



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:30 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 Full wwPDB X-ray Structure Validation 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

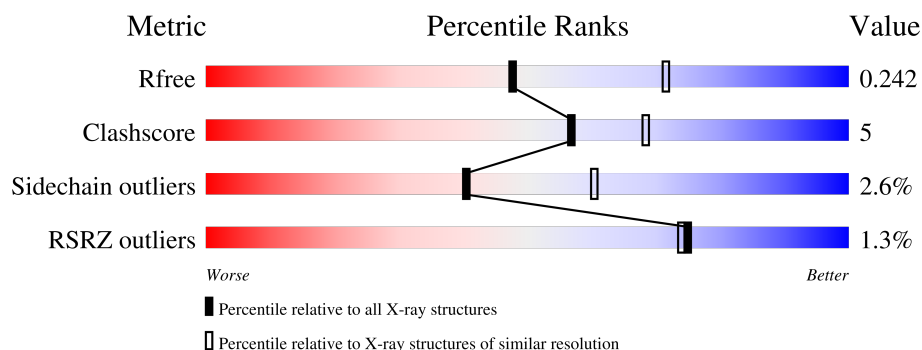
1 Overall quality at a glance

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.



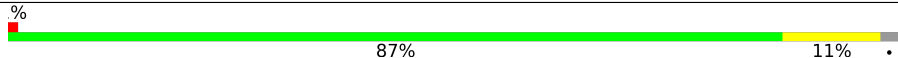
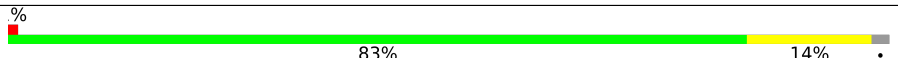
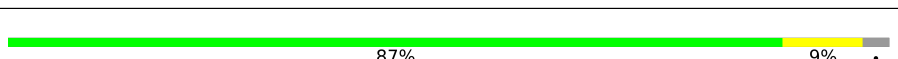
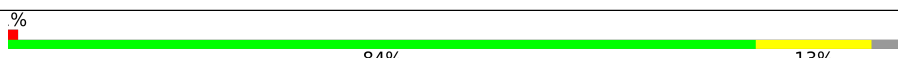
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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).

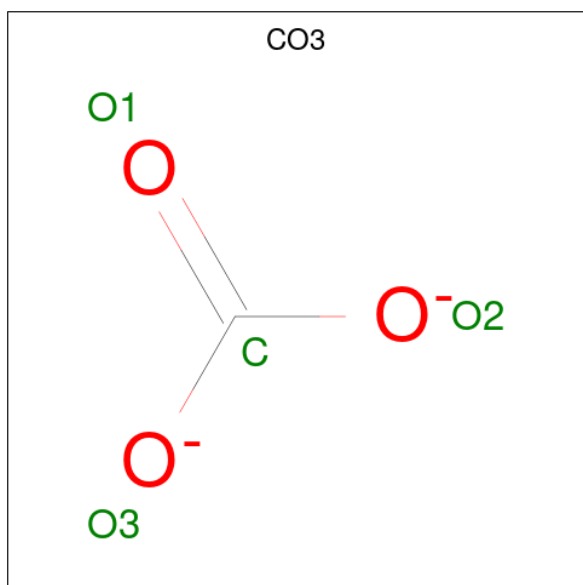
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0

Continued on next page...

Continued from previous page...

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).



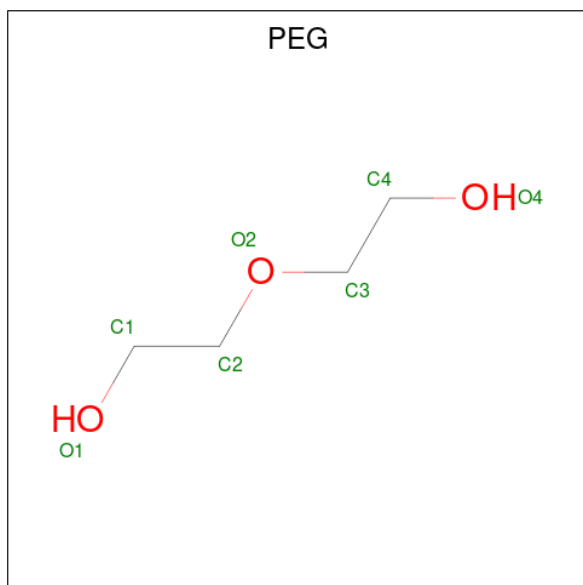
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

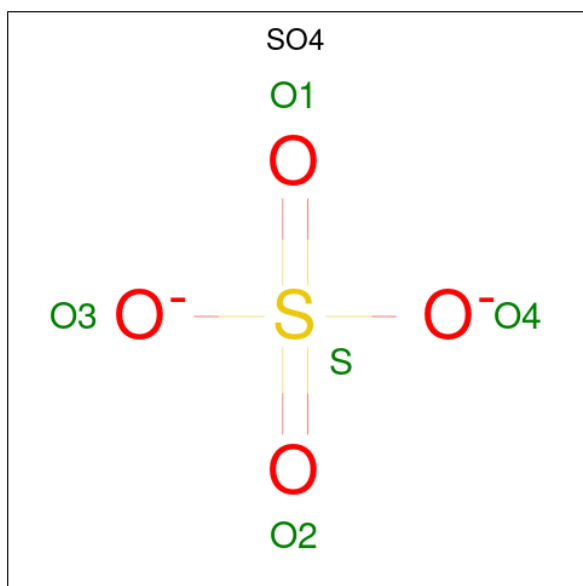
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

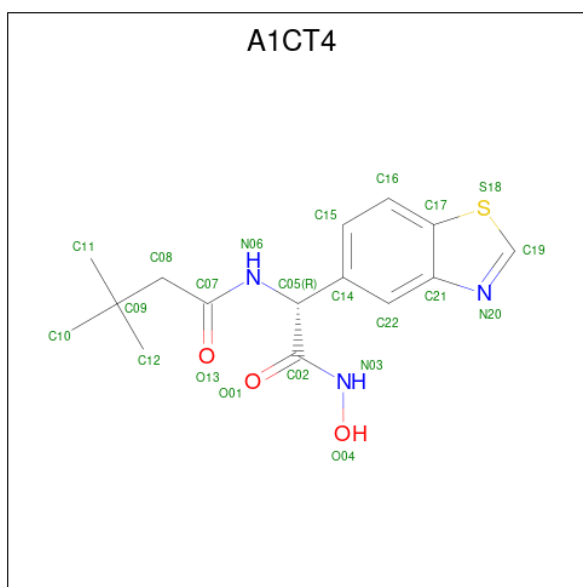
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total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

Continued on next page...

Continued from previous page...

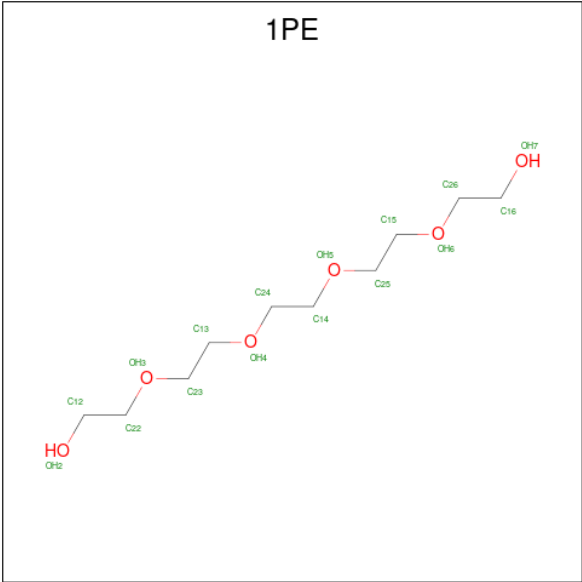
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	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: C₁₀H₂₂O₆).



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		

Continued on next page...

Continued from previous page...

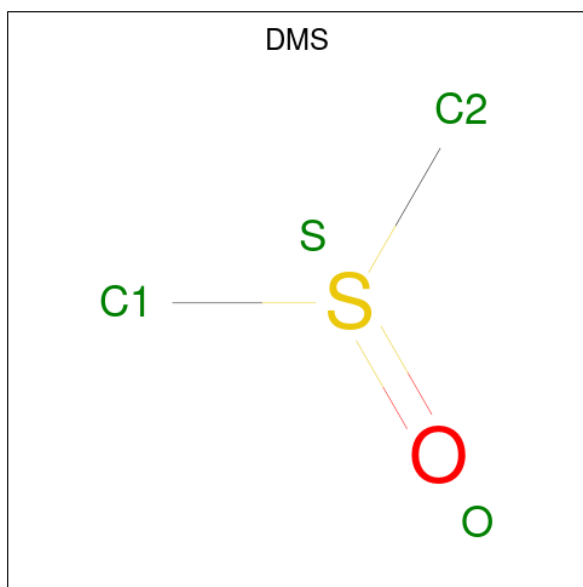
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			10	6	4		
7	F	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			8	5	3		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			6	4	2		
7	G	1	Total	C	O	0	0
			13	8	5		
7	I	1	Total	C	O	0	0
			13	8	5		
7	I	1	Total	C	O	0	0
			10	6	4		
7	I	1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

Continued on next page...

Continued from previous page...

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: C₂H₆OS).



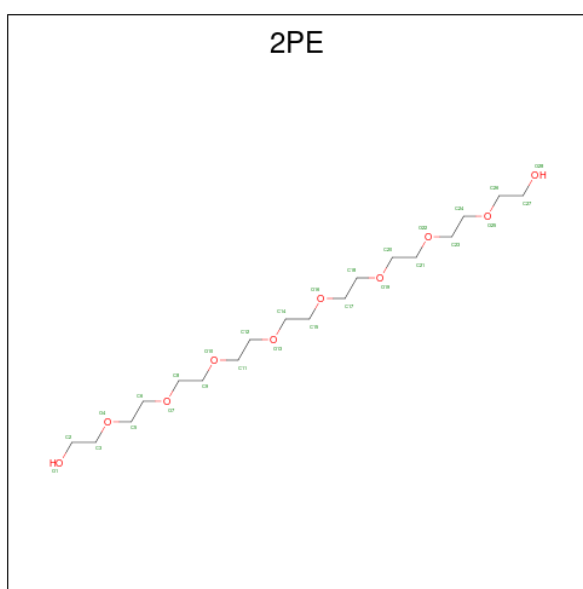
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	B	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	D	1	Total	C	O	S	0	0
			4	2	1	1		
8	G	1	Total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

Continued on next page...

Continued from previous page...

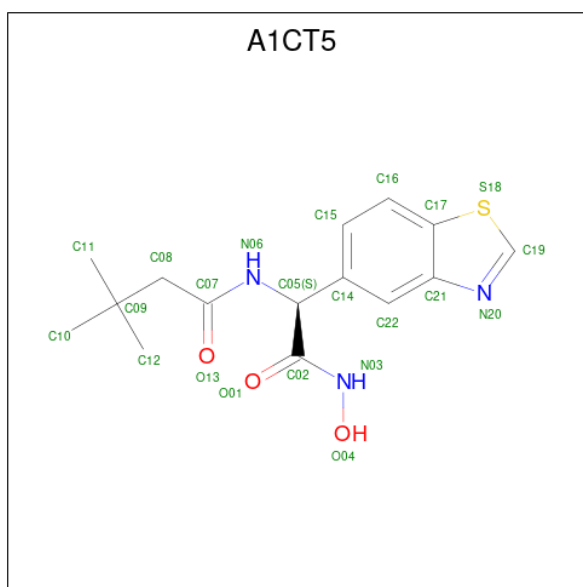
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	I	1	Total	C	O	S	0	0
			4	2	1	1		
8	J	1	Total	C	O	S	0	0
			4	2	1	1		
8	J	1	Total	C	O	S	0	0
			4	2	1	1		
8	L	1	Total	C	O	S	0	0
			4	2	1	1		

- 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		

Continued on next page...

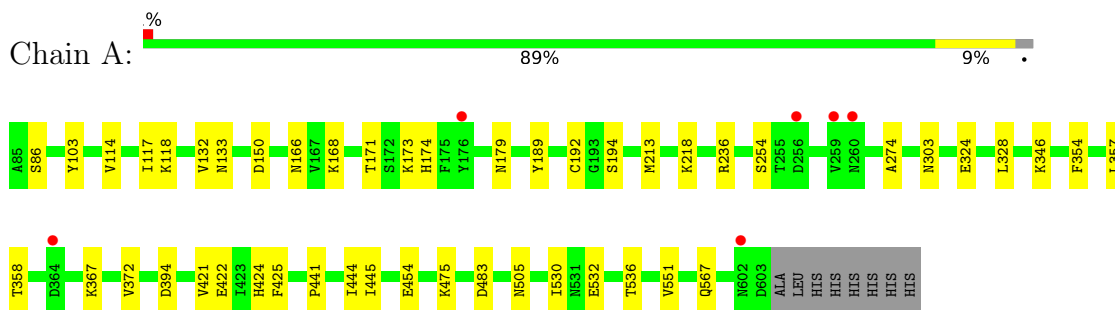
Continued from previous page...

