4	F	710	-	4,4,4	0.23	0	6,6,6	0.08	0
7	1PE	L	714	-	9,9,15	0.09	0	8,8,14	0.16	0
4	PEG	L	709	-	6,6,6	0.12	0	5,5,5	0.09	0
5	SO4	E	714	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	E	710	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	C	717	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	713	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	J	713	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	I	713	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	F	709	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	D	711	-	4,4,4	0.22	0	6,6,6	0.08	0
7	1PE	D	704	-	12,12,15	0.12	0	11,11,14	0.10	0
5	SO4	H	709	-	4,4,4	0.24	0	6,6,6	0.07	0
7	1PE	C	719	-	6,6,15	0.08	0	5,5,14	0.19	0
7	1PE	B	709	-	6,6,15	0.10	0	5,5,14	0.15	0
7	1PE	K	714	-	7,7,15	0.15	0	6,6,14	0.13	0
5	SO4	K	709	-	4,4,4	0.23	0	6,6,6	0.11	0
4	PEG	G	704	-	6,6,6	0.11	0	5,5,5	0.09	0
3	CO3	F	703	-	3,3,3	0.85	0	2,3,3	0.21	0
8	DMS	J	704	-	3,3,3	0.66	0	3,3,3	0.49	0
5	SO4	L	712	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	K	710	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	I	714	-	4,4,4	0.23	0	6,6,6	0.09	0
4	PEG	K	704	-	6,6,6	0.12	0	5,5,5	0.08	0
8	DMS	B	710	-	3,3,3	0.66	0	3,3,3	0.56	0
7	1PE	G	713	-	7,7,15	0.16	0	6,6,14	0.14	0
8	DMS	L	708	-	3,3,3	0.69	0	3,3,3	0.67	0
5	SO4	D	710	-	4,4,4	0.23	0	6,6,6	0.07	0
7	1PE	J	719	-	9,9,15	0.12	0	8,8,14	0.12	0
5	SO4	B	712	-	4,4,4	0.24	0	6,6,6	0.08	0
3	CO3	I	703	-	3,3,3	0.84	0	2,3,3	0.24	0
5	SO4	F	708	-	4,4,4	0.23	0	6,6,6	0.09	0
6	A1CT4	I	708	2	22,23,23	2.83	12 (54%)	26,33,33	2.83	6 (23%)
5	SO4	J	706	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	G	710	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	G	712	-	4,4,4	0.24	0	6,6,6	0.07	0
8	DMS	G	706	-	3,3,3	0.66	0	3,3,3	0.53	0
5	SO4	K	707	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	705	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	E	707	-	4,4,4	0.24	0	6,6,6	0.08	0
7	1PE	J	718	-	9,9,15	0.11	0	8,8,14	0.13	0
4	PEG	C	707	-	6,6,6	0.13	0	5,5,5	0.06	0
4	PEG	C	712	-	6,6,6	0.11	0	5,5,5	0.10	0
6	A1CT4	F	707	2	22,23,23	2.83	12 (54%)	26,33,33	2.86	5 (19%)
6	A1CT4	A	710	2	22,23,23	2.84	12 (54%)	26,33,33	2.82	4 (15%)
8	DMS	C	705	-	3,3,3	0.67	0	3,3,3	0.53	0
3	CO3	B	703	-	3,3,3	0.79	0	2,3,3	0.05	0
6	A1CT4	B	708	2	22,23,23	2.82	12 (54%)	26,33,33	2.90	6 (23%)
7	1PE	A	717	-	6,6,15	0.09	0	5,5,14	0.18	0
3	CO3	L	703	-	3,3,3	0.84	0	2,3,3	0.14	0
7	1PE	J	721	-	8,8,15	0.15	0	7,7,14	0.13	0
5	SO4	J	715	-	4,4,4	0.23	0	6,6,6	0.07	0
7	1PE	D	717	-	4,4,15	0.16	0	3,3,14	0.20	0
4	PEG	A	704	-	6,6,6	0.12	0	5,5,5	0.09	0
5	SO4	K	712	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	G	707	-	4,4,4	0.21	0	6,6,6	0.16	0
8	DMS	B	706	-	3,3,3	0.67	0	3,3,3	0.48	0
3	CO3	A	703	-	3,3,3	0.75	0	2,3,3	0.10	0
3	CO3	E	703	-	3,3,3	0.77	0	2,3,3	0.07	0
5	SO4	A	711	-	4,4,4	0.24	0	6,6,6	0.09	0
7	1PE	G	716	-	12,12,15	0.12	0	11,11,14	0.18	0
6	A1CT4	K	706	2	22,23,23	2.82	12 (54%)	26,33,33	2.83	4 (15%)
4	PEG	D	708	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	I	704	-	6,6,6	0.11	0	5,5,5	0.11	0
5	SO4	A	714	-	4,4,4	0.24	0	6,6,6	0.06	0
7	1PE	C	718	-	9,9,15	0.09	0	8,8,14	0.16	0
6	A1CT4	L	710	2	22,23,23	2.83	12 (54%)	26,33,33	2.86	4 (15%)
5	SO4	H	710	-	4,4,4	0.24	0	6,6,6	0.07	0
4	PEG	C	709	-	6,6,6	0.11	0	5,5,5	0.09	0
7	1PE	E	709	-	12,12,15	0.12	0	11,11,14	0.10	0

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
7	1PE	G	714	-	-	1/3/3/13	-
7	1PE	L	713	-	-	1/7/7/13	-
7	1PE	F	712	-	-	3/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	I	710	-	-	3/4/4/4	-
4	PEG	E	706	-	-	2/4/4/4	-
4	PEG	A	709	-	-	4/4/4/4	-
4	PEG	C	708	-	-	2/4/4/4	-
4	PEG	J	709	-	-	1/4/4/4	-
7	1PE	J	705	-	-	4/7/7/13	-
6	A1CT4	E	708	2	-	2/19/19/19	0/2/2/2
4	PEG	H	704	-	-	3/4/4/4	-
4	PEG	L	705	-	-	2/4/4/4	-
7	1PE	L	715	-	-	4/4/4/13	-
4	PEG	D	706	-	-	1/4/4/4	-
4	PEG	J	708	-	-	0/4/4/4	-
4	PEG	E	704	-	-	2/4/4/4	-
9	2PE	B	714	-	-	6/23/23/25	-
4	PEG	A	708	-	-	3/4/4/4	-
7	1PE	I	716	-	-	1/6/6/13	-
4	PEG	A	707	-	-	2/4/4/4	-
7	1PE	E	717	-	-	2/7/7/13	-
7	1PE	K	717	-	-	1/3/3/13	-
7	1PE	D	716	-	-	2/8/8/13	-
7	1PE	I	715	-	-	2/7/7/13	-
4	PEG	B	704	-	-	0/4/4/4	-
7	1PE	G	715	-	-	2/3/3/13	-
7	1PE	L	707	-	-	3/7/7/13	-
7	1PE	E	716	-	-	4/7/7/13	-
4	PEG	L	704	-	-	3/4/4/4	-
7	1PE	D	714	-	-	1/4/4/13	-
6	A1CT4	D	707	2	-	0/19/19/19	0/2/2/2
7	1PE	F	711	-	-	5/7/7/13	-
4	PEG	C	711	-	-	2/4/4/4	-
4	PEG	J	717	-	-	1/4/4/4	-
4	PEG	B	705	-	-	1/4/4/4	-
7	1PE	J	720	-	-	5/8/8/13	-
6	A1CT4	C	710	2	-	0/19/19/19	0/2/2/2
6	A1CT4	H	705	2	-	0/19/19/19	0/2/2/2
6	A1CT4	J	707	2	-	3/19/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	K	716	-	-	3/8/8/13	-
4	PEG	A	706	-	-	3/4/4/4	-
7	1PE	L	716	-	-	1/8/8/13	-
7	1PE	K	715	-	-	2/7/7/13	-
4	PEG	C	704	-	-	1/4/4/4	-
4	PEG	E	715	-	-	4/4/4/4	-
4	PEG	K	705	-	-	1/4/4/4	-
9	2PE	H	712	-	-	6/22/22/25	-
10	A1CT5	G	705	2	-	8/19/19/19	0/2/2/2
7	1PE	A	716	-	-	1/4/4/13	-
4	PEG	F	704	-	-	2/4/4/4	-
7	1PE	I	707	-	-	5/10/10/13	-
4	PEG	D	705	-	-	3/4/4/4	-
4	PEG	I	706	-	-	3/4/4/4	-
7	1PE	D	715	-	-	5/5/5/13	-
4	PEG	L	711	-	-	1/4/4/4	-
4	PEG	I	709	-	-	3/4/4/4	-
7	1PE	F	706	-	-	2/13/13/13	-
4	PEG	L	706	-	-	3/4/4/4	-
7	1PE	L	714	-	-	4/7/7/13	-
4	PEG	L	709	-	-	1/4/4/4	-
7	1PE	D	704	-	-	1/10/10/13	-
7	1PE	C	719	-	-	2/4/4/13	-
7	1PE	B	709	-	-	1/4/4/13	-
7	1PE	K	714	-	-	1/5/5/13	-
4	PEG	G	704	-	-	2/4/4/4	-
4	PEG	K	704	-	-	3/4/4/4	-
7	1PE	G	713	-	-	3/5/5/13	-
7	1PE	J	719	-	-	1/7/7/13	-
6	A1CT4	I	708	2	-	3/19/19/19	0/2/2/2
7	1PE	J	718	-	-	1/7/7/13	-
4	PEG	C	707	-	-	1/4/4/4	-
4	PEG	C	712	-	-	1/4/4/4	-
6	A1CT4	F	707	2	-	3/19/19/19	0/2/2/2
6	A1CT4	A	710	2	-	3/19/19/19	0/2/2/2
6	A1CT4	B	708	2	-	5/19/19/19	0/2/2/2
7	1PE	A	717	-	-	1/4/4/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	J	721	-	-	3/6/6/13	-
7	1PE	D	717	-	-	1/2/2/13	-
4	PEG	A	704	-	-	3/4/4/4	-
7	1PE	G	716	-	-	4/10/10/13	-
6	A1CT4	K	706	2	-	4/19/19/19	0/2/2/2
4	PEG	D	708	-	-	3/4/4/4	-
4	PEG	I	704	-	-	2/4/4/4	-
7	1PE	C	718	-	-	2/7/7/13	-
6	A1CT4	L	710	2	-	5/19/19/19	0/2/2/2
4	PEG	C	709	-	-	3/4/4/4	-
7	1PE	E	709	-	-	5/10/10/13	-

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	706	A1CT4	C07-N06	7.04	1.49	1.34
10	G	705	A1CT5	C07-N06	7.02	1.48	1.34
6	E	708	A1CT4	C07-N06	7.00	1.48	1.34
6	L	710	A1CT4	C07-N06	6.99	1.48	1.34
6	A	710	A1CT4	C07-N06	6.98	1.48	1.34

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	710	A1CT4	S18-C19-N20	-12.38	109.24	117.01
6	B	708	A1CT4	S18-C19-N20	-12.31	109.28	117.01
6	F	707	A1CT4	S18-C19-N20	-12.30	109.29	117.01
6	E	708	A1CT4	S18-C19-N20	-12.24	109.33	117.01
6	A	710	A1CT4	S18-C19-N20	-12.24	109.33	117.01

There are no chirality outliers.

5 of 213 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	707	A1CT4	C07-C08-C09-C10
6	J	707	A1CT4	C07-C08-C09-C11
6	J	707	A1CT4	C07-C08-C09-C12
6	K	706	A1CT4	C07-C08-C09-C10
6	K	706	A1CT4	C07-C08-C09-C11

There are no ring outliers.