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

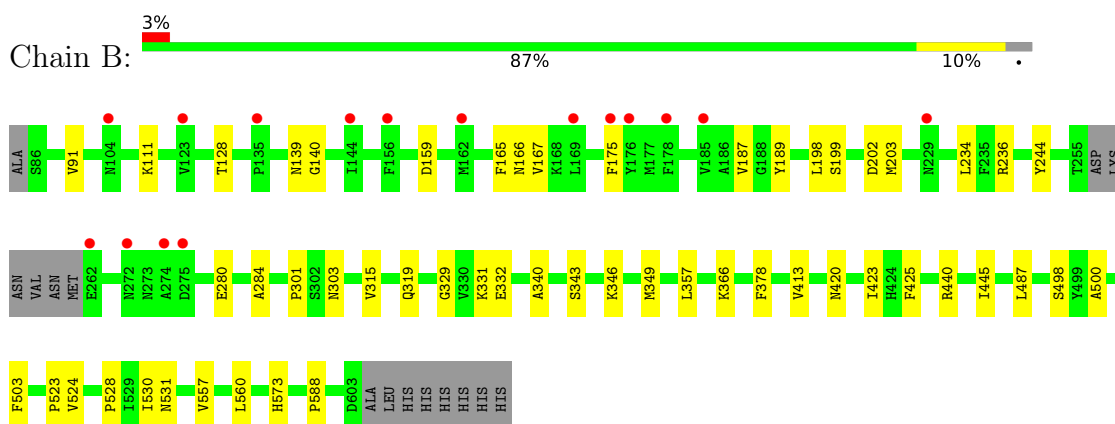
3 Residue-property plots

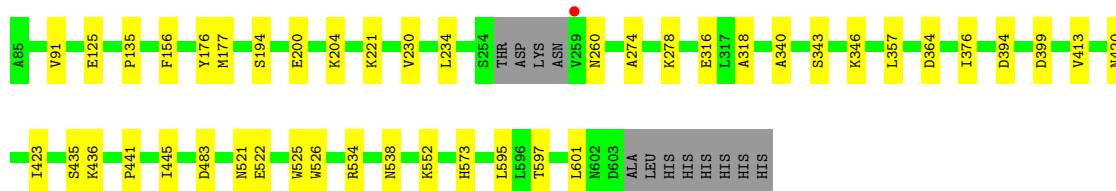
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



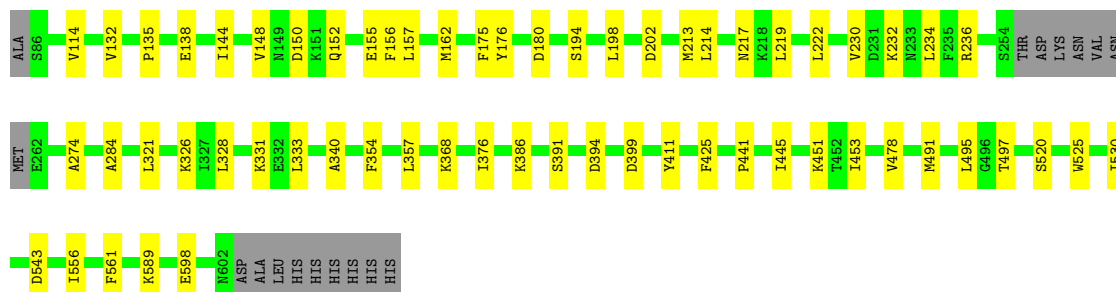
- Molecule 1: M17 leucyl aminopeptidase





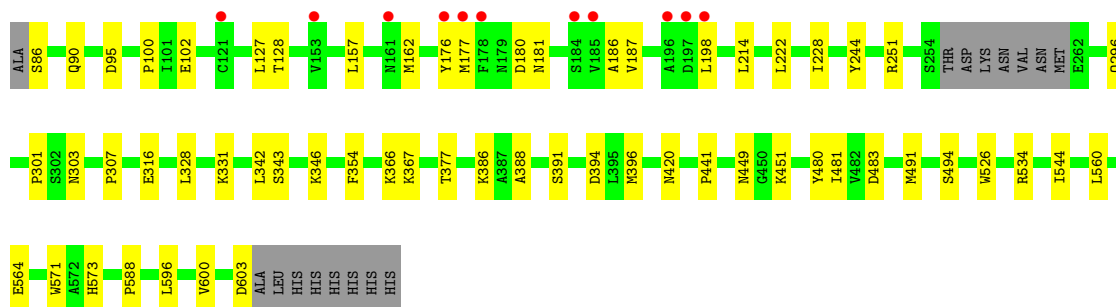
- Molecule 1: M17 leucyl aminopeptidase

Chain E: 85% 12%



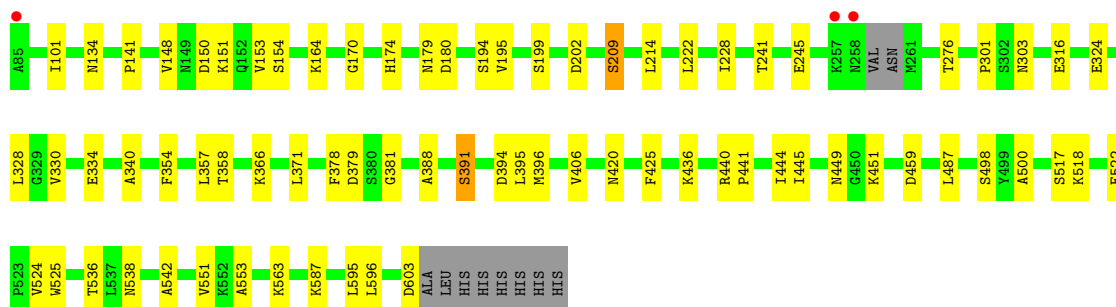
- Molecule 1: M17 leucyl aminopeptidase

Chain F: 86% 11%

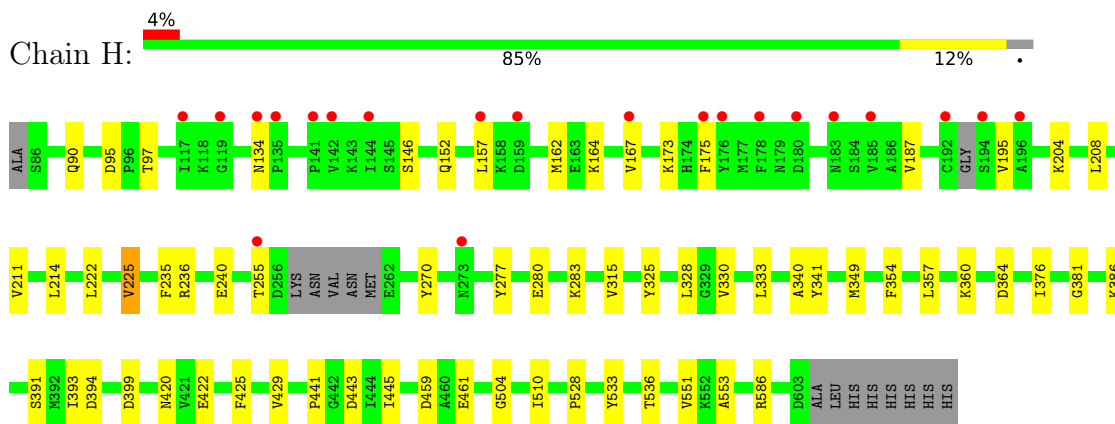


- Molecule 1: M17 leucyl aminopeptidase

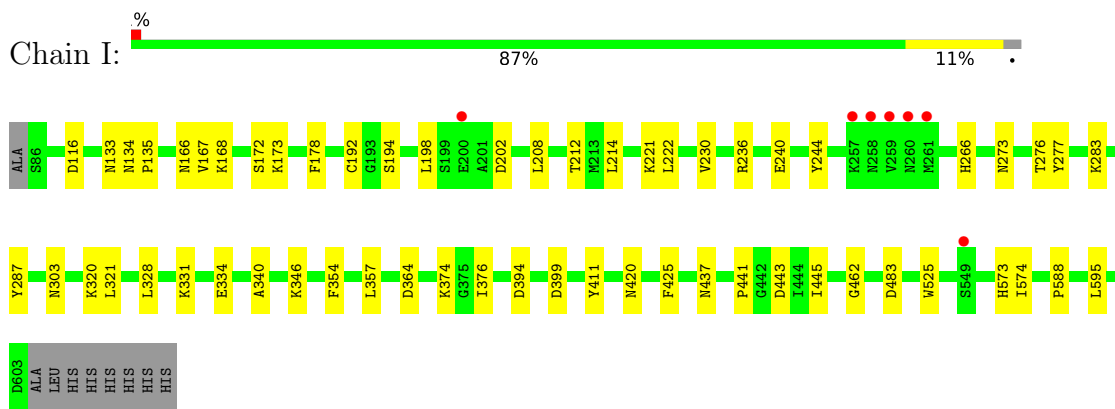
Chain G: 84% 14%



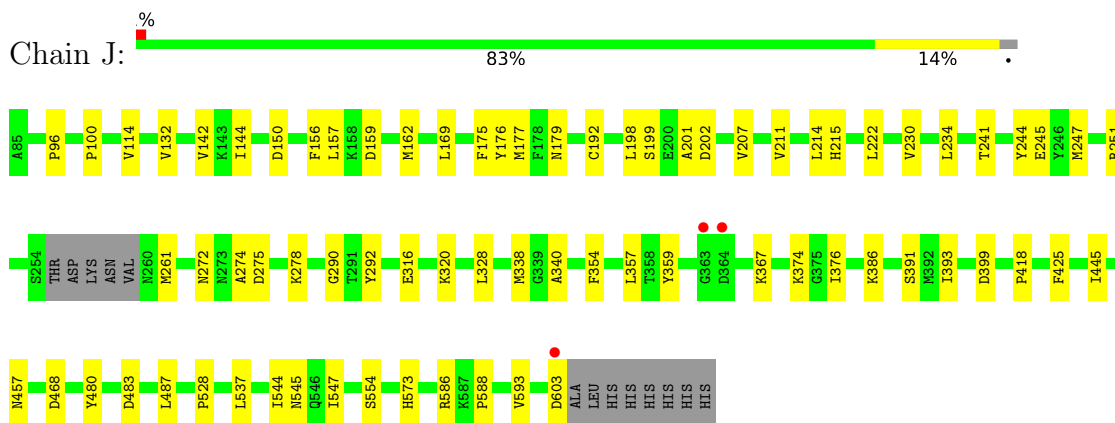
- Molecule 1: M17 leucyl aminopeptidase



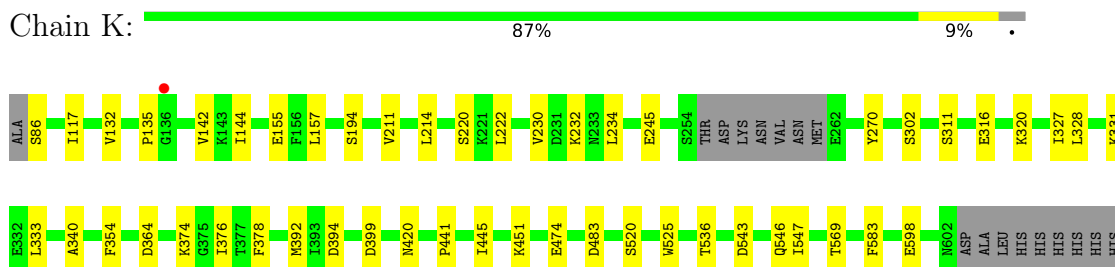
- Molecule 1: M17 leucyl aminopeptidase



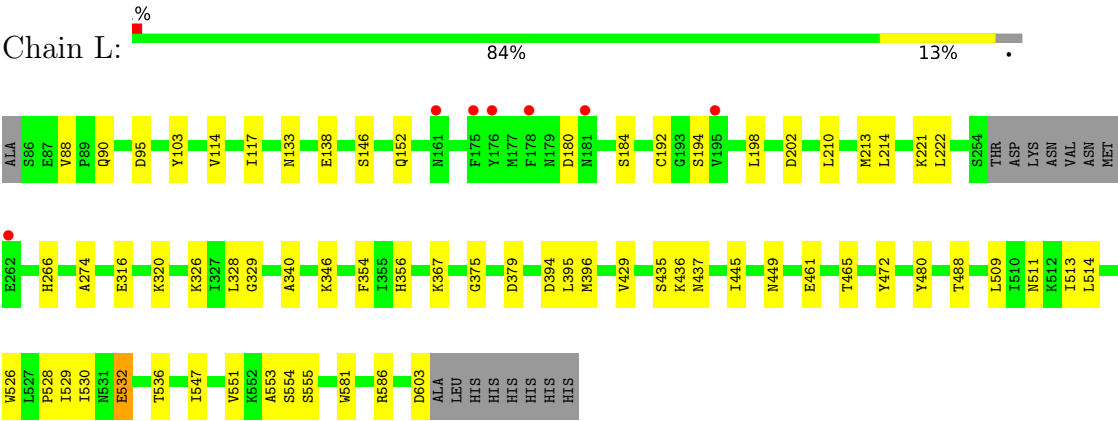
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



● Molecule 1: M17 leucyl aminopeptidase



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 [i](#)

5.1 Standard geometry [i](#)

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 [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	3994	0	3958	30	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