53 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	713	1PE	1	0
8	C	713	DMS	2	0
4	I	710	PEG	2	0
8	J	710	DMS	2	0
4	E	706	PEG	1	0
4	A	709	PEG	1	0
4	J	709	PEG	1	0
8	C	706	DMS	1	0
6	E	708	A1CT4	1	0
5	J	716	SO4	1	0
4	L	705	PEG	1	0
7	L	715	1PE	2	0
4	D	706	PEG	3	0
5	K	711	SO4	1	0
4	J	708	PEG	1	0
8	H	706	DMS	1	0
4	A	708	PEG	1	0
4	A	707	PEG	2	0
7	I	716	1PE	1	0
4	B	704	PEG	2	0
4	L	704	PEG	2	0
4	J	717	PEG	2	0
4	B	705	PEG	1	0
5	J	711	SO4	1	0
7	K	716	1PE	3	0
4	A	706	PEG	1	0
7	L	716	1PE	2	0
7	K	715	1PE	1	0
5	B	711	SO4	1	0
10	G	705	A1CT5	1	0
8	B	707	DMS	1	0
5	H	711	SO4	1	0
7	F	706	1PE	1	0
4	L	706	PEG	3	0
7	L	714	1PE	1	0
7	D	704	1PE	1	0
7	K	714	1PE	1	0
8	J	704	DMS	2	0
7	J	719	1PE	1	0
7	J	718	1PE	1	0

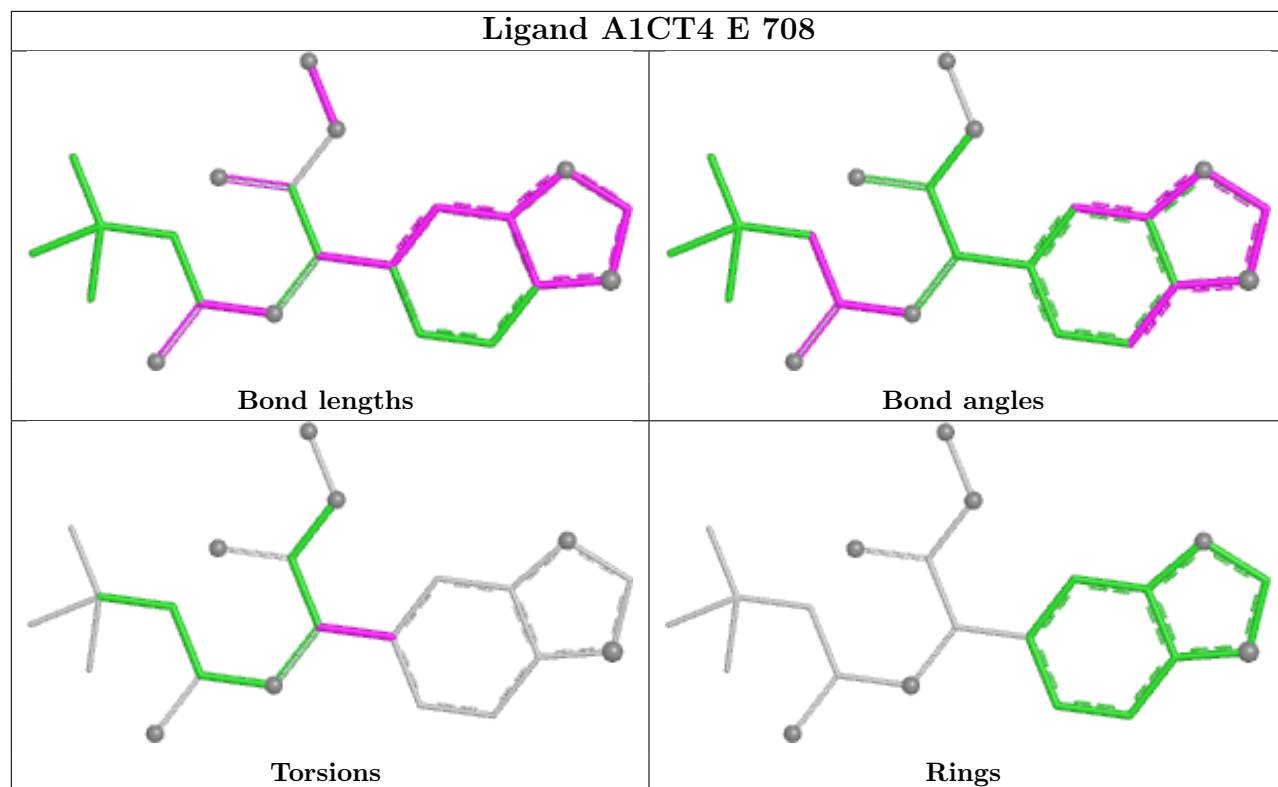
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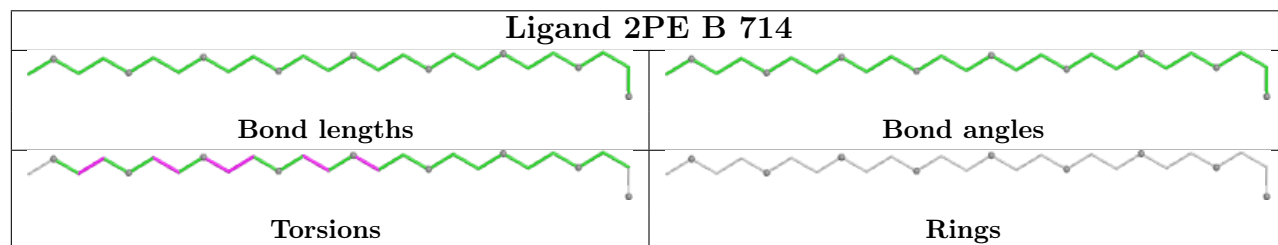
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	707	PEG	1	0
3	B	703	CO3	1	0
6	B	708	A1CT4	2	0
7	A	717	1PE	1	0
3	L	703	CO3	2	0
7	D	717	1PE	2	0
4	A	704	PEG	1	0
3	E	703	CO3	1	0
7	G	716	1PE	1	0
6	K	706	A1CT4	1	0
6	L	710	A1CT4	2	0
4	C	709	PEG	1	0
7	E	709	1PE	2	0

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.