All (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
1:L:326:LYS:HE2	1:L:328:LEU:HD11	1.71	0.71
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.72	0.71
1:K:320:LYS:HB3	7:K:715:1PE:H152	1.72	0.70
1:K:132:VAL:HG21	1:K:142:VAL:HG13	1.74	0.70
1:F:128:THR:HB	1:F:187:VAL:HG12	1.74	0.69
1:F:316:GLU:HG3	7:F:706:1PE:H242	1.77	0.67
1:F:86:SER:N	11:F:803:HOH:O	2.28	0.65
1:H:360:LYS:HG3	1:H:422:GLU:HG3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.78	0.65
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.60	0.65
1:B:531:ASN:H	4:B:704:PEG:H21	1.62	0.64
1:K:316:GLU:HG3	7:K:714:1PE:H152	1.79	0.64
1:C:192:CYS:HB3	1:C:198:LEU:HD11	1.80	0.63
1:C:221:LYS:NZ	11:C:803:HOH:O	2.32	0.62
1:J:215:HIS:HA	1:J:261:MET:HG3	1.83	0.61
1:B:139:ASN:HB3	1:B:166:ASN:HB2	1.82	0.60
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.83	0.60
1:G:164:LYS:NZ	8:J:704:DMS:O	2.28	0.60
1:J:316:GLU:HG3	7:J:719:1PE:H141	1.82	0.60
1:L:581:TRP:HZ2	4:L:706:PEG:H22	1.66	0.60
1:J:386:LYS:HB3	1:J:391:SER:HB3	1.83	0.60
1:H:211:VAL:HA	1:H:214:LEU:HD12	1.84	0.60
1:D:204:LYS:NZ	11:D:811:HOH:O	2.35	0.59
1:D:376:ILE:HB	1:D:399:ASP:HB3	1.85	0.59
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.84	0.59
1:G:563:LYS:NZ	11:G:807:HOH:O	2.36	0.59
1:E:530:ILE:HD12	1:E:556:ILE:HD13	1.85	0.58
1:L:329:GLY:HA3	4:L:705:PEG:H31	1.85	0.58
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.86	0.58
1:H:164:LYS:NZ	1:L:184:SER:OG	2.36	0.58
1:I:483:ASP:OD1	1:I:573:HIS:ND1	2.34	0.58
1:C:331:LYS:HB2	8:C:706:DMS:H21	1.86	0.58
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.86	0.58
1:B:175:PHE:HD1	1:F:176:TYR:HB2	1.69	0.58
1:H:443:ASP:OD2	1:I:303:ASN:HB3	2.03	0.58
1:J:586:ARG:NH1	5:J:711:SO4:O2	2.37	0.57
1:K:392:MET:HE1	1:K:583:PHE:CE1	2.39	0.57
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.85	0.57
1:H:97:THR:HB	8:H:706:DMS:H13	1.87	0.57
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.87	0.57
1:H:214:LEU:HD21	1:H:222:LEU:HD22	1.86	0.57
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.86	0.57
1:C:386:LYS:HB3	1:C:391:SER:HB2	1.87	0.57
1:I:221:LYS:HG3	1:I:266:HIS:HB2	1.87	0.57
1:C:275:ASP:HA	1:C:278:LYS:HD2	1.85	0.57
1:F:483:ASP:OD2	1:F:573:HIS:HD2	1.87	0.57
1:G:487:LEU:O	10:G:705:A1CT5:N03	2.38	0.57
1:K:399:ASP:OD2	6:K:706:A1CT4:O04	2.22	0.56
1:F:180:ASP:C	1:F:181:ASN:HD22	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:483:ASP:OD1	1:J:573:HIS:ND1	2.37	0.56
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.88	0.56
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.88	0.56
1:J:386:LYS:HB2	1:J:393:ILE:HD12	1.88	0.55
1:A:194:SER:H	4:A:704:PEG:H21	1.70	0.55
1:C:395:LEU:HD21	1:C:581:TRP:CG	2.42	0.55
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.88	0.55
1:C:315:VAL:O	1:C:319:GLN:HG3	2.06	0.55
1:E:232:LYS:H	1:E:232:LYS:CD	2.19	0.55
1:H:586:ARG:NH1	5:H:711:SO4:O3	2.39	0.55
1:J:114:VAL:HG12	1:J:274:ALA:HB1	1.88	0.55
1:G:150:ASP:OD2	1:G:179:ASN:HB2	2.06	0.55
1:J:150:ASP:OD2	1:J:179:ASN:HB2	2.07	0.55
4:C:707:PEG:H21	1:D:552:LYS:HZ1	1.71	0.55
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.89	0.55
1:E:451:LYS:HE2	7:E:709:1PE:H132	1.88	0.55
1:H:90:GLN:HB3	1:H:95:ASP:HB2	1.89	0.55
1:C:395:LEU:HD11	1:C:581:TRP:CE2	2.42	0.54
1:C:282:GLU:HA	1:C:282:GLU:OE2	2.07	0.54
1:F:331:LYS:HD3	1:F:331:LYS:N	2.22	0.54
1:L:532:GLU:HB2	4:L:704:PEG:H32	1.89	0.54
1:B:440:ARG:NH1	11:B:804:HOH:O	2.35	0.54
1:I:236:ARG:NE	1:I:240:GLU:OE2	2.34	0.54
1:F:331:LYS:HD3	1:F:331:LYS:H	1.73	0.54
1:B:487:LEU:O	6:B:708:A1CT4:N03	2.41	0.54
1:C:386:LYS:HB2	1:C:393:ILE:HD12	1.89	0.54
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.90	0.54
1:J:338:MET:HE3	1:J:468:ASP:HB3	1.89	0.53
1:D:176:TYR:HB3	7:D:717:1PE:H261	1.91	0.53
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.91	0.53
3:L:703:CO3:O1	6:L:710:A1CT4:O04	2.27	0.53
1:G:199:SER:OG	1:G:202:ASP:OD2	2.24	0.53
1:C:526:TRP:HB3	4:D:706:PEG:H11	1.91	0.53
1:A:475:LYS:NZ	11:A:815:HOH:O	2.42	0.53
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.91	0.53
1:K:331:LYS:H	1:K:331:LYS:HD3	1.73	0.52
1:L:511:ASN:HA	1:L:514:LEU:HD12	1.91	0.52
1:B:236:ARG:HG3	1:B:284:ALA:HB2	1.90	0.52
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.90	0.52
1:L:395:LEU:HD21	4:L:706:PEG:H31	1.91	0.52
1:E:386:LYS:HB3	1:E:391:SER:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:364:ASP:O	1:H:420:ASN:HA	2.10	0.52
1:G:518:LYS:NZ	11:G:812:HOH:O	2.42	0.52
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.92	0.52
1:J:159:ASP:H	4:J:708:PEG:H32	1.75	0.52
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.92	0.51
1:K:364:ASP:O	1:K:420:ASN:HA	2.10	0.51
1:F:386:LYS:HE3	1:F:396:MET:HG3	1.93	0.51
1:H:386:LYS:HB2	1:H:393:ILE:HD12	1.92	0.51
1:F:451:LYS:NZ	11:F:802:HOH:O	2.43	0.51
1:A:86:SER:HA	4:A:706:PEG:H42	1.92	0.51
1:L:103:TYR:HB2	7:L:716:1PE:H161	1.92	0.51
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.93	0.51
1:G:500:ALA:HB3	1:G:524:VAL:HG22	1.93	0.51
1:I:320:LYS:HB3	7:I:716:1PE:H232	1.93	0.51
1:A:174:HIS:CE1	1:A:213:MET:HG2	2.46	0.51
1:A:150:ASP:OD2	1:A:179:ASN:HB2	2.10	0.50
1:L:210:LEU:HA	1:L:213:MET:HE2	1.93	0.50
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.94	0.50
4:I:710:PEG:H42	1:J:201:ALA:HB3	1.92	0.50
1:B:128:THR:HB	1:B:187:VAL:HG22	1.92	0.50
8:C:713:DMS:H13	1:E:176:TYR:HB3	1.94	0.50
1:D:316:GLU:OE2	7:D:704:1PE:H131	2.11	0.50
1:H:175:PHE:N	1:H:187:VAL:O	2.40	0.50
1:B:331:LYS:HB2	8:B:707:DMS:H13	1.93	0.50
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.94	0.50
1:H:504:GLY:HA3	1:H:510:ILE:HD11	1.92	0.50
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.93	0.50
1:D:230:VAL:HG23	1:D:234:LEU:HD23	1.93	0.49
1:D:534:ARG:NH1	1:D:538:ASN:OD1	2.42	0.49
1:G:151:LYS:N	1:G:180:ASP:OD2	2.43	0.49
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.93	0.49
1:K:230:VAL:HG23	1:K:234:LEU:HD23	1.94	0.49
1:J:272:ASN:ND2	5:J:716:SO4:O4	2.44	0.49
1:F:157:LEU:HD23	1:F:162:MET:HE2	1.94	0.49
1:G:440:ARG:NH2	11:G:806:HOH:O	2.35	0.49
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.93	0.49
1:F:90:GLN:NE2	1:F:95:ASP:O	2.46	0.49
1:H:376:ILE:HB	1:H:399:ASP:HB3	1.92	0.49
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.94	0.49
1:A:303:ASN:HB3	1:C:440:ARG:HH12	1.78	0.49
1:L:356:HIS:ND1	1:L:472:TYR:OH	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:LYS:HB3	1:E:478:VAL:HG12	1.94	0.49
1:K:474:GLU:OE2	1:K:569:THR:OG1	2.22	0.49
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.95	0.48
1:D:364:ASP:O	1:D:420:ASN:HA	2.13	0.48
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.95	0.48
1:G:381:GLY:HA2	1:G:459:ASP:OD1	2.12	0.48
1:I:320:LYS:NZ	11:I:820:HOH:O	2.46	0.48
1:C:311:SER:HB2	1:C:327:ILE:HD12	1.95	0.48
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.95	0.48
1:H:236:ARG:HB2	1:H:280:GLU:HG3	1.95	0.48
1:I:376:ILE:HB	1:I:399:ASP:HB3	1.94	0.48
1:L:214:LEU:HD11	1:L:222:LEU:HD22	1.95	0.48
1:L:536:THR:HG21	1:L:551:VAL:HG23	1.95	0.48
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.95	0.48
1:G:449:ASN:HD21	1:G:451:LYS:HD2	1.76	0.48
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.96	0.48
1:E:230:VAL:HG12	1:E:234:LEU:HD23	1.96	0.48
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.95	0.48
1:D:200:GLU:HG2	1:D:521:ASN:HB3	1.95	0.48
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.95	0.48
1:C:260:ASN:ND2	11:C:817:HOH:O	2.46	0.48
1:D:274:ALA:O	1:D:278:LYS:HG3	2.14	0.48
1:H:381:GLY:HA2	1:H:459:ASP:OD1	2.13	0.48
1:L:526:TRP:HE3	7:L:715:1PE:H152	1.77	0.48
1:A:530:ILE:HG23	4:A:707:PEG:H12	1.95	0.48
1:I:198:LEU:HD22	1:I:202:ASP:HB2	1.96	0.48
1:L:138:GLU:HA	1:L:194:SER:HB3	1.95	0.48
1:J:320:LYS:HB3	7:J:718:1PE:H161	1.95	0.48
1:J:367:LYS:HD3	1:J:480:TYR:CE2	2.49	0.48
1:L:90:GLN:HB3	1:L:95:ASP:HB2	1.95	0.47
1:C:226:PHE:HB2	1:C:271:ILE:HG13	1.95	0.47
1:G:371:LEU:HD22	1:G:596:LEU:HD22	1.96	0.47
1:G:316:GLU:HG3	7:G:716:1PE:H131	1.95	0.47
1:E:543:ASP:HB3	7:E:709:1PE:H231	1.96	0.47
1:J:211:VAL:HG21	1:J:245:GLU:HB2	1.96	0.47
1:B:91:VAL:HG23	1:B:349:MET:HE1	1.96	0.47
1:B:199:SER:OG	1:B:202:ASP:OD2	2.30	0.47
1:D:522:GLU:OE1	1:D:595:LEU:N	2.46	0.47
1:F:198:LEU:HD12	1:F:228:ILE:HD13	1.95	0.47
4:A:708:PEG:H21	1:F:526:TRP:HB3	1.96	0.47
1:B:175:PHE:HD2	1:B:187:VAL:HG12	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:PRO:O	1:J:251:ARG:NH1	2.42	0.47
1:J:230:VAL:HG13	1:J:234:LEU:HB3	1.95	0.47
1:L:117:ILE:HD11	1:L:146:SER:HB3	1.97	0.47
1:H:533:TYR:O	1:H:536:THR:OG1	2.32	0.47
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.97	0.47
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.97	0.47
3:L:703:CO3:O1	6:L:710:A1CT4:N03	2.48	0.47
1:D:483:ASP:OD2	1:D:573:HIS:HB2	2.15	0.46
1:E:331:LYS:H	1:E:331:LYS:HD2	1.80	0.46
1:E:520:SER:HB3	1:E:598:GLU:HG3	1.97	0.46
8:J:710:DMS:H11	4:J:717:PEG:H21	1.96	0.46
1:K:331:LYS:HD3	1:K:331:LYS:N	2.30	0.46
1:K:451:LYS:HZ2	7:K:716:1PE:H151	1.79	0.46
1:L:346:LYS:HB3	1:L:437:ASN:O	2.14	0.46
1:B:203:MET:HE3	1:B:234:LEU:HD11	1.96	0.46
1:J:537:LEU:HA	1:J:545:ASN:HB2	1.97	0.46
1:I:364:ASP:O	1:I:420:ASN:HA	2.15	0.46
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.96	0.46
3:B:703:CO3:O2	6:B:708:A1CT4:O04	2.33	0.46
1:C:254:SER:OG	1:C:255:THR:N	2.48	0.46
1:K:220:SER:OG	5:K:711:SO4:O1	2.31	0.46
1:K:451:LYS:NZ	7:K:716:1PE:H151	2.30	0.46
1:L:367:LYS:HE2	1:L:480:TYR:CE2	2.51	0.46
1:A:536:THR:HG21	1:A:551:VAL:HG23	1.97	0.46
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.98	0.46
1:C:298:ILE:HG23	1:C:398:PHE:HA	1.98	0.46
1:K:331:LYS:H	1:K:331:LYS:CD	2.29	0.46
1:L:530:ILE:HG23	4:L:704:PEG:H41	1.98	0.46
1:A:441:PRO:HD2	1:B:378:PHE:CZ	2.50	0.46
1:D:125:GLU:HG2	1:D:221:LYS:HD2	1.96	0.46
1:G:148:VAL:HG12	1:G:150:ASP:H	1.80	0.46
1:A:133:ASN:HB3	1:A:192:CYS:HB2	1.97	0.46
1:B:315:VAL:O	1:B:319:GLN:HG2	2.16	0.46
1:F:214:LEU:HD21	1:F:222:LEU:HD22	1.98	0.46
1:L:133:ASN:HB3	1:L:192:CYS:HB2	1.97	0.46
1:G:170:GLY:O	1:G:209:SER:OG	2.31	0.46
1:G:538:ASN:ND2	11:G:823:HOH:O	2.46	0.46
1:H:386:LYS:HB3	1:H:391:SER:HB2	1.97	0.46
1:J:96:PRO:HA	4:J:709:PEG:H41	1.97	0.46
1:J:244:TYR:OH	1:J:588:PRO:O	2.31	0.46
1:E:135:PRO:HA	1:E:194:SER:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.96	0.46
4:E:706:PEG:H11	4:E:706:PEG:H32	1.76	0.46
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.51	0.46
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.97	0.46
1:C:287:TYR:CD2	1:C:594:ARG:HG2	2.51	0.45
1:C:440:ARG:NH1	1:C:443:ASP:OD2	2.49	0.45
1:D:177:MET:N	7:D:717:1PE:H162	2.31	0.45
1:F:388:ALA:O	1:F:391:SER:OG	2.30	0.45
1:I:133:ASN:HB3	1:I:192:CYS:HB2	1.98	0.45
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.99	0.45
1:B:140:GLY:H	1:B:167:VAL:HG22	1.81	0.45
1:B:500:ALA:HB3	1:B:524:VAL:HG22	1.97	0.45
1:E:497:THR:O	1:E:589:LYS:NZ	2.49	0.45
1:K:135:PRO:HA	1:K:194:SER:O	2.16	0.45
1:E:217:ASN:HB3	1:E:219:LEU:HD21	1.97	0.45
1:G:245:GLU:OE1	1:G:587:LYS:NZ	2.44	0.45
1:I:283:LYS:HE2	1:I:287:TYR:CZ	2.52	0.45
1:I:574:ILE:HD13	1:I:595:LEU:HD21	1.98	0.45
1:G:148:VAL:HG11	1:G:153:VAL:HB	1.99	0.45
1:G:303:ASN:HB3	1:I:443:ASP:OD2	2.17	0.45
1:K:311:SER:HB2	1:K:327:ILE:HD12	1.98	0.45
1:A:367:LYS:HB3	1:A:421:VAL:HG23	1.99	0.45
1:A:567:GLN:OE1	4:A:709:PEG:H31	2.16	0.45
1:C:181:ASN:OD1	1:C:181:ASN:N	2.50	0.45
1:E:214:LEU:HD11	1:E:222:LEU:HD22	1.99	0.45
1:J:198:LEU:HD22	1:J:202:ASP:HB3	1.99	0.45
1:K:374:LYS:HE3	1:K:376:ILE:HG13	1.99	0.45
1:J:156:PHE:CG	1:J:177:MET:HE1	2.51	0.45
1:K:211:VAL:HG21	1:K:245:GLU:HB2	1.98	0.45
1:L:221:LYS:HE2	1:L:266:HIS:HB2	1.99	0.45
1:A:166:ASN:HD21	1:D:260:ASN:ND2	2.15	0.44
1:B:203:MET:HE3	1:B:234:LEU:CD1	2.48	0.44
1:H:236:ARG:HD2	1:H:283:LYS:HG2	1.99	0.44
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.99	0.44
1:I:273:ASN:O	1:I:276:THR:HG22	2.17	0.44
1:J:230:VAL:HG22	1:J:234:LEU:HD23	1.99	0.44
1:C:517:SER:OG	1:C:522:GLU:O	2.31	0.44
1:C:161:ASN:HB3	8:C:713:DMS:H21	1.99	0.44
1:D:343:SER:HA	1:D:346:LYS:HD3	2.00	0.44
1:J:457:ASN:HB2	1:J:547:ILE:HD13	1.99	0.44
1:K:117:ILE:HG12	1:K:270:TYR:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:103:TYR:HB3	7:L:713:1PE:H151	1.98	0.44
1:B:159:ASP:OD1	1:B:159:ASP:N	2.50	0.44
1:C:287:TYR:OH	1:C:598:GLU:OE2	2.35	0.44
1:J:359:TYR:OH	1:J:418:PRO:O	2.24	0.44
1:H:134:ASN:H	1:H:167:VAL:HG21	1.83	0.44
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.52	0.44
1:E:148:VAL:HG12	1:E:150:ASP:H	1.83	0.44
1:J:367:LYS:HD3	1:J:480:TYR:HE2	1.82	0.44
1:B:343:SER:HA	1:B:346:LYS:HD3	2.00	0.44
1:E:357:LEU:HB2	1:E:425:PHE:HB2	2.00	0.44
1:J:275:ASP:HA	1:J:278:LYS:HD2	1.99	0.44
1:C:90:GLN:NE2	1:C:95:ASP:O	2.44	0.44
1:C:174:HIS:HB3	1:E:175:PHE:CD2	2.53	0.44
1:D:135:PRO:HA	1:D:194:SER:O	2.17	0.44
1:F:244:TYR:OH	1:F:588:PRO:O	2.36	0.44
1:H:376:ILE:HG13	1:H:461:GLU:OE2	2.18	0.43
1:I:244:TYR:OH	1:I:588:PRO:O	2.36	0.43
1:I:374:LYS:HZ2	1:I:462:GLY:HA3	1.82	0.43
1:D:526:TRP:H	4:D:706:PEG:H42	1.82	0.43
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.82	0.43
1:L:509:LEU:O	1:L:513:ILE:HG12	2.18	0.43
1:A:444:ILE:HB	1:B:301:PRO:HG2	2.00	0.43
1:E:376:ILE:HB	1:E:399:ASP:HB3	2.00	0.43
3:E:703:CO3:O3	6:E:708:A1CT4:N03	2.51	0.43
1:F:366:LYS:HG3	1:F:420:ASN:HB3	2.00	0.43
1:F:483:ASP:OD2	1:F:573:HIS:CD2	2.70	0.43
1:F:534:ARG:HB2	1:F:560:LEU:HD22	1.99	0.43
1:G:150:ASP:O	1:G:154:SER:OG	2.28	0.43
1:I:134:ASN:HB2	1:I:167:VAL:HG21	1.99	0.43
4:I:710:PEG:H31	1:J:199:SER:OG	2.19	0.43
1:B:366:LYS:HG3	1:B:420:ASN:HB3	1.99	0.43
1:E:491:MET:HE1	1:E:495:LEU:HD12	2.00	0.43
1:H:236:ARG:NE	1:H:240:GLU:OE2	2.49	0.43
1:J:376:ILE:HB	1:J:399:ASP:HB3	2.00	0.43
8:J:710:DMS:H21	4:J:717:PEG:H22	2.01	0.43
1:A:103:TYR:CD1	7:A:717:1PE:H251	2.54	0.43
1:C:114:VAL:HG12	1:C:274:ALA:HB1	2.01	0.43
1:K:543:ASP:HB3	7:K:716:1PE:H231	2.00	0.43
1:L:221:LYS:NZ	11:L:819:HOH:O	2.52	0.43
1:D:156:PHE:CG	1:D:177:MET:HE1	2.53	0.43
1:D:318:ALA:HB2	1:D:357:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:ASP:O	1:G:396:MET:HG3	2.19	0.43
1:J:156:PHE:O	1:J:162:MET:HE3	2.19	0.43
1:B:236:ARG:HB2	1:B:280:GLU:HB3	2.00	0.43
1:F:367:LYS:HD3	1:F:367:LYS:HA	1.86	0.43
1:L:198:LEU:HD22	1:L:202:ASP:HB3	2.00	0.43
1:E:156:PHE:O	1:E:162:MET:HE3	2.18	0.42
1:I:230:VAL:O	1:I:277:TYR:OH	2.27	0.42
1:I:525:TRP:CZ3	1:J:528:PRO:HB3	2.54	0.42
1:J:374:LYS:HZ2	1:J:487:LEU:HD12	1.84	0.42
1:B:503:PHE:O	1:B:573:HIS:N	2.46	0.42
1:D:435:SER:OG	1:D:436:LYS:N	2.52	0.42
1:J:156:PHE:CD2	1:J:177:MET:HE1	2.53	0.42
1:B:165:PHE:HB3	1:B:189:TYR:OH	2.19	0.42
1:C:500:ALA:HB3	1:C:524:VAL:HG22	2.02	0.42
1:E:326:LYS:HE2	1:E:326:LYS:HB3	1.73	0.42
1:F:596:LEU:HD23	1:F:596:LEU:HA	1.87	0.42
1:H:341:TYR:OH	1:H:429:VAL:O	2.34	0.42
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.01	0.42
1:J:328:LEU:HB2	1:J:354:PHE:HB3	2.01	0.42
1:A:372:VAL:O	1:A:483:ASP:HA	2.18	0.42
1:B:198:LEU:HD22	1:B:203:MET:CE	2.49	0.42
1:D:91:VAL:HB	1:F:346:LYS:HE3	2.02	0.42
1:F:481:ILE:O	1:F:571:TRP:HA	2.19	0.42
1:G:330:VAL:O	1:G:334:GLU:HG3	2.18	0.42
1:G:340:ALA:HA	1:G:445:ILE:HD12	2.02	0.42
1:H:157:LEU:HA	1:H:162:MET:HE3	2.02	0.42
1:H:204:LYS:O	1:H:208:LEU:HG	2.20	0.42
1:A:346:LYS:HB3	1:A:346:LYS:HE2	1.83	0.42
1:L:152:GLN:HG2	1:L:180:ASP:OD1	2.19	0.42
1:C:346:LYS:HB3	1:C:437:ASN:O	2.19	0.42
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.55	0.42
1:E:213:MET:HE3	1:E:213:MET:HB2	1.92	0.42
1:F:307:PRO:HD3	1:F:377:THR:OG1	2.20	0.42
1:G:436:LYS:HD3	1:H:349:MET:HB3	2.02	0.42
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.54	0.42
1:J:144:ILE:HG21	1:J:157:LEU:HD13	2.02	0.42
1:K:331:LYS:NZ	11:K:2718:HOH:O	2.39	0.42
1:K:333:LEU:HD21	1:K:354:PHE:HB2	2.01	0.42
1:G:366:LYS:HG3	1:G:420:ASN:HB3	2.01	0.42
1:H:236:ARG:HB2	1:H:280:GLU:CG	2.50	0.42
1:H:528:PRO:HB3	1:K:525:TRP:CZ3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:SER:OG	1:K:378:PHE:HB2	2.20	0.42
4:B:705:PEG:H12	4:B:705:PEG:H32	1.85	0.42
1:F:214:LEU:HD11	1:F:222:LEU:HD22	2.00	0.42
1:G:301:PRO:HB2	1:G:303:ASN:OD1	2.20	0.42
1:G:444:ILE:HD13	1:G:542:ALA:HB2	2.01	0.42
1:I:116:ASP:O	11:I:801:HOH:O	2.21	0.42
1:K:132:VAL:HG11	1:K:144:ILE:HD13	2.00	0.42
1:B:498:SER:O	1:B:523:PRO:HG2	2.20	0.42
1:C:173:LYS:HA	1:C:173:LYS:HD3	1.93	0.42
1:G:536:THR:HG21	1:G:551:VAL:HG23	2.01	0.42
1:H:225:VAL:HG13	1:H:270:TYR:HB2	2.02	0.42
1:K:376:ILE:HB	1:K:399:ASP:HB3	2.02	0.42
1:B:487:LEU:HD12	1:B:487:LEU:HA	1.90	0.42
1:C:150:ASP:OD2	1:C:179:ASN:HB2	2.19	0.42
1:D:413:VAL:HG11	1:D:423:ILE:HD13	2.02	0.42
1:F:100:PRO:O	1:F:251:ARG:HD2	2.20	0.42
1:L:461:GLU:O	1:L:465:THR:HG23	2.20	0.42
1:A:173:LYS:HB2	1:A:189:TYR:CE1	2.55	0.41
1:B:530:ILE:HG23	4:B:704:PEG:H12	2.01	0.41
1:H:551:VAL:HG12	1:H:553:ALA:H	1.84	0.41
1:L:435:SER:OG	1:L:436:LYS:N	2.53	0.41
1:A:454:GLU:OE2	11:A:801:HOH:O	2.21	0.41
1:A:505:ASN:ND2	11:A:818:HOH:O	2.43	0.41
1:F:331:LYS:H	1:F:331:LYS:CD	2.32	0.41
1:F:449:ASN:HD21	1:F:451:LYS:HD2	1.84	0.41
1:K:520:SER:HB3	1:K:598:GLU:HG3	2.02	0.41
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.01	0.41
1:B:557:VAL:HA	1:B:560:LEU:HD12	2.02	0.41
1:E:152:GLN:HG2	1:E:180:ASP:OD1	2.20	0.41
1:F:301:PRO:HB2	1:F:303:ASN:OD1	2.20	0.41
1:I:208:LEU:O	1:I:212:THR:HG23	2.20	0.41
7:L:715:1PE:H251	7:L:715:1PE:H241	1.71	0.41
1:B:413:VAL:HG11	1:B:423:ILE:HD13	2.01	0.41
1:G:134:ASN:ND2	1:G:141:PRO:HD2	2.36	0.41
1:G:378:PHE:CZ	1:I:441:PRO:HD2	2.55	0.41
1:H:235:PHE:CE2	1:H:277:TYR:HB3	2.55	0.41
1:L:379:ASP:O	1:L:396:MET:HG3	2.21	0.41
1:L:551:VAL:HG12	1:L:553:ALA:H	1.85	0.41
1:A:324:GLU:HB2	1:A:358:THR:HB	2.02	0.41
1:B:111:LYS:HA	1:B:111:LYS:HD3	1.86	0.41
1:D:526:TRP:HB3	4:D:706:PEG:H22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:GLU:HG2	1:F:296:GLN:OE1	2.19	0.41
1:F:343:SER:HA	1:F:346:LYS:HD3	2.02	0.41
1:G:395:LEU:HD12	1:G:395:LEU:HA	1.94	0.41
1:L:320:LYS:HZ2	1:L:320:LYS:HG2	1.78	0.41
1:L:375:GLY:O	1:L:429:VAL:HA	2.20	0.41
1:B:329:GLY:H	1:B:332:GLU:CD	2.28	0.41
1:E:333:LEU:HD21	1:E:354:PHE:HB2	2.03	0.41
1:H:333:LEU:HD21	1:H:354:PHE:HB2	2.03	0.41
1:L:449:ASN:O	7:L:714:1PE:H141	2.21	0.41
1:A:303:ASN:HB3	1:C:443:ASP:OD2	2.21	0.41
1:C:451:LYS:NZ	4:C:709:PEG:H11	2.36	0.41
1:E:138:GLU:HA	1:E:194:SER:OG	2.20	0.41
1:E:453:ILE:HD13	1:E:561:PHE:HZ	1.85	0.41
1:F:177:MET:HE2	1:F:177:MET:HB3	1.86	0.41
1:G:324:GLU:HB2	1:G:358:THR:HB	2.03	0.41
1:G:551:VAL:HG12	1:G:553:ALA:H	1.86	0.41
1:H:315:VAL:HG22	1:H:325:TYR:CD1	2.54	0.41
1:J:247:MET:HG3	1:J:292:TYR:CZ	2.56	0.41
1:K:546:GLN:HG2	1:K:547:ILE:HG23	2.03	0.41
1:L:488:THR:HG21	1:L:555:SER:HA	2.02	0.41
5:B:711:SO4:O3	1:C:436:LYS:HG2	2.21	0.41
1:F:386:LYS:HB3	1:F:391:SER:HB2	2.03	0.41
1:I:331:LYS:HD2	1:I:334:GLU:OE1	2.21	0.41
1:L:316:GLU:CD	7:L:716:1PE:H141	2.46	0.41
1:A:532:GLU:N	4:A:707:PEG:O1	2.53	0.41
1:J:169:LEU:HD12	1:J:192:CYS:HA	2.03	0.41
1:A:236:ARG:NH2	11:A:838:HOH:O	2.54	0.41
1:E:236:ARG:HG3	1:E:284:ALA:HB2	2.03	0.41
1:G:517:SER:OG	1:G:522:GLU:O	2.32	0.41
1:J:340:ALA:HA	1:J:445:ILE:HD12	2.03	0.41
1:A:422:GLU:OE2	1:A:424:HIS:NE2	2.54	0.40
1:E:132:VAL:HG21	1:E:144:ILE:HD13	2.02	0.40
1:G:388:ALA:O	1:G:391:SER:OG	2.30	0.40
1:I:331:LYS:HD2	1:I:331:LYS:HA	1.85	0.40
1:K:232:LYS:HB3	1:K:232:LYS:HE3	1.79	0.40
1:A:168:LYS:HD3	1:D:260:ASN:HD21	1.86	0.40
1:B:303:ASN:OD1	1:B:303:ASN:N	2.54	0.40
1:I:172:SER:O	1:I:173:LYS:HD2	2.22	0.40
1:J:207:VAL:HG11	1:J:241:THR:HG22	2.02	0.40
1:F:127:LEU:HA	1:F:186:ALA:O	2.21	0.40
1:F:544:ILE:HD12	1:F:564:GLU:HG3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:LYS:HB3	1:I:437:ASN:O	2.21	0.40
1:J:176:TYR:HB3	8:J:704:DMS:H12	2.04	0.40
1:E:441:PRO:HB2	1:F:394:ASP:HA	2.04	0.40
1:F:367:LYS:HE2	1:F:480:TYR:CE2	2.56	0.40
1:F:491:MET:HA	1:F:494:SER:OG	2.21	0.40
1:B:244:TYR:OH	1:B:588:PRO:O	2.36	0.40
1:D:597:THR:O	1:D:601:LEU:HG	2.22	0.40
1:F:342:LEU:O	1:F:346:LYS:HG3	2.21	0.40
1:I:135:PRO:HA	1:I:194:SER:O	2.22	0.40
1:I:166:ASN:OD1	1:I:168:LYS:HB2	2.22	0.40
1:J:290:GLY:C	1:J:593:VAL:HG11	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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	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

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	118	LYS
1	A	132	VAL
1	A	171	THR
1	A	218	LYS
1	A	254	SER
1	A	445	ILE
1	F	600	VAL
1	F	603	ASP
1	G	101	ILE
1	G	194	SER
1	G	195	VAL
1	G	209	SER
1	G	228	ILE
1	G	241	THR
1	G	276	THR
1	G	391	SER
1	G	406	VAL
1	G	498	SER
1	G	595	LEU
1	G	603	ASP
1	H	146	SER
1	H	152	GLN
1	H	173	LYS
1	H	195	VAL
1	H	225	VAL
1	H	255	THR
1	H	330	VAL
1	J	544	ILE
1	J	554	SER
1	J	603	ASP
1	K	86	SER
1	K	394	ASP
1	K	483	ASP
1	K	536	THR
1	L	88	VAL
1	L	529	ILE
1	L	532	GLU
1	L	547	ILE
1	L	554	SER
1	L	603	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	573	HIS
1	G	104	ASN
1	G	437	ASN
1	G	567	GLN
1	H	174	HIS
1	H	322	ASN
1	J	568	ASN
1	K	531	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-
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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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
6	I	708	A1CT4	C07-N06	6.94	1.48	1.34
6	D	707	A1CT4	C07-N06	6.94	1.48	1.34
6	J	707	A1CT4	C07-N06	6.94	1.48	1.34
6	F	707	A1CT4	C07-N06	6.91	1.48	1.34
6	H	705	A1CT4	C07-N06	6.88	1.48	1.34
6	C	710	A1CT4	C07-N06	6.88	1.48	1.34
6	B	708	A1CT4	C07-N06	6.85	1.48	1.34
6	H	705	A1CT4	C19-N20	6.50	1.38	1.29
6	I	708	A1CT4	C19-N20	6.47	1.38	1.29
6	C	710	A1CT4	C19-N20	6.47	1.38	1.29
6	D	707	A1CT4	C19-N20	6.46	1.38	1.29
6	E	708	A1CT4	C19-N20	6.45	1.38	1.29
6	A	710	A1CT4	C19-N20	6.45	1.38	1.29
6	J	707	A1CT4	C19-N20	6.44	1.38	1.29
6	F	707	A1CT4	C19-N20	6.44	1.38	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	708	A1CT4	C19-N20	6.40	1.38	1.29
6	L	710	A1CT4	C19-N20	6.38	1.38	1.29
6	K	706	A1CT4	C19-N20	6.35	1.38	1.29
10	G	705	A1CT5	C19-N20	6.26	1.38	1.29
10	G	705	A1CT5	C19-S18	-5.12	1.66	1.73
6	A	710	A1CT4	C19-S18	-5.12	1.66	1.73
6	L	710	A1CT4	C19-S18	-5.11	1.66	1.73
6	B	708	A1CT4	C19-S18	-5.09	1.66	1.73
6	J	707	A1CT4	C19-S18	-5.08	1.66	1.73
6	E	708	A1CT4	C19-S18	-5.08	1.66	1.73
6	F	707	A1CT4	C19-S18	-5.08	1.66	1.73
6	H	705	A1CT4	C19-S18	-5.08	1.66	1.73
6	I	708	A1CT4	C19-S18	-5.07	1.66	1.73
6	K	706	A1CT4	C19-S18	-5.07	1.66	1.73
6	D	707	A1CT4	C19-S18	-5.06	1.66	1.73
6	C	710	A1CT4	C19-S18	-5.04	1.66	1.73
6	A	710	A1CT4	C14-C05	2.90	1.57	1.52
6	C	710	A1CT4	C14-C05	2.84	1.57	1.52
6	H	705	A1CT4	C14-C05	2.83	1.57	1.52
6	B	708	A1CT4	C14-C05	2.81	1.57	1.52
6	D	707	A1CT4	C14-C05	2.81	1.57	1.52
6	C	710	A1CT4	C21-N20	2.76	1.44	1.39
6	E	708	A1CT4	C21-N20	2.75	1.44	1.39
6	H	705	A1CT4	C21-N20	2.73	1.44	1.39
10	G	705	A1CT5	C22-C14	-2.73	1.35	1.39
6	J	707	A1CT4	C21-N20	2.73	1.44	1.39
6	I	708	A1CT4	C21-N20	2.73	1.44	1.39
6	B	708	A1CT4	C21-N20	2.72	1.44	1.39
6	F	707	A1CT4	C21-N20	2.72	1.44	1.39
6	K	706	A1CT4	C22-C14	-2.71	1.35	1.39
6	D	707	A1CT4	C21-N20	2.71	1.44	1.39
6	L	710	A1CT4	C21-N20	2.71	1.44	1.39
6	A	710	A1CT4	C21-N20	2.70	1.44	1.39
6	F	707	A1CT4	C14-C05	2.69	1.57	1.52
6	J	707	A1CT4	C14-C05	2.68	1.57	1.52
6	K	706	A1CT4	C21-N20	2.68	1.44	1.39
10	G	705	A1CT5	C21-N20	2.65	1.44	1.39
6	K	706	A1CT4	O01-C02	-2.64	1.18	1.23
6	E	708	A1CT4	C14-C05	2.63	1.56	1.52
6	L	710	A1CT4	O01-C02	-2.59	1.18	1.23
6	L	710	A1CT4	C14-C05	2.59	1.56	1.52
6	L	710	A1CT4	C22-C14	-2.58	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	708	A1CT4	C14-C05	2.56	1.56	1.52
6	E	708	A1CT4	C22-C14	-2.55	1.35	1.39
6	F	707	A1CT4	C22-C14	-2.53	1.35	1.39
6	J	707	A1CT4	C22-C14	-2.53	1.35	1.39
6	B	708	A1CT4	C22-C14	-2.52	1.35	1.39
10	G	705	A1CT5	C14-C05	2.51	1.56	1.52
6	E	708	A1CT4	O01-C02	-2.50	1.18	1.23
6	K	706	A1CT4	C14-C05	2.50	1.56	1.52
6	A	710	A1CT4	C22-C14	-2.50	1.35	1.39
6	I	708	A1CT4	O01-C02	-2.49	1.18	1.23
6	I	708	A1CT4	C22-C14	-2.49	1.35	1.39
6	D	707	A1CT4	C22-C14	-2.49	1.35	1.39
6	C	710	A1CT4	C22-C14	-2.48	1.35	1.39
6	F	707	A1CT4	C17-S18	-2.48	1.67	1.73
6	C	710	A1CT4	O01-C02	-2.48	1.18	1.23
6	D	707	A1CT4	O01-C02	-2.48	1.18	1.23
6	J	707	A1CT4	O01-C02	-2.47	1.18	1.23
6	A	710	A1CT4	O01-C02	-2.47	1.18	1.23
6	H	705	A1CT4	C22-C14	-2.45	1.35	1.39
6	F	707	A1CT4	O01-C02	-2.44	1.18	1.23
6	H	705	A1CT4	O01-C02	-2.44	1.18	1.23
6	B	708	A1CT4	O01-C02	-2.43	1.18	1.23
6	H	705	A1CT4	C22-C21	2.43	1.43	1.40
6	I	708	A1CT4	C17-S18	-2.42	1.67	1.73
10	G	705	A1CT5	C17-S18	-2.42	1.67	1.73
10	G	705	A1CT5	O01-C02	-2.41	1.18	1.23
6	D	707	A1CT4	C22-C21	2.41	1.43	1.40
6	I	708	A1CT4	C22-C21	2.40	1.43	1.40
6	L	710	A1CT4	C17-S18	-2.39	1.67	1.73
6	D	707	A1CT4	C17-S18	-2.38	1.67	1.73
6	E	708	A1CT4	C17-S18	-2.38	1.67	1.73
6	C	710	A1CT4	C17-S18	-2.37	1.67	1.73
6	H	705	A1CT4	C17-S18	-2.37	1.67	1.73
6	J	707	A1CT4	C17-S18	-2.37	1.67	1.73
6	B	708	A1CT4	C17-S18	-2.36	1.67	1.73
6	K	706	A1CT4	C17-S18	-2.36	1.67	1.73
6	A	710	A1CT4	C22-C21	2.34	1.43	1.40
6	E	708	A1CT4	C22-C21	2.34	1.43	1.40
6	A	710	A1CT4	C17-S18	-2.34	1.67	1.73
6	L	710	A1CT4	O04-N03	2.32	1.45	1.40
6	D	707	A1CT4	O04-N03	2.32	1.45	1.40
6	J	707	A1CT4	C22-C21	2.31	1.43	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	710	A1CT4	O04-N03	2.31	1.45	1.40
10	G	705	A1CT5	O04-N03	2.31	1.45	1.40
6	J	707	A1CT4	O04-N03	2.29	1.45	1.40
6	F	707	A1CT4	C22-C21	2.29	1.43	1.40
6	E	708	A1CT4	O04-N03	2.28	1.45	1.40
6	C	710	A1CT4	C22-C21	2.28	1.43	1.40
6	I	708	A1CT4	O04-N03	2.27	1.45	1.40
6	B	708	A1CT4	O04-N03	2.27	1.45	1.40
6	A	710	A1CT4	O04-N03	2.27	1.45	1.40
6	H	705	A1CT4	O04-N03	2.27	1.45	1.40
6	B	708	A1CT4	C22-C21	2.25	1.43	1.40
6	F	707	A1CT4	O04-N03	2.25	1.45	1.40
6	K	706	A1CT4	O04-N03	2.21	1.45	1.40
6	L	710	A1CT4	C22-C21	2.17	1.43	1.40
6	C	710	A1CT4	O13-C07	-2.16	1.19	1.23
6	L	710	A1CT4	C21-C17	-2.16	1.37	1.40
6	B	708	A1CT4	O13-C07	-2.15	1.19	1.23
6	K	706	A1CT4	C21-C17	-2.14	1.37	1.40
10	G	705	A1CT5	C21-C17	-2.14	1.37	1.40
6	F	707	A1CT4	O13-C07	-2.14	1.19	1.23
6	H	705	A1CT4	O13-C07	-2.14	1.19	1.23
6	J	707	A1CT4	C21-C17	-2.13	1.37	1.40
6	L	710	A1CT4	O13-C07	-2.13	1.19	1.23
6	I	708	A1CT4	O13-C07	-2.13	1.19	1.23
6	A	710	A1CT4	C21-C17	-2.13	1.37	1.40
6	B	708	A1CT4	C21-C17	-2.12	1.37	1.40
6	C	710	A1CT4	C21-C17	-2.11	1.37	1.40
6	F	707	A1CT4	C21-C17	-2.11	1.37	1.40
6	D	707	A1CT4	C21-C17	-2.10	1.37	1.40
6	D	707	A1CT4	O13-C07	-2.10	1.19	1.23
10	G	705	A1CT5	O13-C07	-2.10	1.19	1.23
6	K	706	A1CT4	C22-C21	2.10	1.43	1.40
6	E	708	A1CT4	C21-C17	-2.09	1.37	1.40
6	J	707	A1CT4	O13-C07	-2.09	1.19	1.23
6	E	708	A1CT4	O13-C07	-2.08	1.19	1.23
6	A	710	A1CT4	O13-C07	-2.08	1.19	1.23
6	K	706	A1CT4	O13-C07	-2.07	1.19	1.23
6	I	708	A1CT4	C21-C17	-2.05	1.37	1.40
10	G	705	A1CT5	C22-C21	2.04	1.43	1.40
6	H	705	A1CT4	C21-C17	-2.03	1.37	1.40