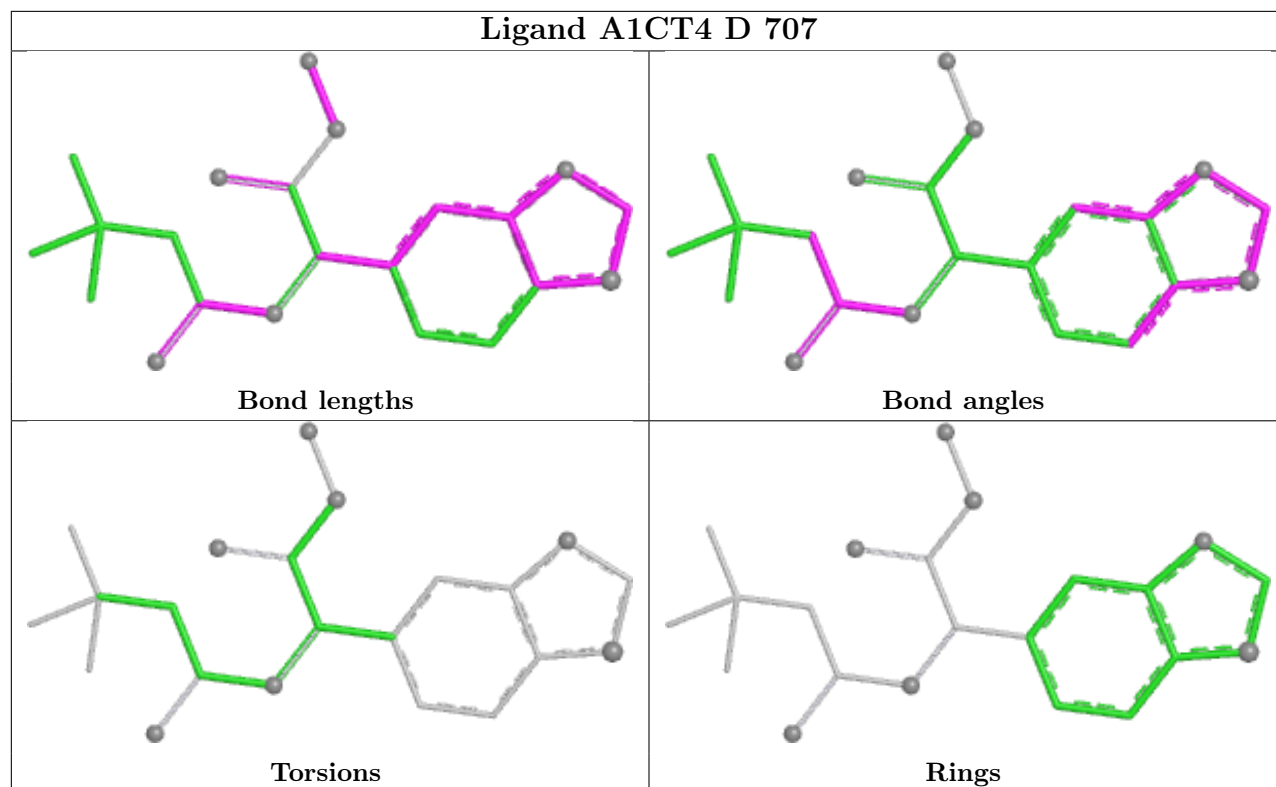
Ligand A1CT4 E 708



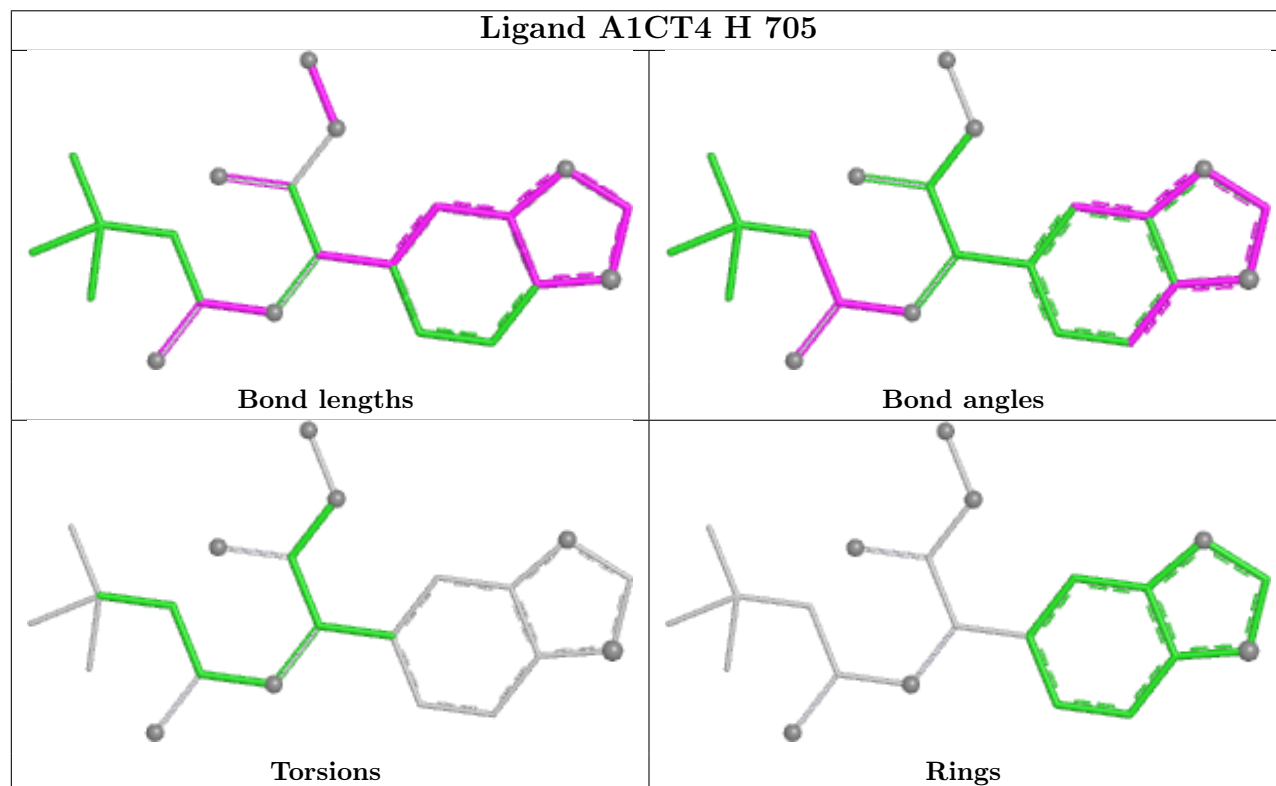
Ligand 2PE B 714



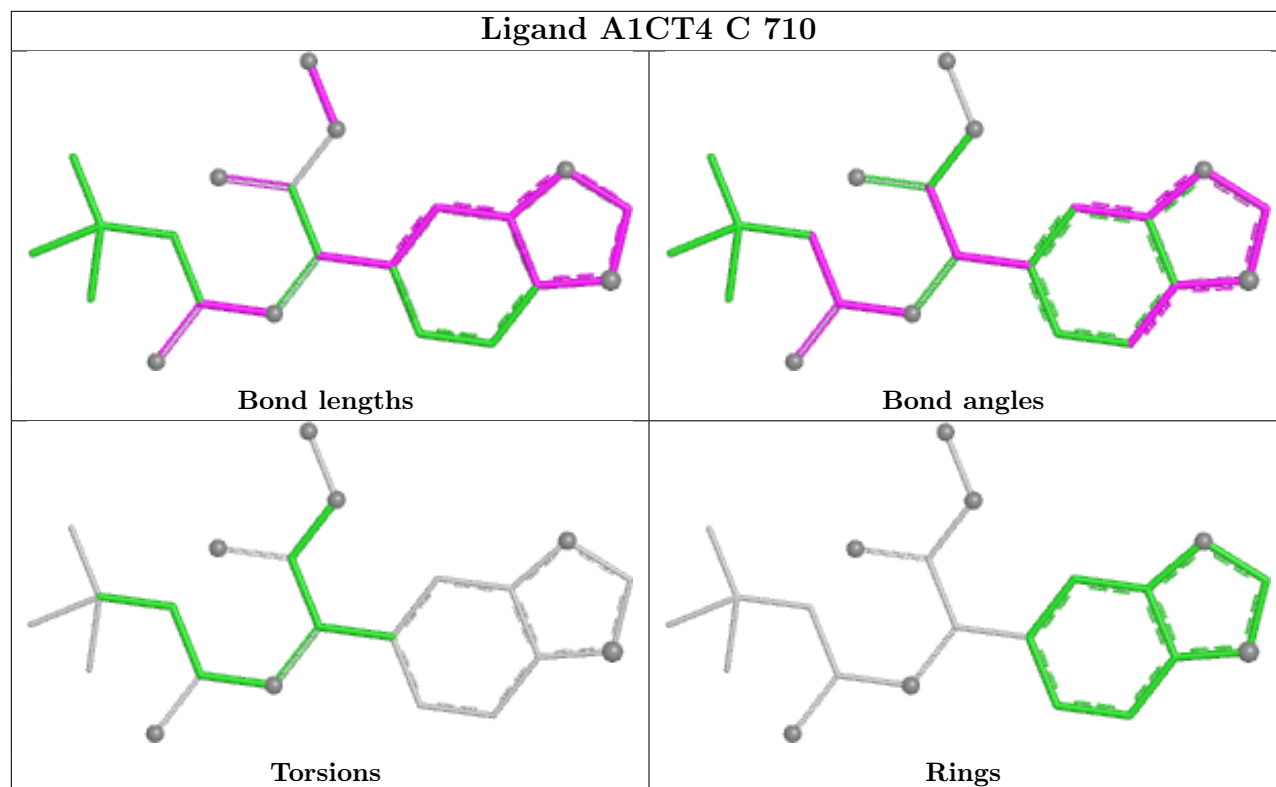
Ligand A1CT4 D 707



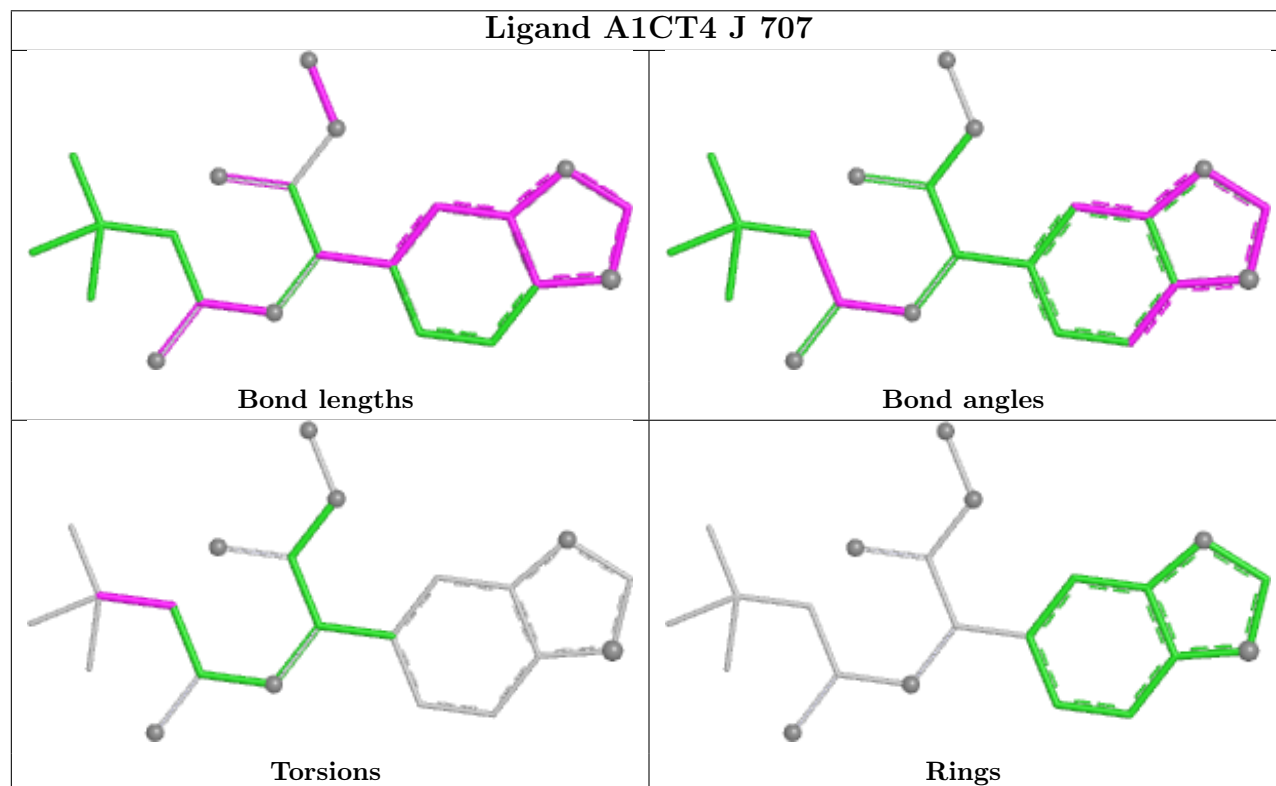
Ligand A1CT4 H 705



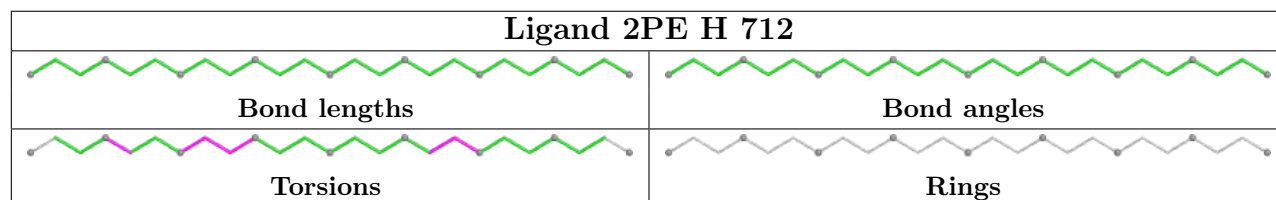
Ligand A1CT4 C 710



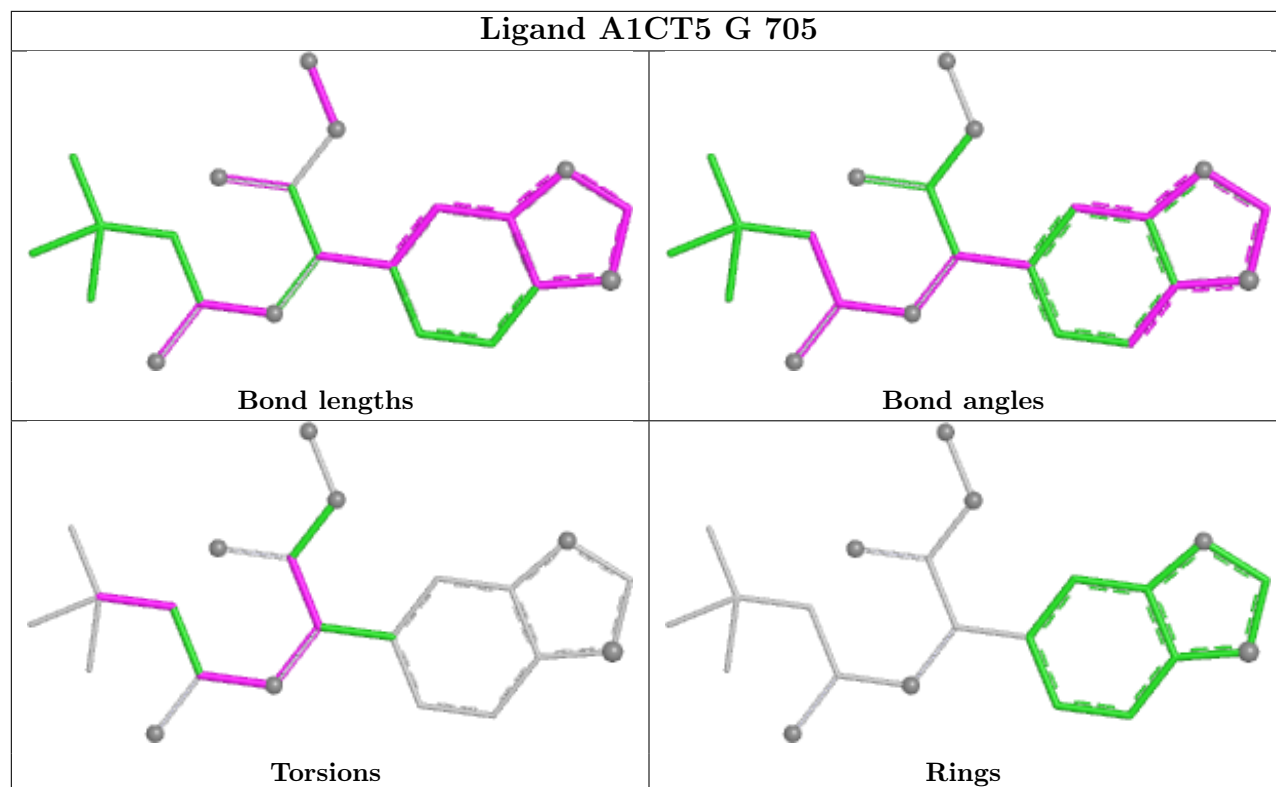
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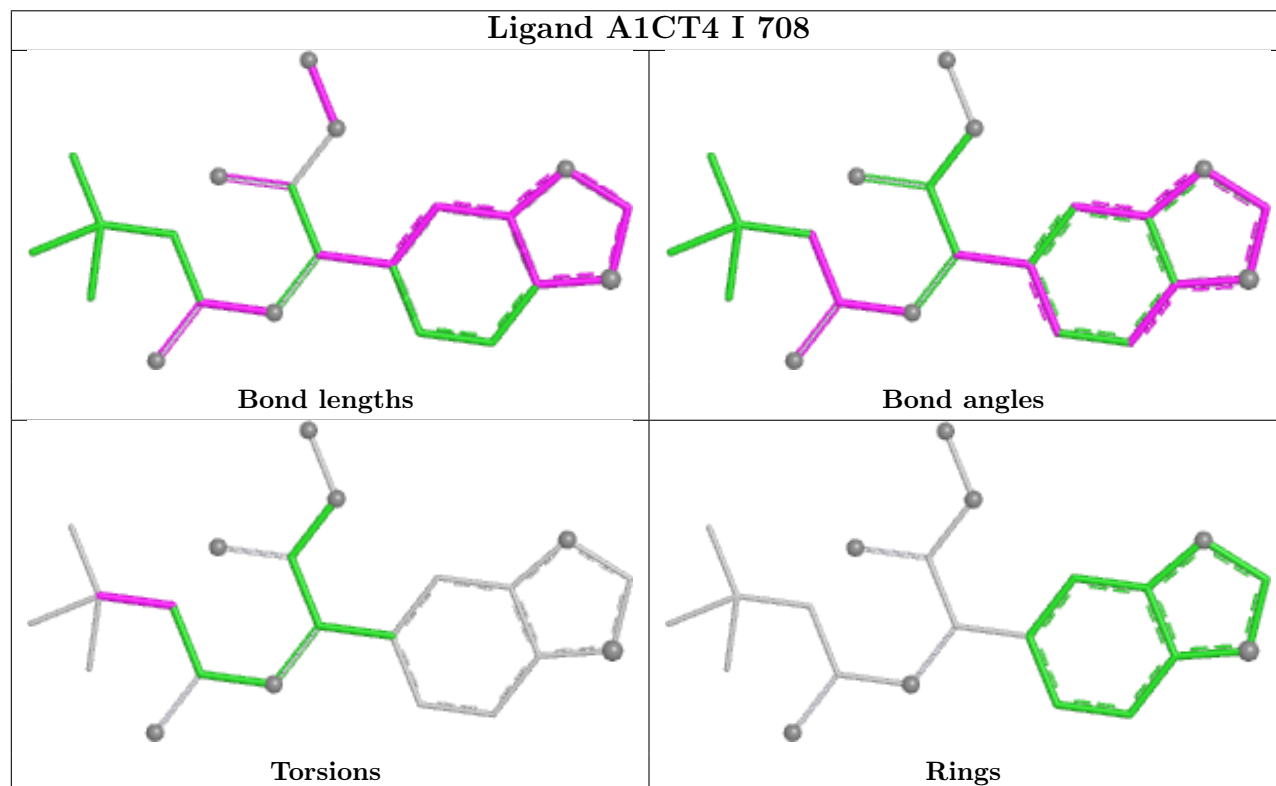
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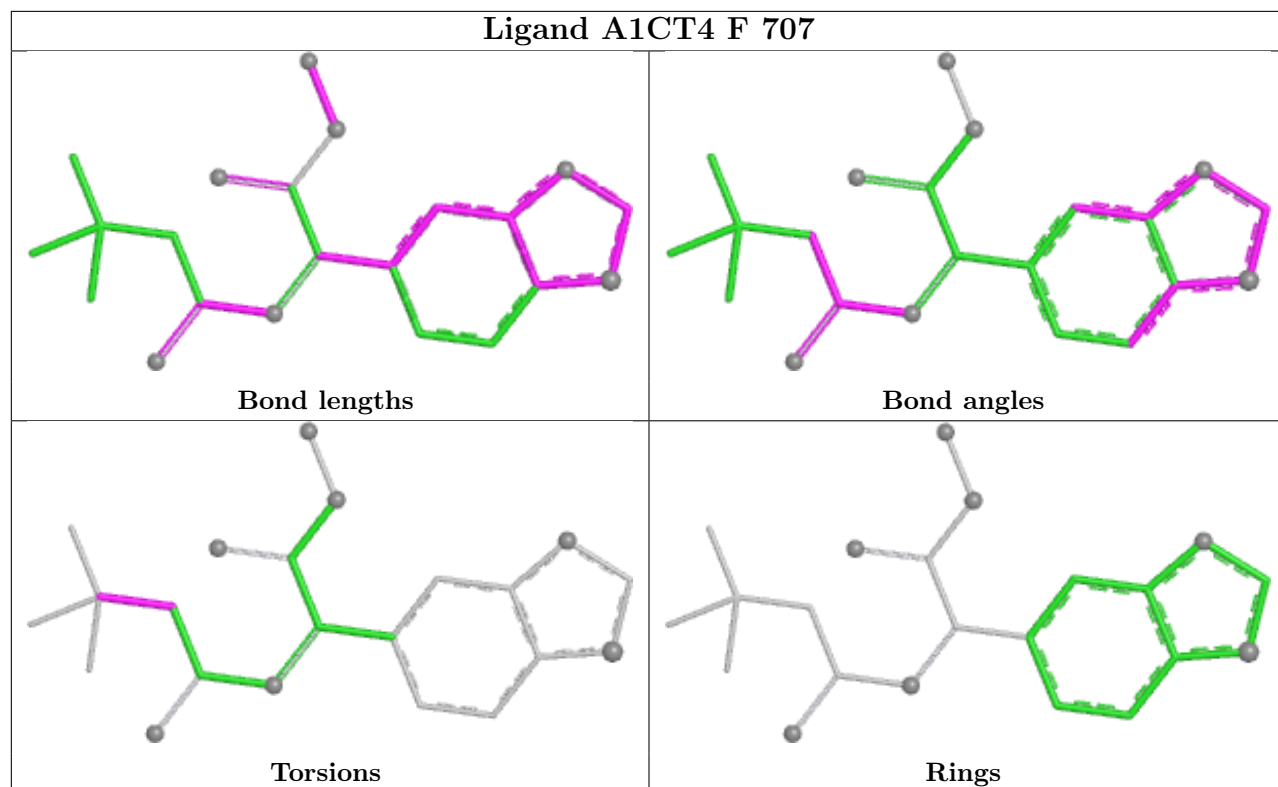
Ligand A1CT5 G 705