All (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
6	K	706	A1CT4	S18-C19-N20	-12.23	109.33	117.01
6	J	707	A1CT4	S18-C19-N20	-12.20	109.35	117.01
6	C	710	A1CT4	S18-C19-N20	-12.19	109.36	117.01
10	G	705	A1CT5	S18-C19-N20	-12.14	109.39	117.01
6	I	708	A1CT4	S18-C19-N20	-12.06	109.44	117.01
6	H	705	A1CT4	S18-C19-N20	-11.98	109.49	117.01
6	D	707	A1CT4	S18-C19-N20	-11.95	109.51	117.01
10	G	705	A1CT5	C22-C21-N20	-4.70	122.61	130.51
6	K	706	A1CT4	C22-C21-N20	-4.59	122.79	130.51
6	L	710	A1CT4	C22-C21-N20	-4.52	122.92	130.51
6	B	708	A1CT4	C22-C21-N20	-4.49	122.96	130.51
6	J	707	A1CT4	C22-C21-N20	-4.47	122.99	130.51
6	E	708	A1CT4	C22-C21-N20	-4.43	123.07	130.51
6	A	710	A1CT4	C22-C21-N20	-4.42	123.08	130.51
6	C	710	A1CT4	C22-C21-N20	-4.42	123.08	130.51
6	D	707	A1CT4	C22-C21-N20	-4.40	123.12	130.51
6	F	707	A1CT4	C22-C21-N20	-4.39	123.12	130.51
6	I	708	A1CT4	C22-C21-N20	-4.38	123.14	130.51
6	H	705	A1CT4	C22-C21-N20	-4.36	123.18	130.51
6	L	710	A1CT4	C16-C17-S18	4.06	134.49	127.36
10	G	705	A1CT5	C16-C17-S18	4.05	134.48	127.36
6	K	706	A1CT4	C16-C17-S18	4.04	134.46	127.36
6	B	708	A1CT4	C16-C17-S18	4.01	134.41	127.36
6	J	707	A1CT4	C16-C17-S18	3.99	134.37	127.36
6	E	708	A1CT4	C16-C17-S18	3.95	134.30	127.36
6	C	710	A1CT4	C16-C17-S18	3.94	134.29	127.36
6	A	710	A1CT4	C16-C17-S18	3.93	134.27	127.36
6	D	707	A1CT4	C16-C17-S18	3.81	134.06	127.36
6	F	707	A1CT4	C16-C17-S18	3.81	134.06	127.36
6	H	705	A1CT4	C16-C17-S18	3.80	134.04	127.36
6	I	708	A1CT4	C16-C17-S18	3.75	133.95	127.36
6	H	705	A1CT4	C08-C07-N06	3.33	121.21	115.65
6	B	708	A1CT4	C08-C07-N06	3.31	121.18	115.65
6	C	710	A1CT4	C08-C07-N06	3.05	120.73	115.65
10	G	705	A1CT5	C08-C07-N06	2.99	120.64	115.65
6	I	708	A1CT4	C08-C07-N06	2.99	120.63	115.65
6	F	707	A1CT4	C08-C07-N06	2.96	120.59	115.65
6	E	708	A1CT4	C08-C07-N06	2.78	120.28	115.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	708	A1CT4	O13-C07-N06	-2.72	118.35	122.95
6	D	707	A1CT4	C08-C07-N06	2.71	120.18	115.65
6	L	710	A1CT4	C08-C07-N06	2.65	120.08	115.65
6	H	705	A1CT4	O13-C07-N06	-2.57	118.60	122.95
10	G	705	A1CT5	O13-C07-N06	-2.51	118.71	122.95
6	J	707	A1CT4	C08-C07-N06	2.45	119.74	115.65
6	K	706	A1CT4	C08-C07-N06	2.44	119.71	115.65
6	C	710	A1CT4	O13-C07-N06	-2.37	118.94	122.95
6	A	710	A1CT4	C08-C07-N06	2.26	119.42	115.65
6	I	708	A1CT4	O13-C07-N06	-2.23	119.18	122.95
10	G	705	A1CT5	C14-C05-N06	-2.17	107.28	112.75
6	I	708	A1CT4	C15-C14-C05	-2.14	117.34	120.78
6	F	707	A1CT4	O13-C07-N06	-2.11	119.38	122.95
6	C	710	A1CT4	C14-C05-C02	2.09	113.35	108.42
6	B	708	A1CT4	C14-C05-C02	2.08	113.33	108.42
6	E	708	A1CT4	O13-C07-N06	-2.06	119.46	122.95
6	D	707	A1CT4	O13-C07-N06	-2.02	119.54	122.95

There are no chirality outliers.

All (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
6	K	706	A1CT4	C07-C08-C09-C12
10	G	705	A1CT5	N03-C02-C05-N06
10	G	705	A1CT5	O01-C02-C05-N06
10	G	705	A1CT5	C08-C07-N06-C05
10	G	705	A1CT5	O13-C07-N06-C05
7	D	715	1PE	OH6-C15-C25-OH5
7	F	712	1PE	OH6-C15-C25-OH5
7	J	721	1PE	OH5-C14-C24-OH4
7	I	707	1PE	OH6-C15-C25-OH5
4	A	708	PEG	O1-C1-C2-O2
7	J	705	1PE	OH6-C15-C25-OH5
7	J	720	1PE	OH5-C14-C24-OH4
4	D	705	PEG	O2-C3-C4-O4
4	E	704	PEG	O1-C1-C2-O2
4	G	704	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	710	PEG	O1-C1-C2-O2
4	I	710	PEG	O2-C3-C4-O4
4	L	706	PEG	O1-C1-C2-O2
7	C	719	1PE	OH4-C13-C23-OH3
7	E	716	1PE	OH4-C13-C23-OH3
7	I	707	1PE	OH7-C16-C26-OH6
7	I	715	1PE	OH6-C15-C25-OH5
7	E	709	1PE	OH6-C15-C25-OH5
7	G	713	1PE	OH5-C14-C24-OH4
7	L	716	1PE	OH6-C15-C25-OH5
4	C	709	PEG	O2-C3-C4-O4
4	E	715	PEG	O2-C3-C4-O4
4	H	704	PEG	O1-C1-C2-O2
4	H	704	PEG	O2-C3-C4-O4
4	K	704	PEG	O2-C3-C4-O4
7	E	716	1PE	OH6-C15-C25-OH5
7	E	717	1PE	OH6-C15-C25-OH5
7	K	714	1PE	OH6-C15-C25-OH5
7	L	714	1PE	OH6-C15-C25-OH5
7	L	715	1PE	OH6-C15-C25-OH5
7	D	715	1PE	C15-C25-OH5-C14
4	A	704	PEG	O2-C3-C4-O4
4	I	709	PEG	O2-C3-C4-O4
7	J	705	1PE	OH7-C16-C26-OH6
9	B	714	2PE	O13-C14-C15-O16
7	J	720	1PE	C23-C13-OH4-C24
7	G	716	1PE	OH6-C15-C25-OH5
7	J	719	1PE	OH6-C15-C25-OH5
4	D	705	PEG	O1-C1-C2-O2
4	D	708	PEG	O1-C1-C2-O2
7	A	717	1PE	OH6-C15-C25-OH5
7	D	714	1PE	OH5-C14-C24-OH4
7	F	711	1PE	OH7-C16-C26-OH6
7	F	711	1PE	OH6-C15-C25-OH5
4	L	705	PEG	C1-C2-O2-C3
7	G	713	1PE	OH4-C13-C23-OH3
7	G	716	1PE	OH5-C14-C24-OH4
4	A	708	PEG	O2-C3-C4-O4
4	C	709	PEG	O1-C1-C2-O2
4	J	709	PEG	O2-C3-C4-O4
7	L	715	1PE	OH5-C14-C24-OH4
7	L	714	1PE	OH5-C14-C24-OH4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	710	A1CT4	C07-C08-C09-C11
6	A	710	A1CT4	C07-C08-C09-C12
4	H	704	PEG	C1-C2-O2-C3
4	C	707	PEG	O1-C1-C2-O2
7	F	711	1PE	OH5-C14-C24-OH4
4	I	710	PEG	C4-C3-O2-C2
9	B	714	2PE	O16-C17-C18-O19
4	A	709	PEG	O2-C3-C4-O4
7	I	716	1PE	OH4-C13-C23-OH3
9	B	714	2PE	O22-C23-C24-O25
7	K	716	1PE	OH6-C15-C25-OH5
7	J	705	1PE	C24-C14-OH5-C25
7	F	706	1PE	OH5-C14-C24-OH4
7	L	713	1PE	OH7-C16-C26-OH6
7	J	721	1PE	C15-C25-OH5-C14
7	G	714	1PE	C24-C14-OH5-C25
4	E	706	PEG	C1-C2-O2-C3
4	C	708	PEG	O1-C1-C2-O2
4	K	705	PEG	O2-C3-C4-O4
7	G	716	1PE	OH7-C16-C26-OH6
7	E	717	1PE	C23-C13-OH4-C24
4	I	709	PEG	C1-C2-O2-C3
7	E	716	1PE	C15-C25-OH5-C14
7	I	707	1PE	C14-C24-OH4-C13
4	I	706	PEG	C1-C2-O2-C3
4	D	705	PEG	C1-C2-O2-C3
7	E	709	1PE	C24-C14-OH5-C25
7	E	709	1PE	C16-C26-OH6-C15
7	F	711	1PE	C24-C14-OH5-C25
4	C	708	PEG	C4-C3-O2-C2
4	L	706	PEG	C1-C2-O2-C3
7	E	716	1PE	OH5-C14-C24-OH4
7	L	715	1PE	C24-C14-OH5-C25
7	K	717	1PE	C24-C14-OH5-C25
4	A	708	PEG	C4-C3-O2-C2
4	A	706	PEG	C1-C2-O2-C3
7	J	720	1PE	C24-C14-OH5-C25
4	A	709	PEG	O1-C1-C2-O2
4	E	706	PEG	O2-C3-C4-O4
4	I	706	PEG	O2-C3-C4-O4
7	L	707	1PE	OH2-C12-C22-OH3
4	E	715	PEG	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	L	714	1PE	C23-C13-OH4-C24
9	H	712	2PE	C23-C24-O25-C26
7	D	715	1PE	C24-C14-OH5-C25
4	C	711	PEG	C4-C3-O2-C2
4	G	704	PEG	C4-C3-O2-C2
7	A	716	1PE	OH4-C13-C23-OH3
7	K	715	1PE	OH4-C13-C23-OH3
4	A	706	PEG	C4-C3-O2-C2
6	B	708	A1CT4	C07-C08-C09-C12
6	F	707	A1CT4	C07-C08-C09-C10
6	F	707	A1CT4	C07-C08-C09-C11
6	I	708	A1CT4	C07-C08-C09-C10
6	L	710	A1CT4	C07-C08-C09-C10
6	L	710	A1CT4	C07-C08-C09-C11
10	G	705	A1CT5	C07-C08-C09-C12
7	G	716	1PE	C23-C13-OH4-C24
7	J	720	1PE	C14-C24-OH4-C13
7	C	718	1PE	C23-C13-OH4-C24
4	I	704	PEG	C1-C2-O2-C3
4	D	708	PEG	C1-C2-O2-C3
9	H	712	2PE	C12-C11-O10-C9
7	B	709	1PE	OH2-C12-C22-OH3
4	F	704	PEG	C1-C2-O2-C3
4	L	705	PEG	C4-C3-O2-C2
7	F	711	1PE	C16-C26-OH6-C15
7	J	721	1PE	C14-C24-OH4-C13
4	E	704	PEG	O2-C3-C4-O4
4	I	706	PEG	O1-C1-C2-O2
4	L	709	PEG	O1-C1-C2-O2
7	F	712	1PE	C25-C15-OH6-C26
4	D	708	PEG	C4-C3-O2-C2
4	C	704	PEG	C1-C2-O2-C3
9	H	712	2PE	O10-C11-C12-O13
7	I	715	1PE	OH4-C13-C23-OH3
7	C	719	1PE	C23-C13-OH4-C24
4	D	706	PEG	C4-C3-O2-C2
4	K	704	PEG	C1-C2-O2-C3
6	B	708	A1CT4	N06-C05-C14-C15
7	F	706	1PE	C15-C25-OH5-C14
9	B	714	2PE	O19-C20-C21-O22
7	K	715	1PE	C15-C25-OH5-C14
7	G	715	1PE	C24-C14-OH5-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	705	PEG	C1-C2-O2-C3
6	K	706	A1CT4	O01-C02-C05-C14
4	A	706	PEG	O1-C1-C2-O2
6	L	710	A1CT4	N03-C02-C05-N06
4	L	704	PEG	C1-C2-O2-C3
6	B	708	A1CT4	N06-C05-C14-C22
7	J	705	1PE	C16-C26-OH6-C15
7	L	714	1PE	C24-C14-OH5-C25
4	L	704	PEG	O1-C1-C2-O2
7	L	707	1PE	C13-C23-OH3-C22
4	F	704	PEG	C4-C3-O2-C2
4	E	715	PEG	C4-C3-O2-C2
7	D	715	1PE	C25-C15-OH6-C26
4	A	707	PEG	C4-C3-O2-C2
4	C	712	PEG	O2-C3-C4-O4
7	J	720	1PE	C15-C25-OH5-C14
10	G	705	A1CT5	C02-C05-N06-C07
9	B	714	2PE	C11-C12-O13-C14
7	G	713	1PE	C24-C14-OH5-C25
9	H	712	2PE	C21-C20-O19-C18
6	A	710	A1CT4	C07-C08-C09-C10
6	B	708	A1CT4	C07-C08-C09-C10
6	F	707	A1CT4	C07-C08-C09-C12
6	I	708	A1CT4	C07-C08-C09-C11
6	L	710	A1CT4	C07-C08-C09-C12
10	G	705	A1CT5	C07-C08-C09-C10
4	I	709	PEG	C4-C3-O2-C2
7	J	718	1PE	C25-C15-OH6-C26
6	E	708	A1CT4	N06-C05-C14-C22
6	L	710	A1CT4	O01-C02-C05-N06
4	L	706	PEG	C4-C3-O2-C2
7	E	709	1PE	C15-C25-OH5-C14
6	E	708	A1CT4	N06-C05-C14-C15
4	I	704	PEG	C4-C3-O2-C2
7	D	716	1PE	C24-C14-OH5-C25
9	B	714	2PE	C17-C18-O19-C20
4	A	704	PEG	C4-C3-O2-C2
4	J	717	PEG	C1-C2-O2-C3
4	A	709	PEG	C1-C2-O2-C3
7	C	718	1PE	C24-C14-OH5-C25
4	E	715	PEG	O1-C1-C2-O2
7	I	707	1PE	C15-C25-OH5-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	H	712	2PE	C20-C21-O22-C23
7	K	716	1PE	OH5-C14-C24-OH4
7	D	715	1PE	OH5-C14-C24-OH4
7	G	715	1PE	OH6-C15-C25-OH5
4	C	711	PEG	C1-C2-O2-C3
4	L	704	PEG	C4-C3-O2-C2
4	K	704	PEG	C4-C3-O2-C2
7	D	716	1PE	C23-C13-OH4-C24
4	A	707	PEG	O2-C3-C4-O4
7	F	712	1PE	OH7-C16-C26-OH6
9	H	712	2PE	O19-C20-C21-O22
7	D	704	1PE	OH6-C15-C25-OH5
7	K	716	1PE	C23-C13-OH4-C24
7	D	717	1PE	C16-C26-OH6-C15
7	E	709	1PE	C14-C24-OH4-C13
7	I	707	1PE	OH4-C13-C23-OH3
6	B	708	A1CT4	C07-C08-C09-C11
6	I	708	A1CT4	C07-C08-C09-C12
10	G	705	A1CT5	C07-C08-C09-C11
7	L	715	1PE	C15-C25-OH5-C14
4	A	704	PEG	O1-C1-C2-O2
4	C	709	PEG	C1-C2-O2-C3
4	L	711	PEG	C1-C2-O2-C3
7	L	707	1PE	C14-C24-OH4-C13
4	A	709	PEG	C4-C3-O2-C2