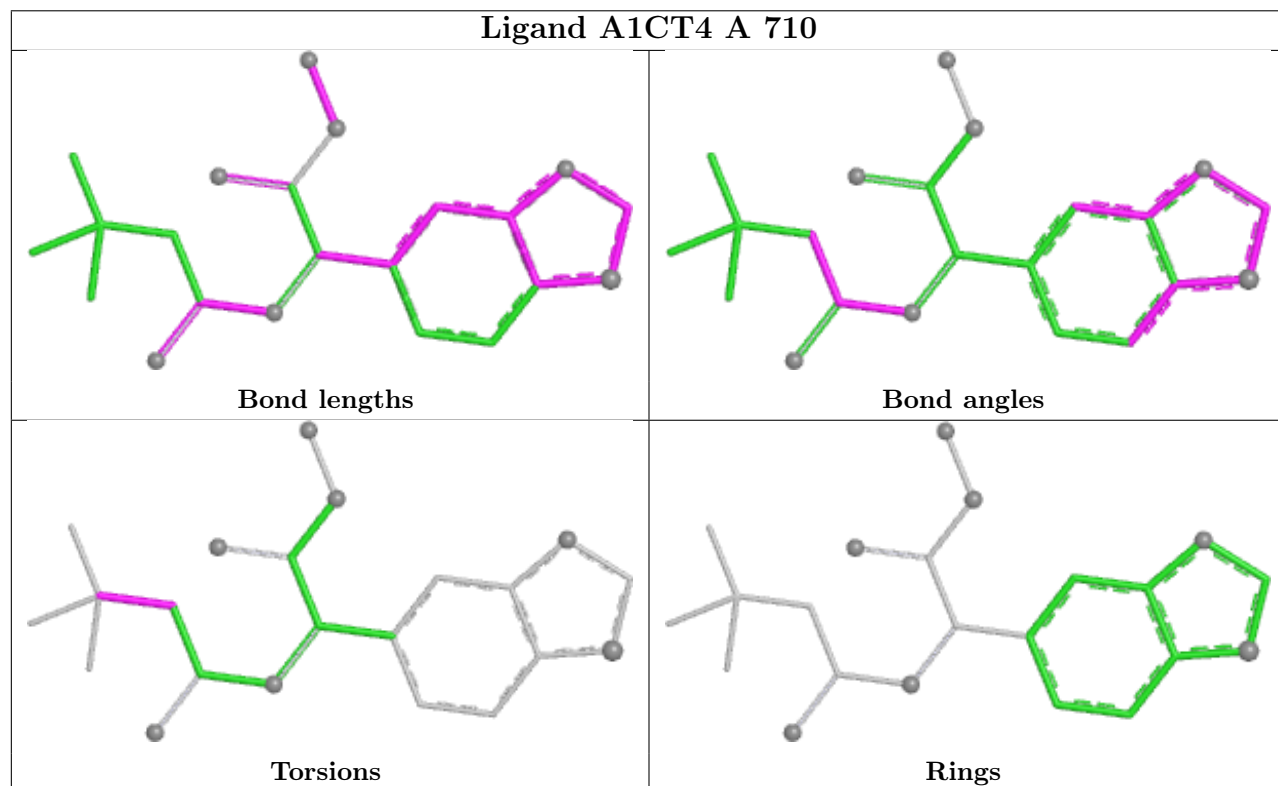
Ligand A1CT4 I 708



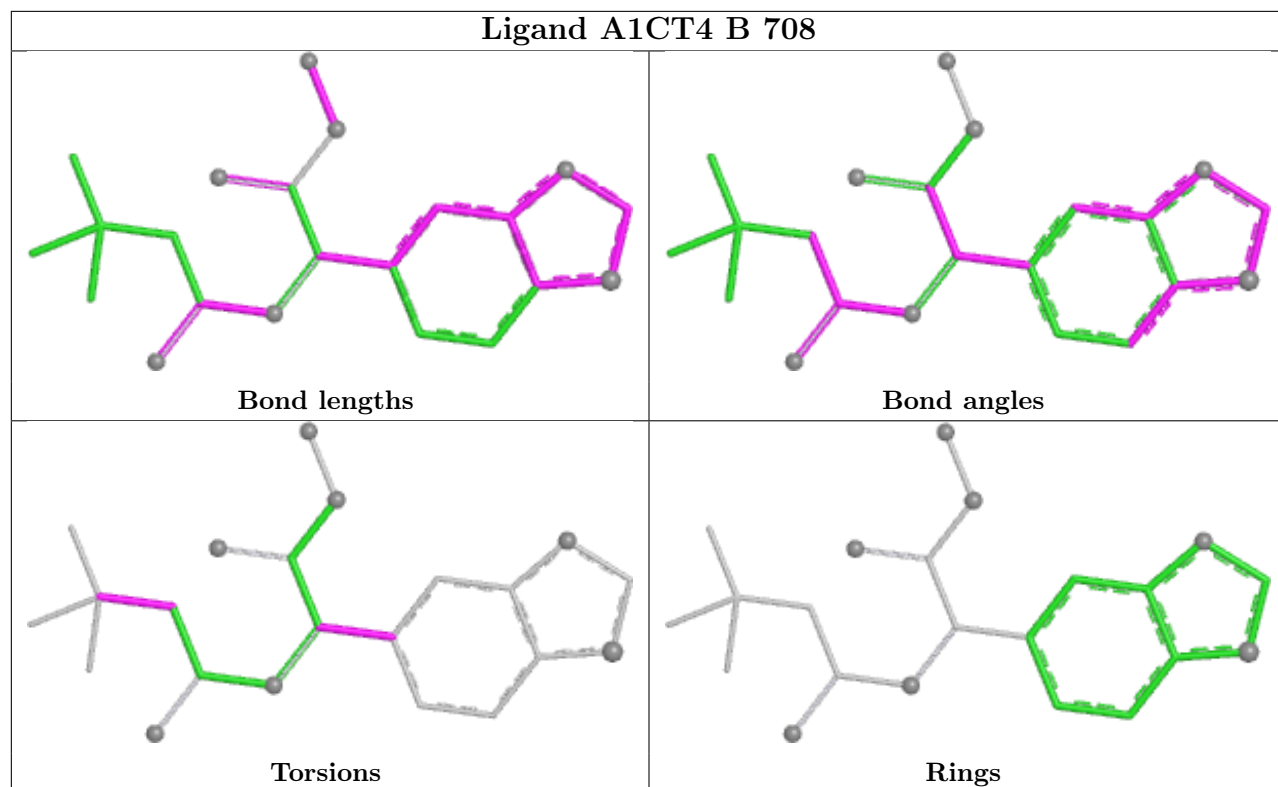
Ligand A1CT4 F 707



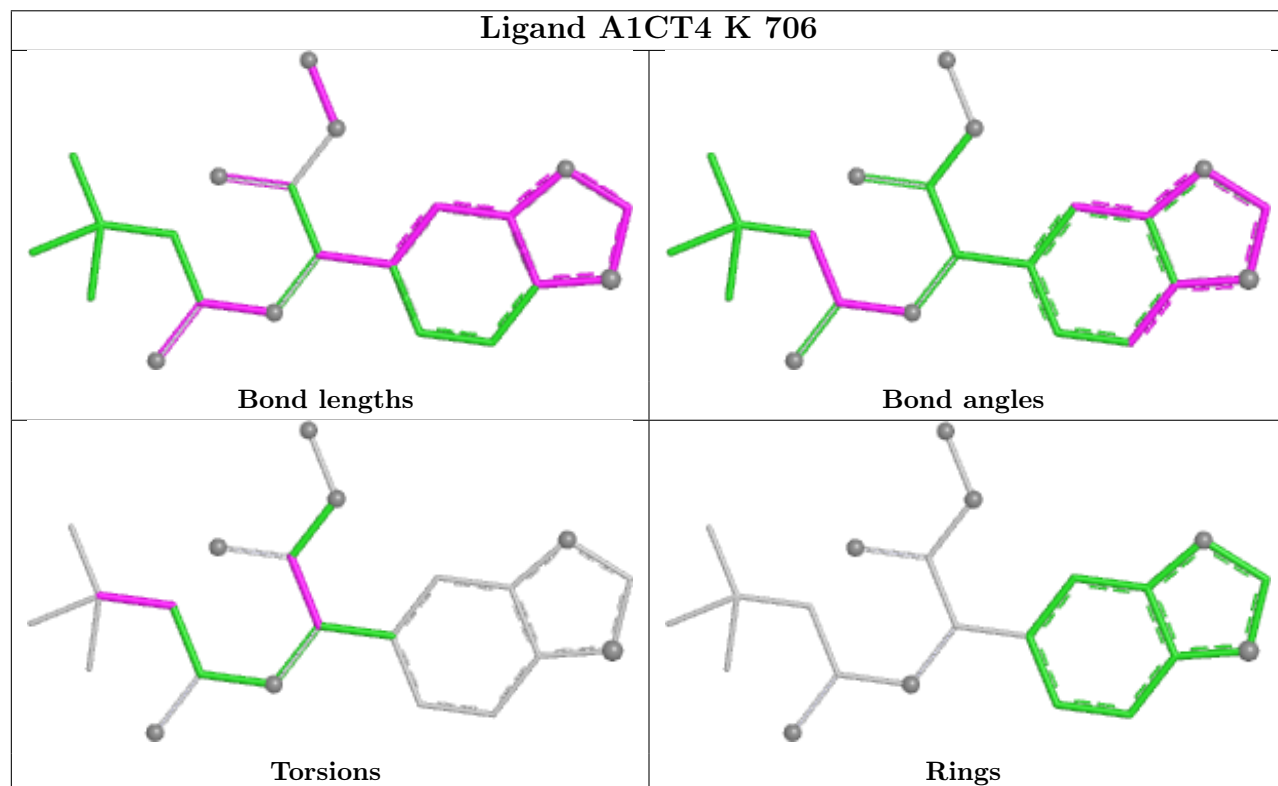
Ligand A1CT4 A 710

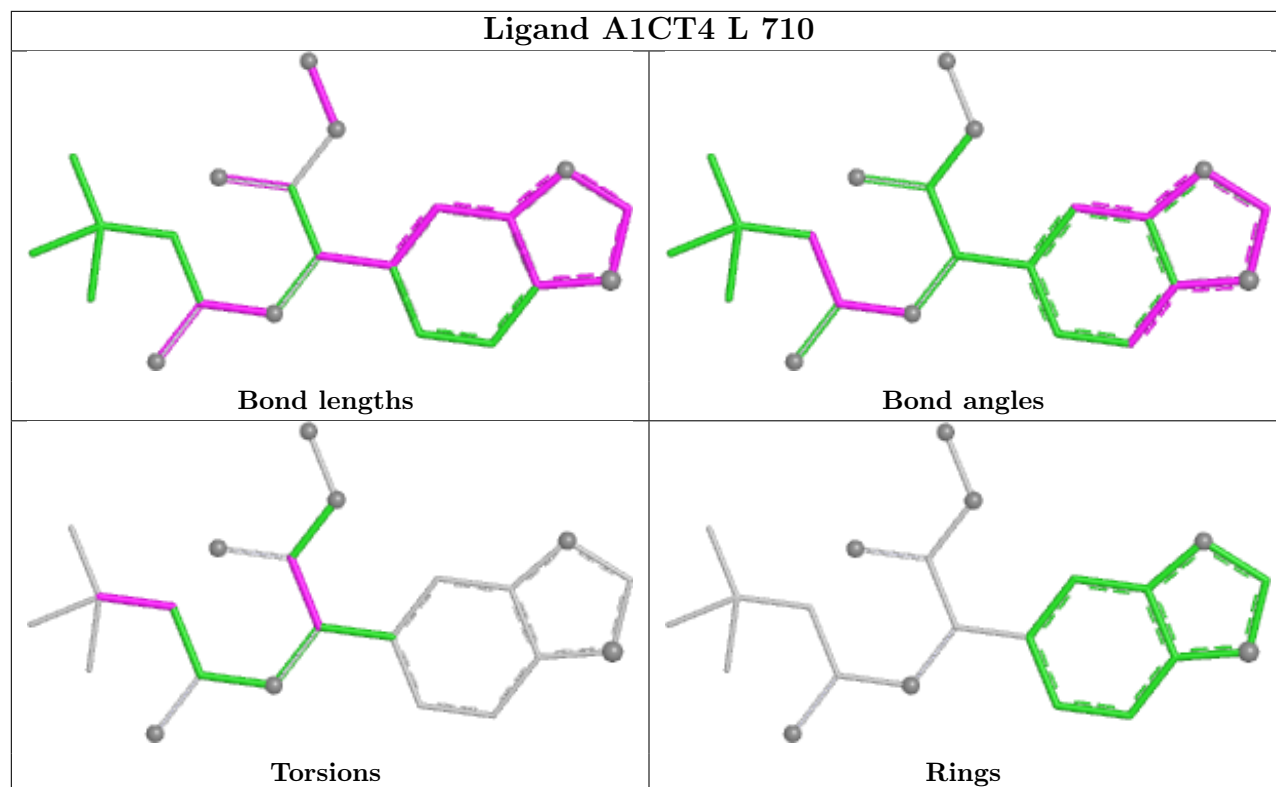


Ligand A1CT4 B 708



Ligand A1CT4 K 706





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	519/527 (98%)	-0.09	6 (1%) 76 76	22, 32, 55, 95	0
1	B	512/527 (97%)	0.13	16 (3%) 51 51	22, 34, 81, 105	2 (0%)
1	C	518/527 (98%)	-0.08	3 (0%) 85 85	21, 32, 59, 96	0
1	D	515/527 (97%)	-0.21	1 (0%) 91 90	21, 30, 52, 79	0
1	E	510/527 (96%)	-0.23	0 100 100	22, 30, 46, 80	0
1	F	511/527 (96%)	0.12	11 (2%) 62 61	22, 35, 74, 100	0
1	G	517/527 (98%)	-0.16	3 (0%) 85 85	21, 30, 52, 73	0
1	H	512/527 (97%)	0.11	21 (4%) 41 41	19, 33, 81, 113	0
1	I	518/527 (98%)	-0.09	7 (1%) 73 72	20, 32, 59, 107	0
1	J	514/527 (97%)	-0.17	3 (0%) 85 85	21, 31, 51, 87	0
1	K	510/527 (96%)	-0.21	1 (0%) 91 90	22, 31, 47, 67	0
1	L	511/527 (96%)	0.02	7 (1%) 73 72	20, 32, 70, 92	0
All	All	6167/6324 (97%)	-0.07	79 (1%) 75 74	19, 31, 65, 113	2 (0%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	VAL	4.8
1	H	176	TYR	4.2
1	A	259	VAL	3.8
1	F	176	TYR	3.4
1	L	176	TYR	3.3

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(Å ²)	Q<0.9
4	PEG	F	704	7/7	0.62	0.13	60,63,76,78	0
5	SO4	E	707	5/5	0.69	0.14	80,86,92,114	0
8	DMS	C	705	4/4	0.69	0.22	57,62,70,95	0
5	SO4	F	709	5/5	0.71	0.13	111,115,135,140	0
4	PEG	A	706	7/7	0.71	0.20	56,59,74,74	0
5	SO4	G	711	5/5	0.72	0.14	76,77,88,110	0
7	1PE	D	715	8/16	0.74	0.20	60,71,76,76	0
4	PEG	L	711	7/7	0.74	0.17	40,52,57,70	0
5	SO4	J	706	5/5	0.75	0.14	83,87,103,115	0
4	PEG	E	715	7/7	0.75	0.14	49,62,67,71	0
4	PEG	L	706	7/7	0.75	0.19	50,51,62,65	0
7	1PE	B	709	7/16	0.77	0.17	46,49,54,56	0
4	PEG	I	709	7/7	0.78	0.15	43,59,65,69	0
5	SO4	F	705	5/5	0.78	0.13	85,93,99,112	0
5	SO4	K	707	5/5	0.79	0.16	87,88,98,105	0
7	1PE	J	705	10/16	0.79	0.18	62,71,79,86	0
7	1PE	J	721	9/16	0.79	0.17	41,51,66,67	0
5	SO4	H	710	5/5	0.79	0.11	88,89,99,112	0
5	SO4	H	707	5/5	0.80	0.15	92,95,107,136	0
4	PEG	A	704	7/7	0.80	0.15	40,47,57,57	0
7	1PE	D	716	11/16	0.80	0.14	35,41,51,52	0
8	DMS	G	706	4/4	0.80	0.20	56,59,75,95	0
7	1PE	K	717	6/16	0.81	0.15	51,55,59,59	0
4	PEG	D	708	7/7	0.81	0.17	53,62,73,82	0
8	DMS	C	706	4/4	0.81	0.14	47,52,61,77	0
5	SO4	E	714	5/5	0.81	0.13	66,71,81,85	0
5	SO4	K	711	5/5	0.82	0.11	54,65,80,89	0
4	PEG	C	704	7/7	0.82	0.16	50,54,59,64	0
7	1PE	J	720	11/16	0.82	0.12	32,41,46,55	0
5	SO4	K	708	5/5	0.82	0.11	74,79,92,100	0
8	DMS	I	705	4/4	0.82	0.18	50,56,59,76	0
4	PEG	L	709	7/7	0.83	0.13	41,46,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	K	704	7/7	0.83	0.12	21,31,49,52	0
8	DMS	H	706	4/4	0.83	0.17	56,69,74,74	0
5	SO4	F	710	5/5	0.83	0.11	88,95,96,117	0
4	PEG	C	709	7/7	0.84	0.12	49,64,68,69	0
5	SO4	A	705	5/5	0.84	0.11	74,91,102,104	0
5	SO4	B	712	5/5	0.84	0.12	68,68,83,94	0
4	PEG	C	712	7/7	0.84	0.14	46,55,65,66	0
4	PEG	A	709	7/7	0.84	0.14	61,64,70,73	0
6	A1CT4	L	710	22/22	0.84	0.13	35,46,50,61	0
5	SO4	H	708	5/5	0.85	0.12	66,69,83,87	0
4	PEG	B	705	7/7	0.85	0.11	38,45,61,61	0
8	DMS	B	707	4/4	0.85	0.15	52,52,52,77	0
8	DMS	B	710	4/4	0.85	0.19	43,45,73,83	0
7	1PE	C	719	7/16	0.85	0.13	24,37,41,43	0
4	PEG	G	704	7/7	0.85	0.14	52,54,69,69	0
5	SO4	D	712	5/5	0.85	0.10	72,74,82,88	0
3	CO3	J	703	4/4	0.85	0.18	25,35,41,50	0
4	PEG	J	708	7/7	0.85	0.11	41,52,56,63	0
8	DMS	J	710	4/4	0.85	0.16	54,55,62,65	0
4	PEG	I	704	7/7	0.86	0.11	43,52,65,74	0
5	SO4	K	713	5/5	0.86	0.17	54,56,69,78	0
6	A1CT4	D	707	22/22	0.86	0.12	28,48,55,60	0
6	A1CT4	I	708	22/22	0.86	0.14	38,49,58,60	0
4	PEG	L	705	7/7	0.86	0.12	35,40,44,49	0
4	PEG	E	706	7/7	0.86	0.17	43,46,50,57	0
5	SO4	J	714	5/5	0.86	0.10	55,67,82,85	0
4	PEG	H	704	7/7	0.86	0.15	56,60,66,69	0
4	PEG	J	717	7/7	0.86	0.12	38,42,48,61	0
7	1PE	E	709	13/16	0.86	0.12	28,41,47,52	0
7	1PE	E	716	10/16	0.86	0.11	27,38,46,50	0
7	1PE	F	706	16/16	0.86	0.11	34,49,57,57	0
9	2PE	B	714	26/28	0.86	0.13	35,52,66,70	0
7	1PE	K	714	8/16	0.87	0.11	30,43,55,61	0