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

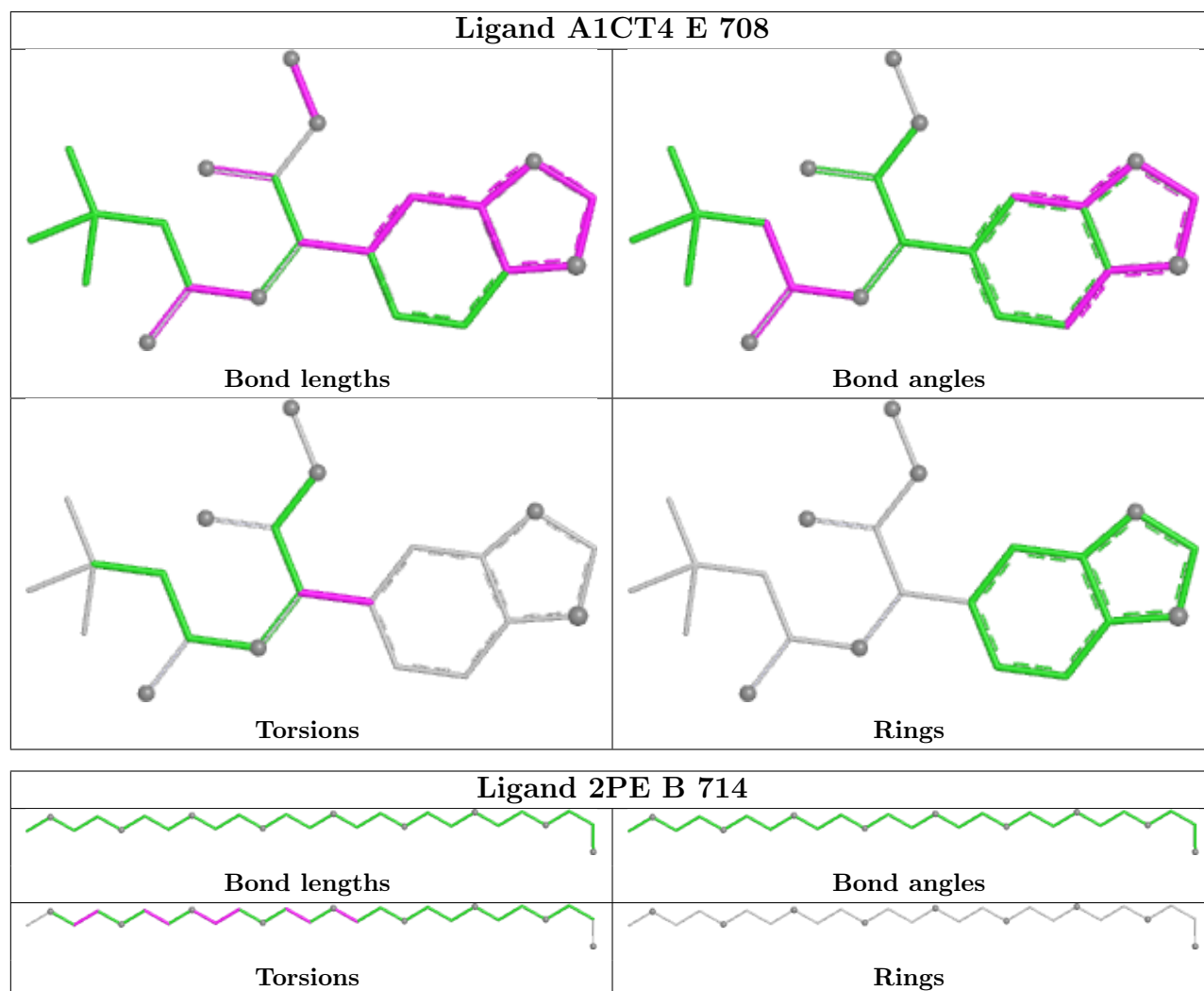
Continued on next page...

Continued from previous page...

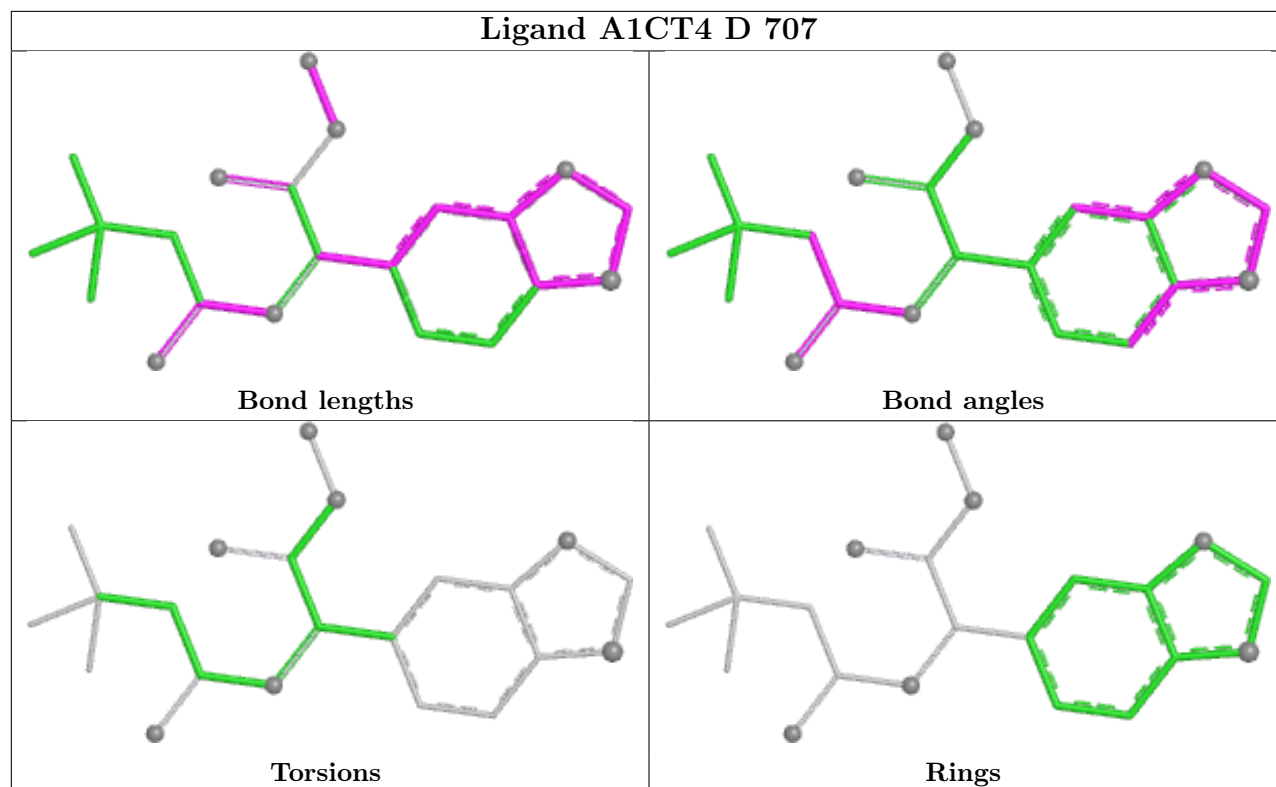
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	706	PEG	3	0
5	K	711	SO4	1	0
4	J	708	PEG	1	0
8	H	706	DMS	1	0
4	A	708	PEG	1	0
4	A	707	PEG	2	0
7	I	716	1PE	1	0
4	B	704	PEG	2	0
4	L	704	PEG	2	0
4	J	717	PEG	2	0
4	B	705	PEG	1	0
5	J	711	SO4	1	0
7	K	716	1PE	3	0
4	A	706	PEG	1	0
7	L	716	1PE	2	0
7	K	715	1PE	1	0
5	B	711	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
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,

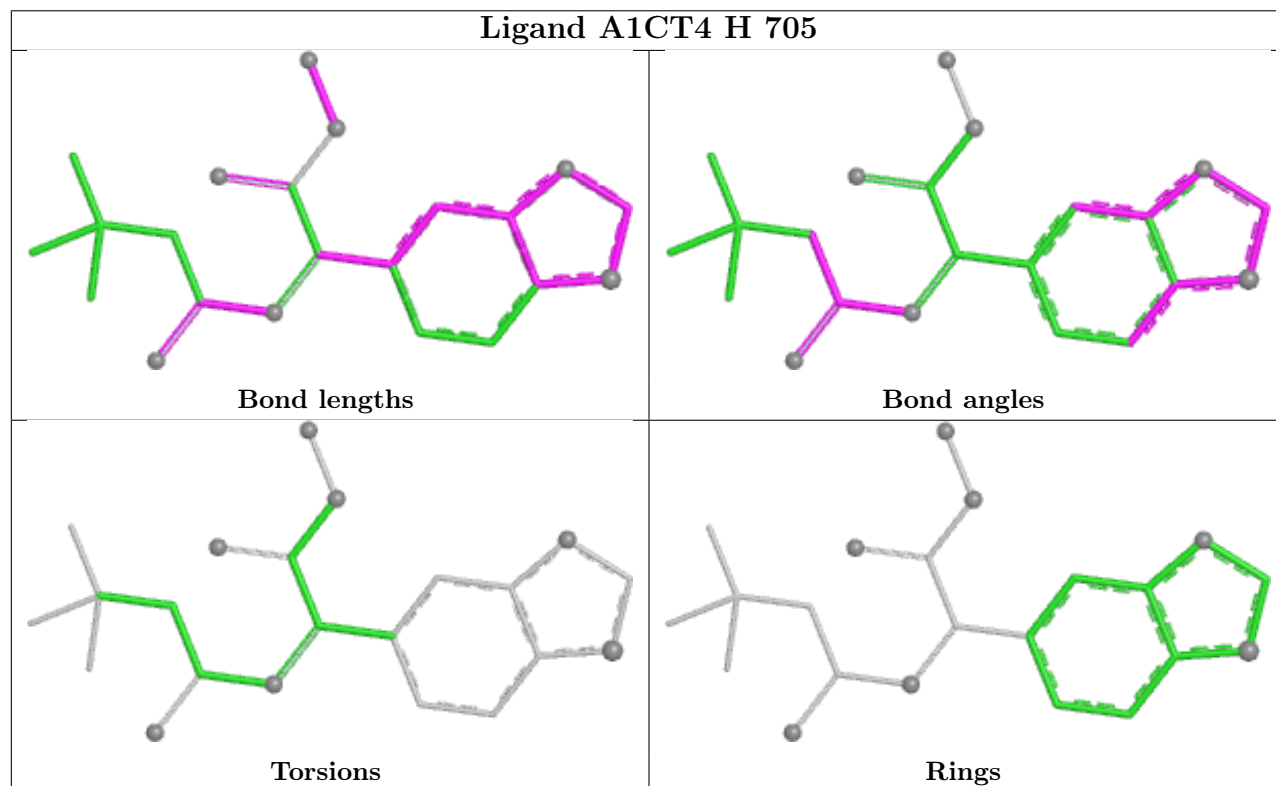
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