7	1PE	K	716	11/16	0.87	0.11	30,41,46,54	0
4	PEG	I	706	7/7	0.87	0.11	28,33,40,45	0
7	1PE	L	707	10/16	0.87	0.12	41,51,54,61	0
7	1PE	L	716	11/16	0.87	0.12	40,45,76,77	0
5	SO4	E	710	5/5	0.87	0.12	83,83,106,113	0
5	SO4	I	712	5/5	0.87	0.09	62,66,76,87	0
7	1PE	D	717	5/16	0.87	0.14	40,43,48,53	0
5	SO4	I	713	5/5	0.87	0.11	56,57,63,74	0
6	A1CT4	B	708	22/22	0.87	0.12	30,43,53,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	714	5/5	0.87	0.10	80,80,86,104	0
5	SO4	J	711	5/5	0.87	0.13	67,70,84,89	0
4	PEG	C	711	7/7	0.87	0.14	38,55,64,80	0
5	SO4	J	715	5/5	0.87	0.07	69,70,89,96	0
10	A1CT5	G	705	22/22	0.87	0.12	35,43,53,59	0
4	PEG	I	710	7/7	0.88	0.18	18,44,47,54	0
5	SO4	E	712	5/5	0.88	0.10	52,67,73,94	0
6	A1CT4	K	706	22/22	0.88	0.12	44,50,58,68	0
7	1PE	I	716	9/16	0.88	0.10	24,29,36,38	0
5	SO4	B	713	5/5	0.88	0.09	55,64,83,86	0
8	DMS	D	718	4/4	0.88	0.15	49,59,64,76	0
7	1PE	A	717	7/16	0.88	0.11	46,52,58,58	0
4	PEG	A	707	7/7	0.88	0.12	35,36,46,52	0
3	CO3	K	703	4/4	0.88	0.15	28,31,35,43	0
5	SO4	D	713	5/5	0.88	0.09	62,68,81,85	0
5	SO4	A	714	5/5	0.88	0.12	54,65,81,94	0
9	2PE	H	712	25/28	0.88	0.11	32,44,52,63	0
6	A1CT4	C	710	22/22	0.88	0.12	31,43,52,66	0
7	1PE	G	715	6/16	0.89	0.10	26,29,36,36	0
4	PEG	C	707	7/7	0.89	0.12	46,60,62,67	0
5	SO4	A	715	5/5	0.89	0.10	65,68,76,85	0
5	SO4	E	705	5/5	0.89	0.19	57,67,71,75	0
6	A1CT4	A	710	22/22	0.89	0.11	29,39,52,55	0
4	PEG	D	705	7/7	0.89	0.14	40,43,52,58	0
5	SO4	G	710	5/5	0.89	0.10	57,63,71,84	0
3	CO3	A	703	4/4	0.89	0.17	45,46,49,54	0
8	DMS	L	708	4/4	0.89	0.12	33,33,34,76	0
4	PEG	B	704	7/7	0.89	0.12	27,35,55,58	0
6	A1CT4	J	707	22/22	0.89	0.11	33,43,53,55	0
5	SO4	E	713	5/5	0.89	0.09	69,71,83,97	0
7	1PE	I	715	10/16	0.90	0.10	33,43,47,49	0
5	SO4	J	716	5/5	0.90	0.12	44,60,79,82	0
3	CO3	D	703	4/4	0.90	0.15	29,29,30,42	0
6	A1CT4	E	708	22/22	0.90	0.12	37,49,58,58	0
6	A1CT4	F	707	22/22	0.90	0.12	33,42,56,66	0
3	CO3	F	703	4/4	0.90	0.14	41,44,48,48	0
5	SO4	C	716	5/5	0.90	0.09	56,65,79,84	0
5	SO4	D	709	5/5	0.90	0.14	58,60,71,72	0
5	SO4	H	709	5/5	0.90	0.09	56,61,78,78	0
7	1PE	L	714	10/16	0.90	0.10	31,40,52,57	0
4	PEG	D	706	7/7	0.90	0.11	39,43,46,46	0
7	1PE	I	707	13/16	0.90	0.10	32,47,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	A1CT4	H	705	22/22	0.91	0.10	26,37,45,56	0
7	1PE	D	704	13/16	0.91	0.09	32,39,51,55	0
5	SO4	I	711	5/5	0.91	0.13	59,60,64,77	0
2	ZN	L	701	1/1	0.91	0.12	85,85,85,85	0
8	DMS	C	713	4/4	0.91	0.17	53,53,53,70	0
4	PEG	C	708	7/7	0.91	0.08	37,40,44,46	0
4	PEG	A	708	7/7	0.91	0.10	46,48,52,61	0
7	1PE	A	716	7/16	0.91	0.11	27,31,40,43	0
5	SO4	G	709	5/5	0.91	0.09	51,51,54,67	0
7	1PE	F	711	10/16	0.91	0.10	23,37,47,50	0
7	1PE	F	712	10/16	0.91	0.10	28,42,51,66	0
7	1PE	G	714	6/16	0.91	0.09	38,39,42,42	0
7	1PE	L	715	7/16	0.91	0.09	26,32,37,37	0
2	ZN	K	701	1/1	0.91	0.10	152,152,152,152	0
7	1PE	L	713	10/16	0.92	0.09	24,32,42,49	0
7	1PE	G	713	8/16	0.92	0.09	29,33,34,43	0
7	1PE	J	719	10/16	0.92	0.09	36,44,53,53	0
5	SO4	A	713	5/5	0.92	0.15	56,60,63,70	0
5	SO4	I	714	5/5	0.92	0.14	42,52,56,82	0
7	1PE	G	716	13/16	0.92	0.09	36,41,49,50	0
4	PEG	L	704	7/7	0.92	0.11	30,32,41,44	0
4	PEG	K	705	7/7	0.92	0.11	32,37,49,54	0
5	SO4	A	712	5/5	0.92	0.09	56,58,73,84	0
7	1PE	J	718	10/16	0.93	0.08	25,33,41,45	0
2	ZN	D	701	1/1	0.93	0.09	83,83,83,83	0
3	CO3	L	703	4/4	0.93	0.09	22,35,39,42	0
5	SO4	H	711	5/5	0.93	0.11	56,65,75,80	0
5	SO4	C	715	5/5	0.93	0.09	49,53,59,66	0
7	1PE	C	718	10/16	0.93	0.09	38,42,50,57	0
3	CO3	G	703	4/4	0.93	0.15	20,31,39,46	0
4	PEG	J	709	7/7	0.93	0.09	39,44,51,54	0
7	1PE	D	714	7/16	0.93	0.10	28,31,37,38	0
5	SO4	K	710	5/5	0.93	0.11	38,60,67,71	0
3	CO3	H	703	4/4	0.93	0.10	18,33,34,43	0
5	SO4	K	712	5/5	0.93	0.12	66,68,74,76	0
3	CO3	E	703	4/4	0.93	0.12	21,30,38,44	0
2	ZN	B	702	1/1	0.94	0.07	100,100,100,100	0
2	ZN	B	701	1/1	0.94	0.09	86,86,86,86	0
8	DMS	J	704	4/4	0.94	0.16	34,44,52,63	0
2	ZN	E	702	1/1	0.94	0.08	80,80,80,80	0
5	SO4	G	712	5/5	0.94	0.10	39,47,60,64	0
3	CO3	B	703	4/4	0.94	0.09	24,26,27,34	0

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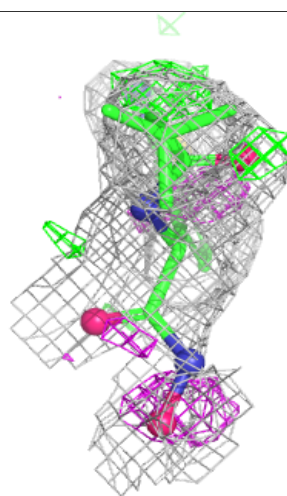
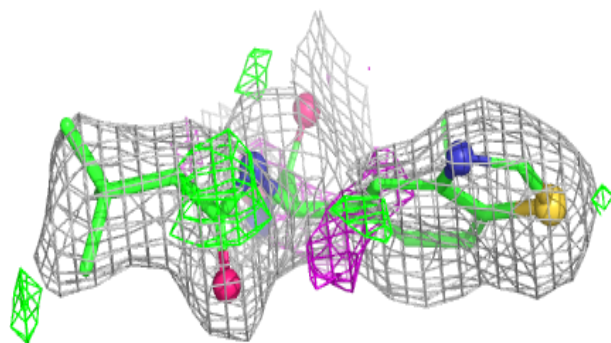
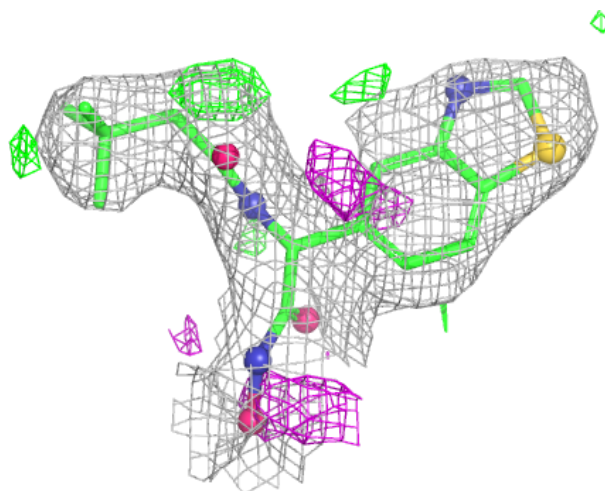
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CO3	C	703	4/4	0.94	0.13	38,43,47,48	0
3	CO3	I	703	4/4	0.94	0.09	21,26,35,41	0
2	ZN	H	701	1/1	0.95	0.10	88,88,88,88	0
2	ZN	K	702	1/1	0.95	0.07	100,100,100,100	0
5	SO4	E	711	5/5	0.95	0.11	46,48,64,69	0
2	ZN	I	701	1/1	0.95	0.07	90,90,90,90	0
8	DMS	B	706	4/4	0.95	0.12	45,47,48,58	0
7	1PE	E	717	10/16	0.95	0.07	26,30,40,46	0
7	1PE	K	715	10/16	0.95	0.07	26,31,36,39	0
5	SO4	K	709	5/5	0.95	0.10	40,43,50,58	0
5	SO4	J	713	5/5	0.95	0.09	43,52,58,62	0
2	ZN	J	701	1/1	0.95	0.10	82,82,82,82	0
5	SO4	C	717	5/5	0.96	0.08	27,29,50,51	0
5	SO4	L	712	5/5	0.96	0.10	41,41,52,60	0
4	PEG	E	704	7/7	0.96	0.06	35,36,42,45	0
5	SO4	D	710	5/5	0.96	0.08	45,51,62,63	0
2	ZN	G	702	1/1	0.96	0.06	85,85,85,85	0
2	ZN	I	702	1/1	0.96	0.09	75,75,75,75	0
2	ZN	E	701	1/1	0.97	0.08	85,85,85,85	0
2	ZN	J	702	1/1	0.97	0.09	71,71,71,71	0
2	ZN	A	702	1/1	0.97	0.07	72,72,72,72	0
5	SO4	F	708	5/5	0.97	0.08	42,46,56,62	0
2	ZN	F	701	1/1	0.97	0.07	80,80,80,80	0
5	SO4	A	711	5/5	0.97	0.07	43,45,55,58	0
5	SO4	G	707	5/5	0.97	0.06	24,27,29,32	0
5	SO4	G	708	5/5	0.97	0.07	38,40,52,53	0
2	ZN	G	701	1/1	0.97	0.07	73,73,73,73	0
2	ZN	A	701	1/1	0.98	0.06	75,75,75,75	0
2	ZN	F	702	1/1	0.98	0.06	75,75,75,75	0
2	ZN	L	702	1/1	0.98	0.06	67,67,67,67	0
5	SO4	B	711	5/5	0.98	0.06	23,24,31,32	0
5	SO4	J	712	5/5	0.98	0.05	25,27,29,39	0
2	ZN	D	702	1/1	0.98	0.11	75,75,75,75	0
5	SO4	D	711	5/5	0.98	0.05	23,23,30,30	0
2	ZN	C	701	1/1	0.98	0.10	59,59,59,59	0
2	ZN	C	702	1/1	0.98	0.13	63,63,63,63	0
2	ZN	H	702	1/1	0.99	0.06	58,58,58,58	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.

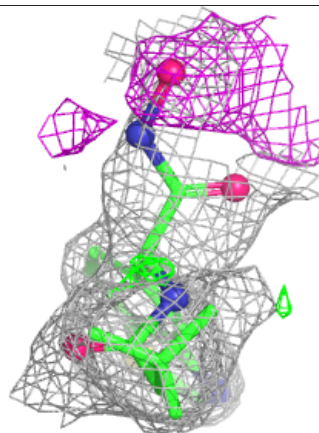
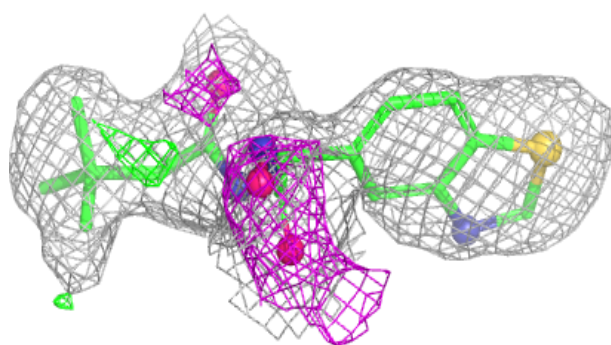
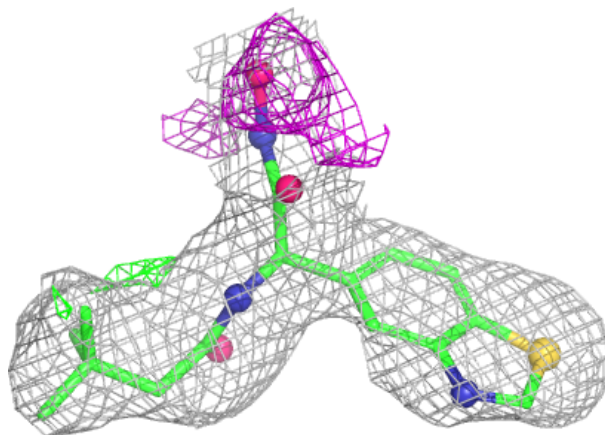
Electron density around A1CT4 L 710:

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



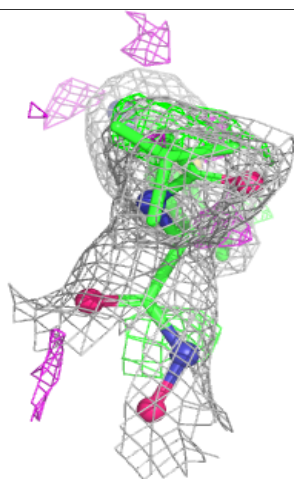
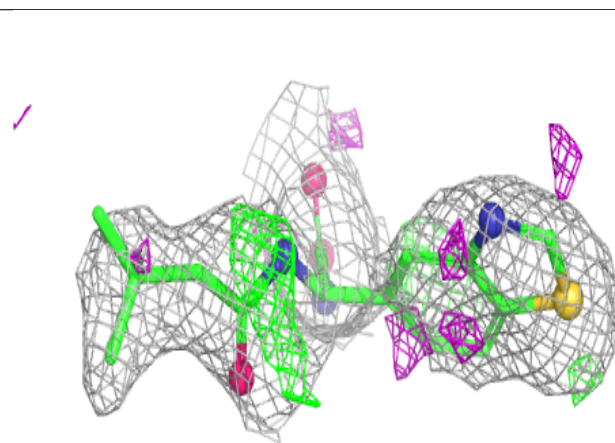
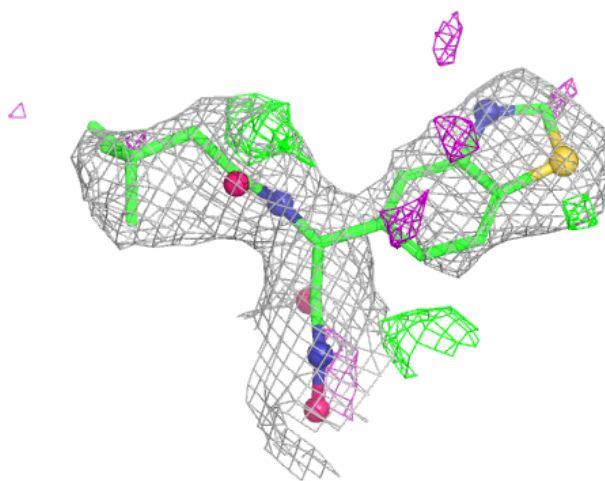
Electron density around A1CT4 D 707:

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



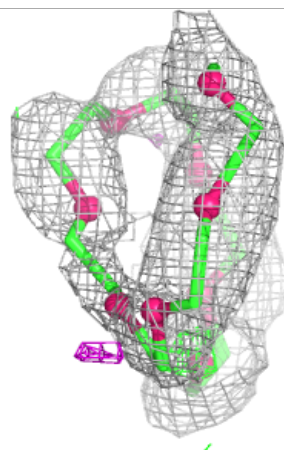
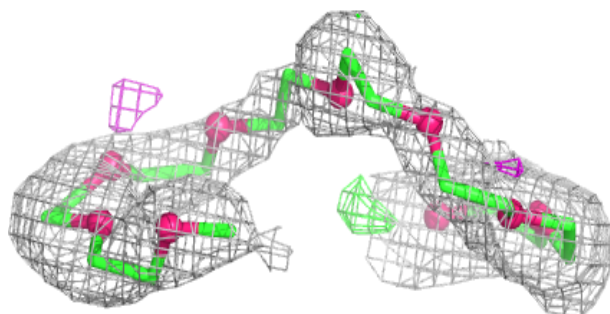
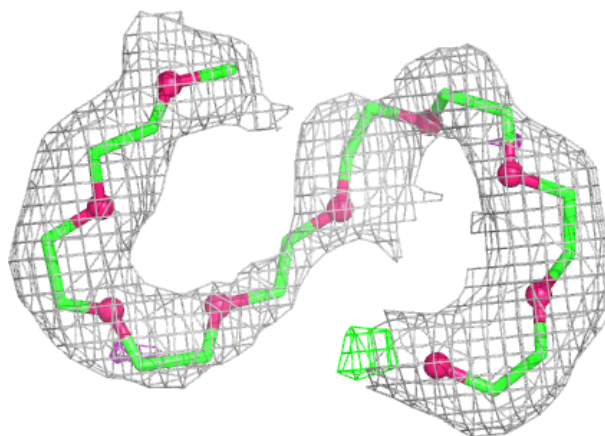
Electron density around A1CT4 I 708:

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



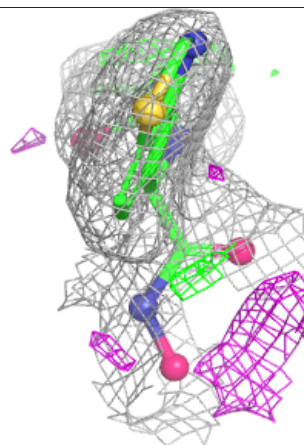
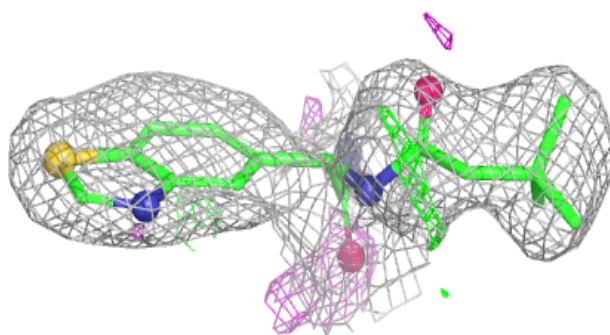
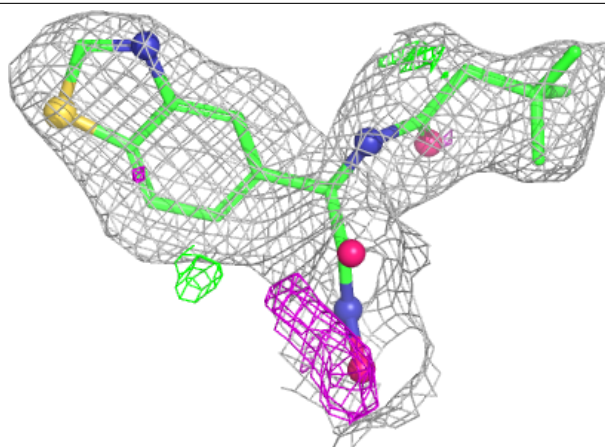
Electron density around 2PE B 714:

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



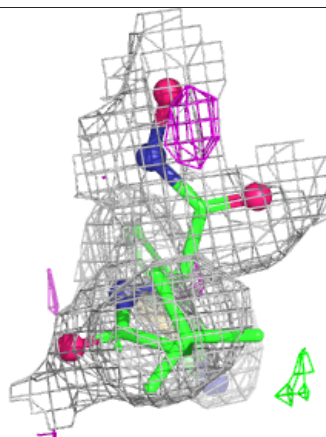
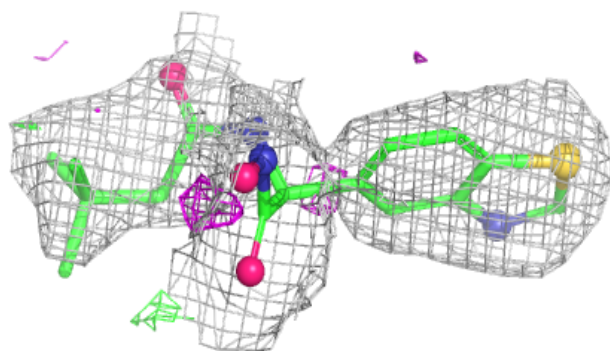
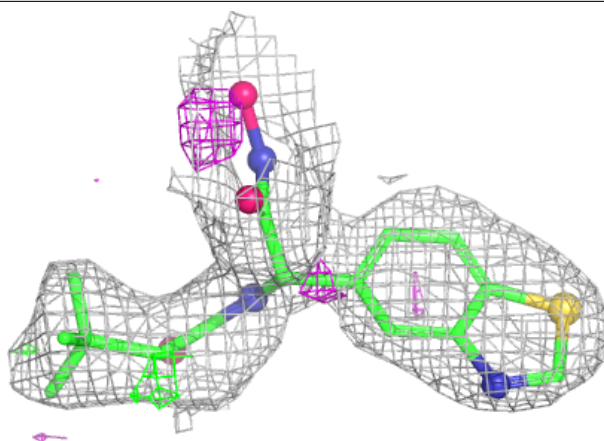
Electron density around A1CT4 B 708:

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



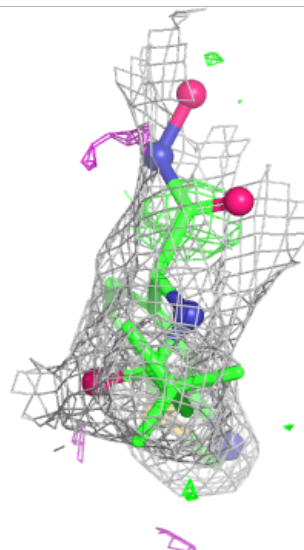
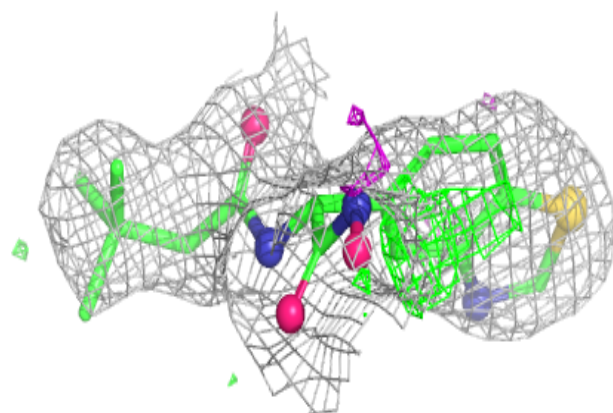
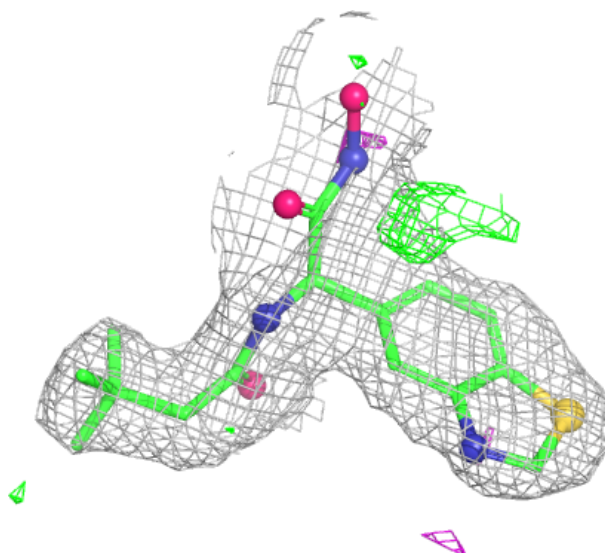
Electron density around A1CT5 G 705:

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



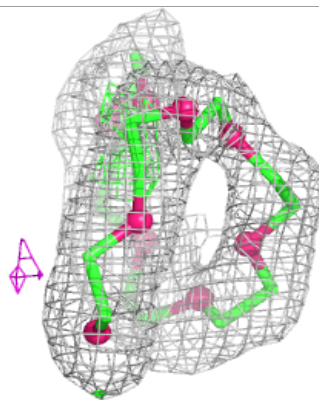
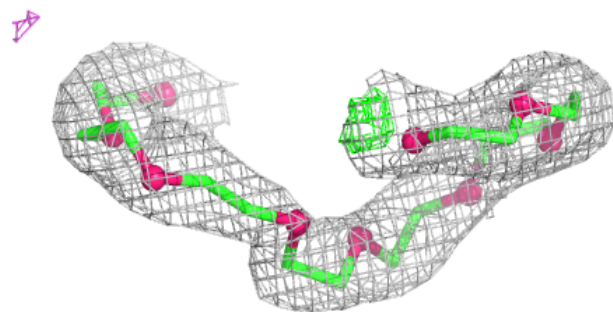
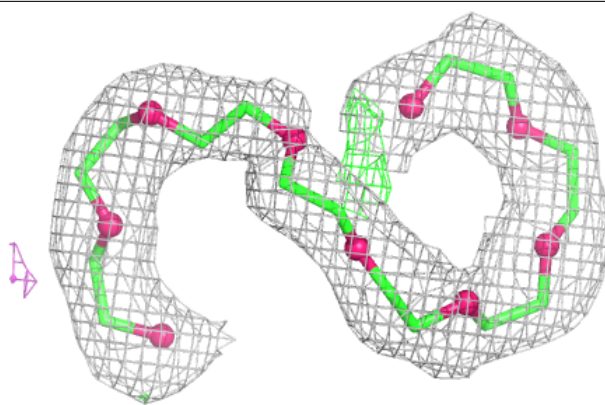
Electron density around A1CT4 K 706:

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



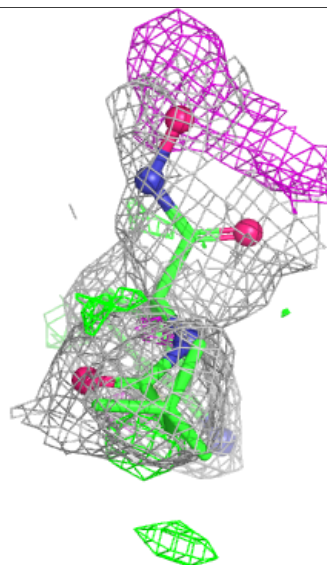
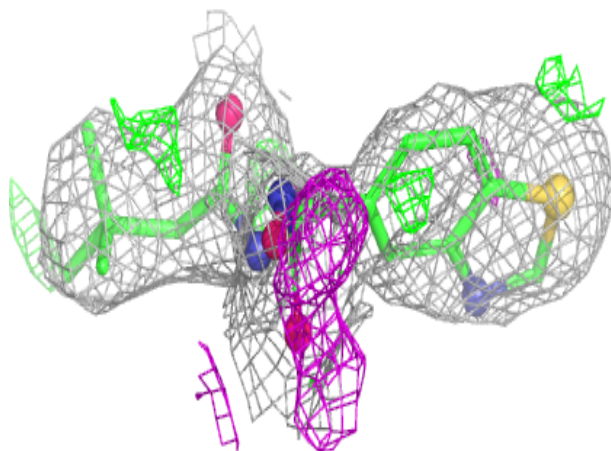
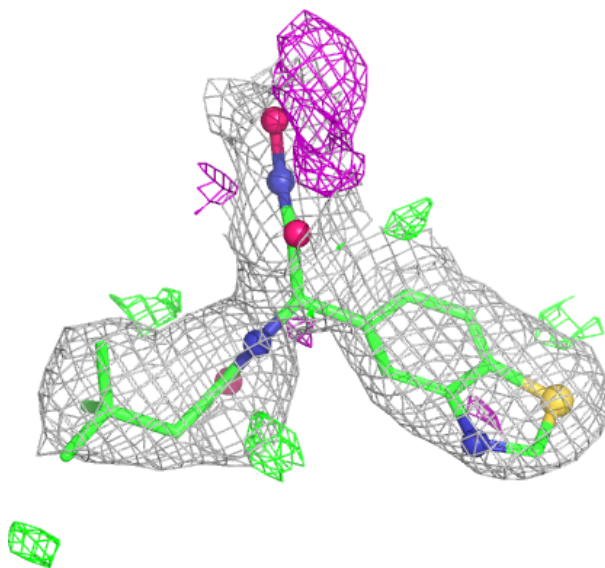
Electron density around 2PE H 712:

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



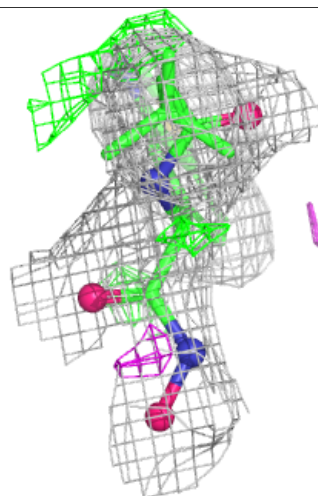
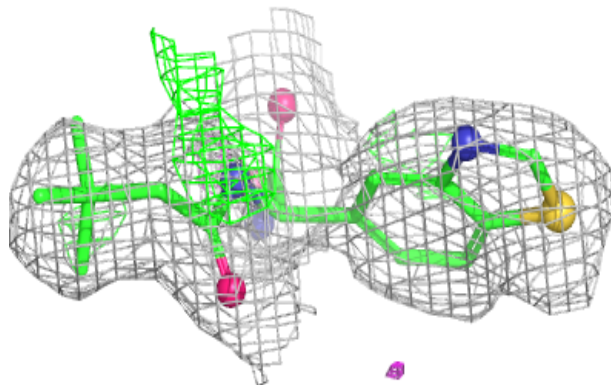
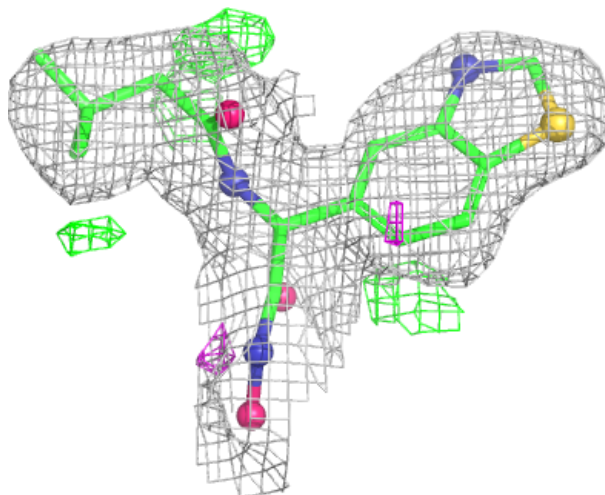
Electron density around A1CT4 C 710:

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



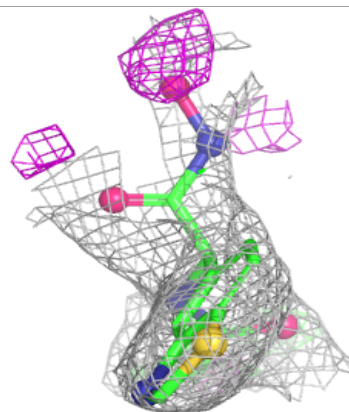
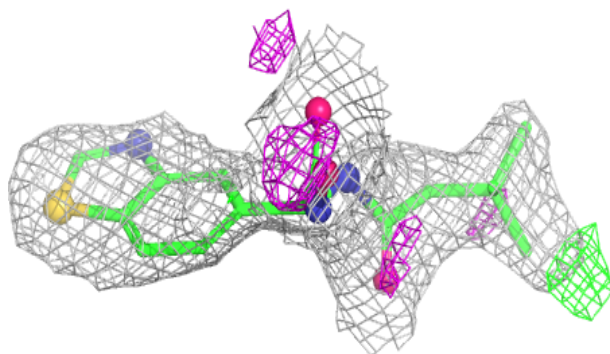
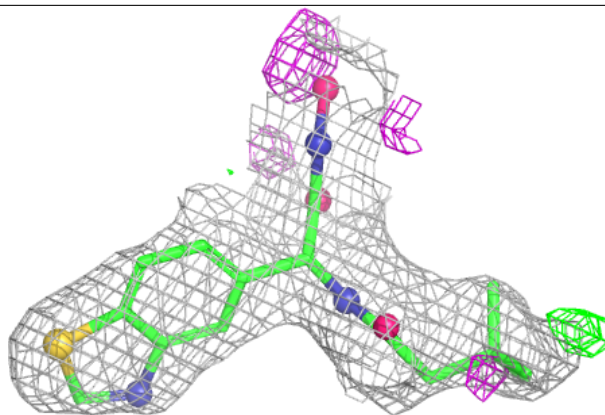
Electron density around A1CT4 A 710:

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



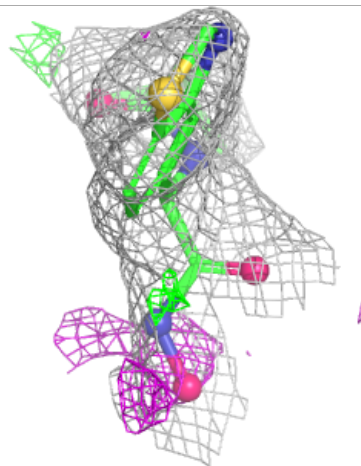
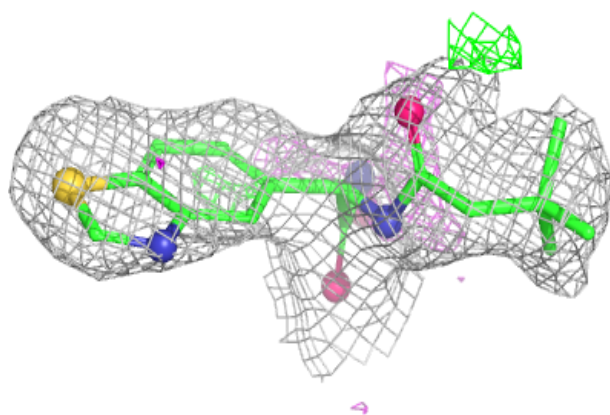
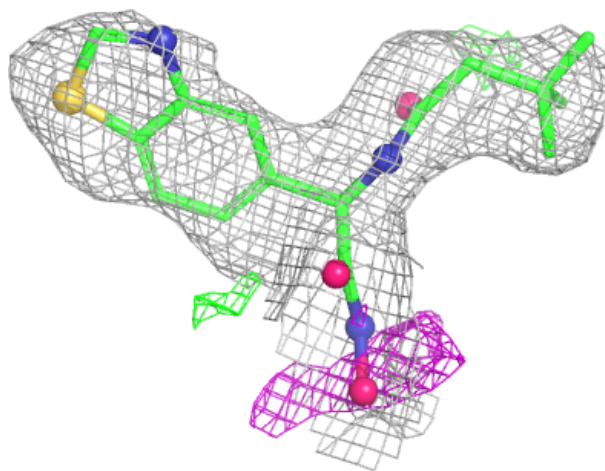
Electron density around A1CT4 J 707:

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



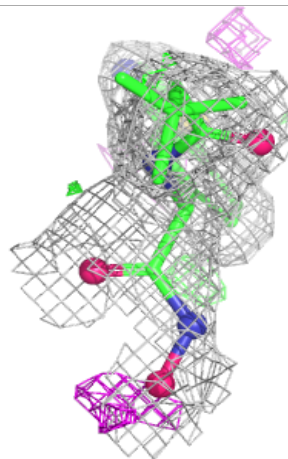
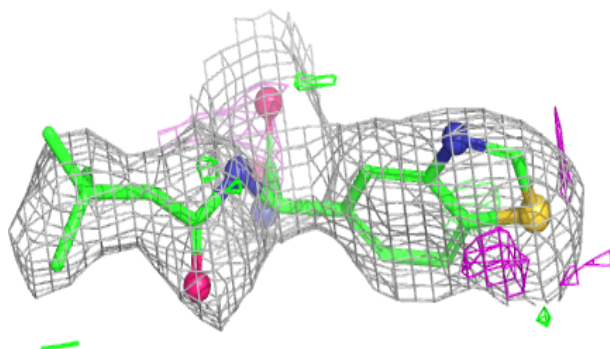
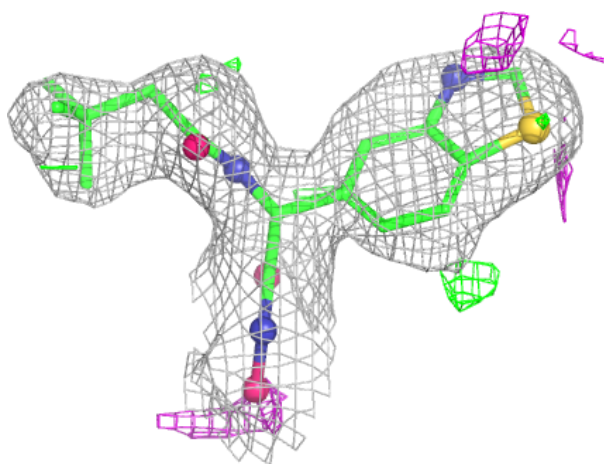
Electron density around A1CT4 E 708:

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



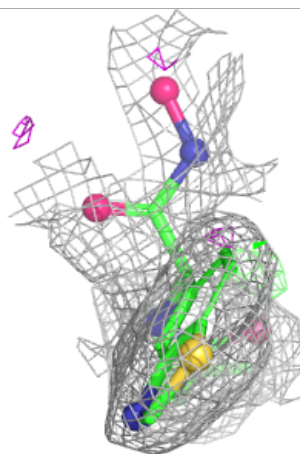
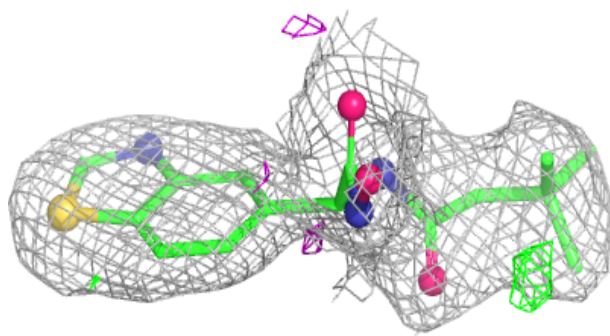
Electron density around A1CT4 F 707:

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



Electron density around A1CT4 H 705:

$2mF_o-DF_c$ (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.