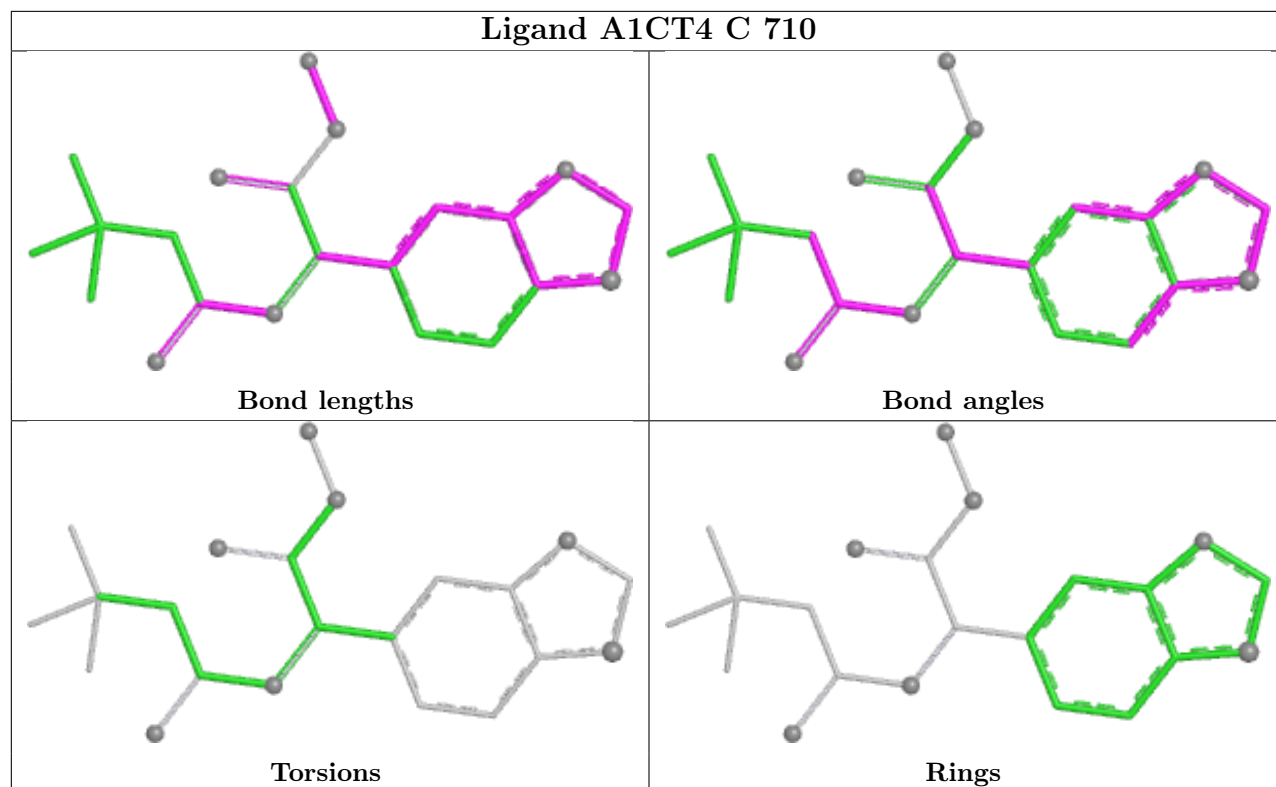
Ligand A1CT4 D 707



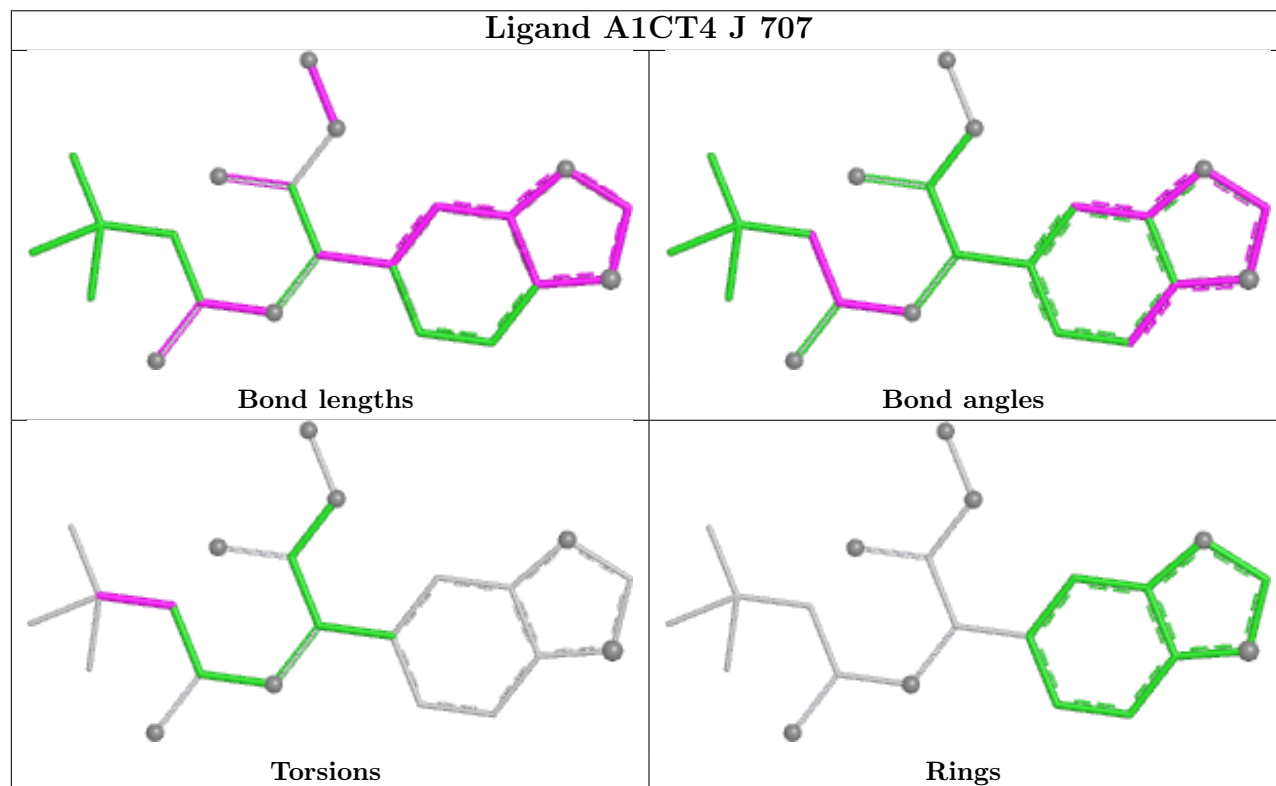
Ligand A1CT4 H 705



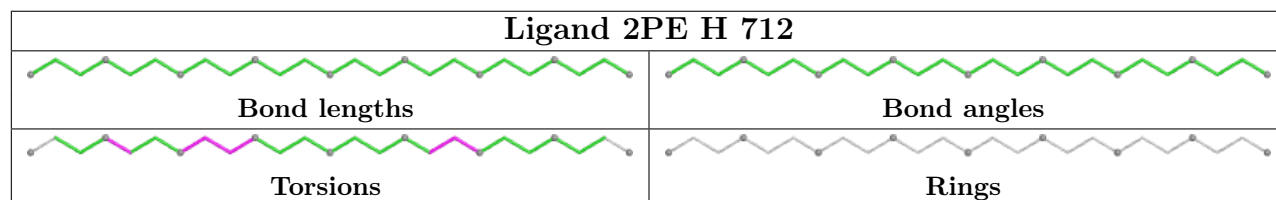
Ligand A1CT4 C 710



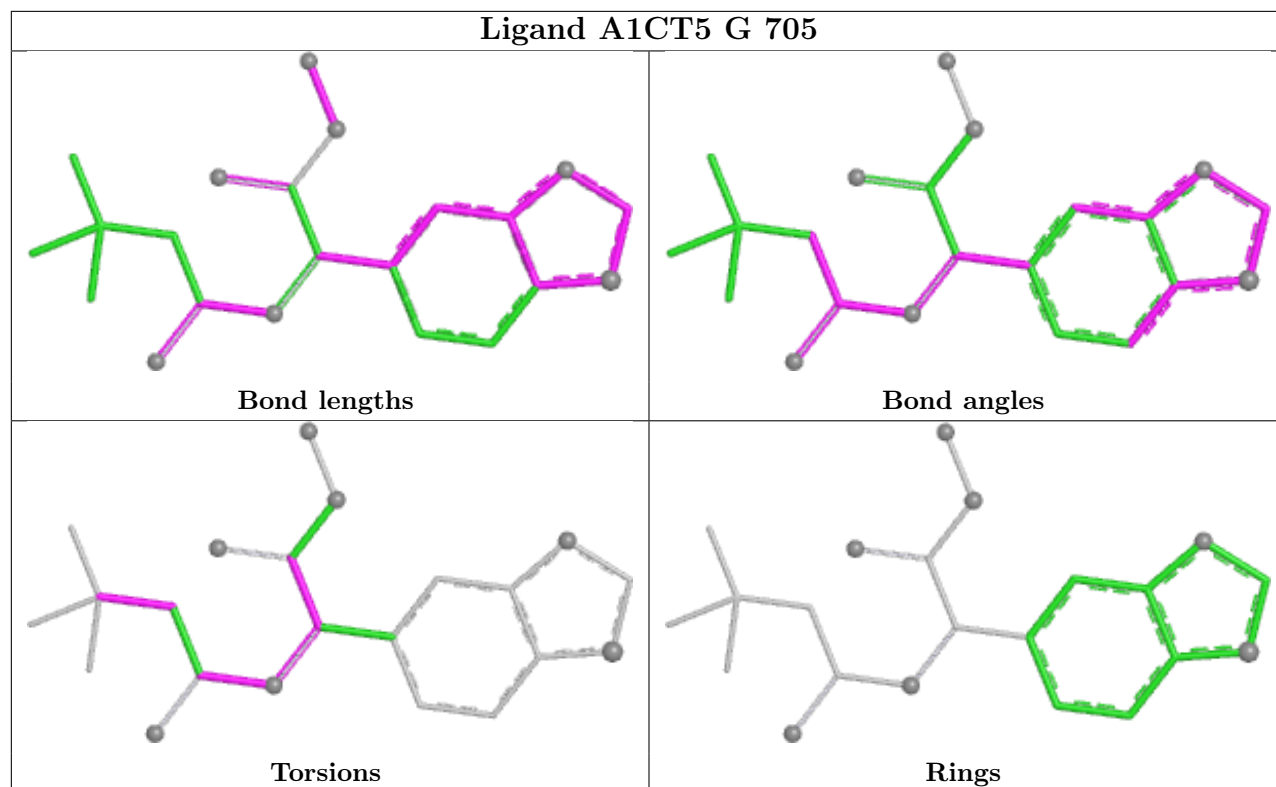
Ligand A1CT4 J 707



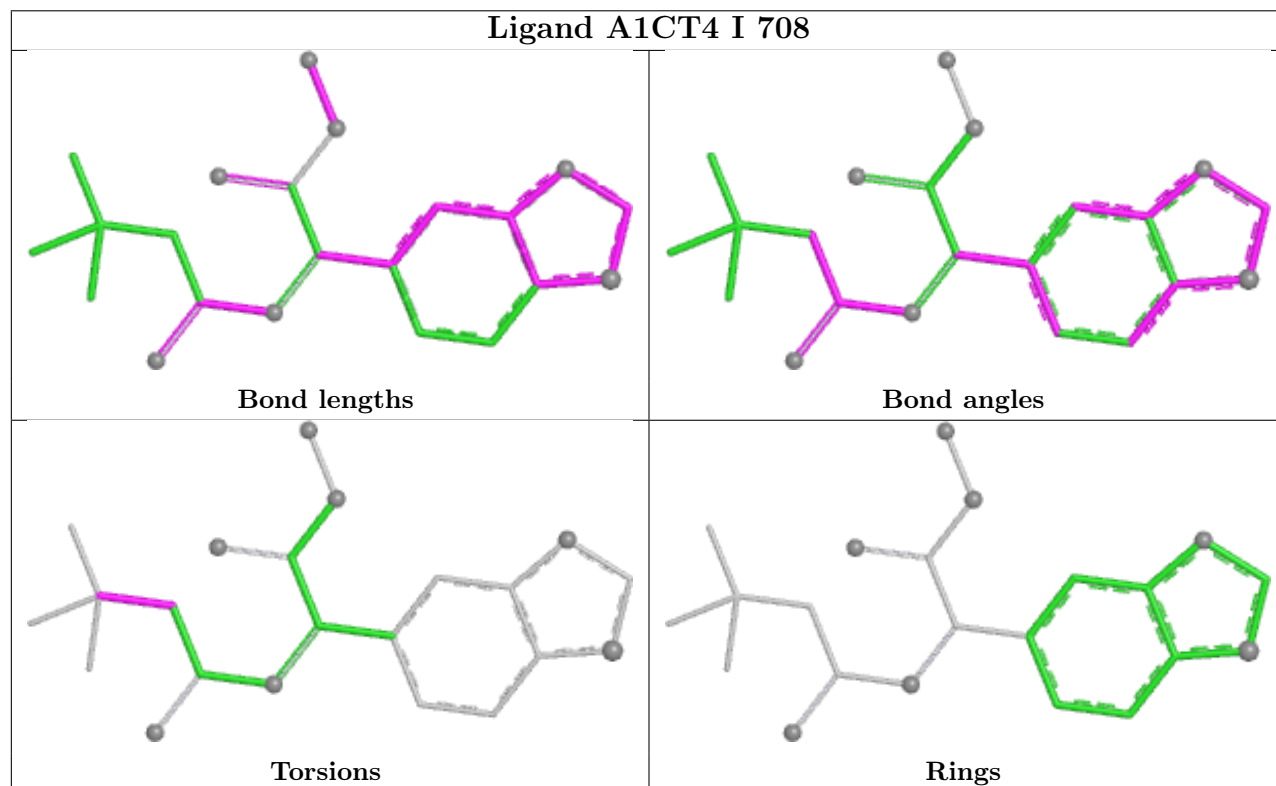
Ligand 2PE H 712



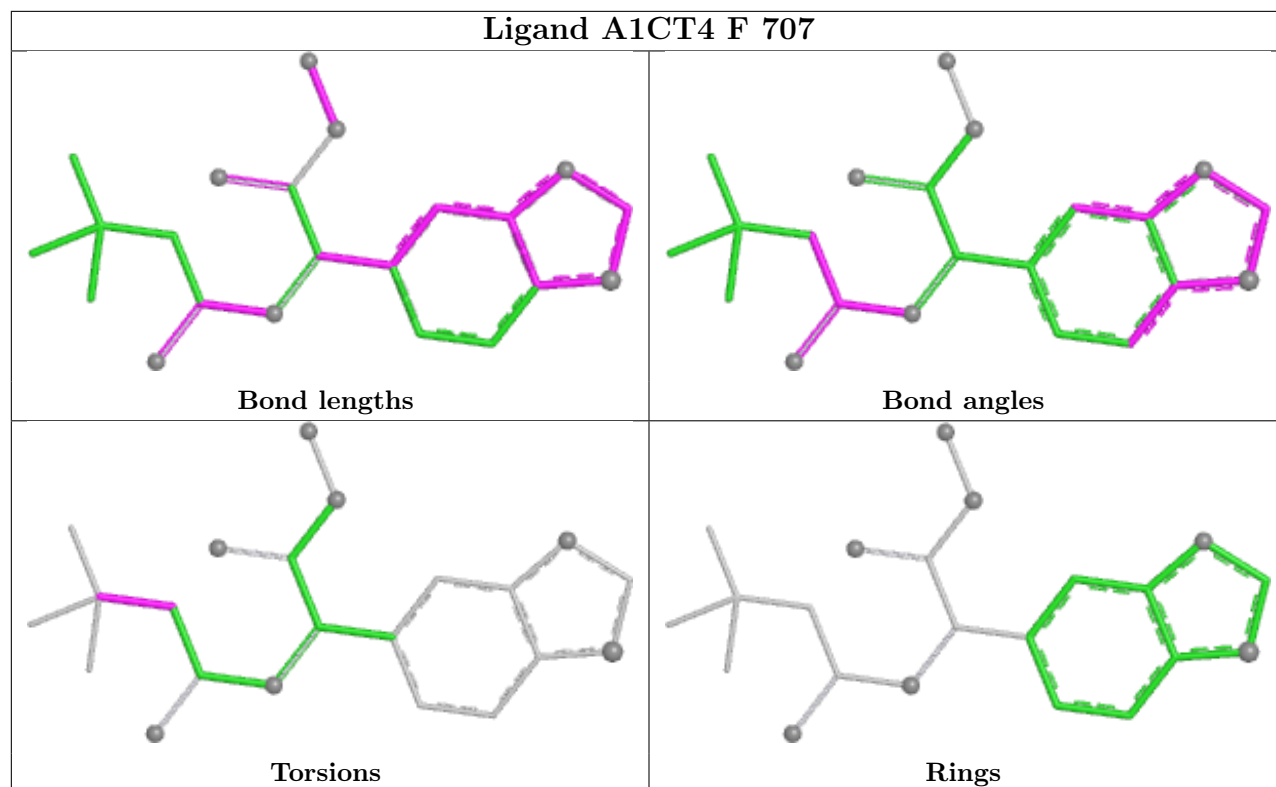
Ligand A1CT5 G 705



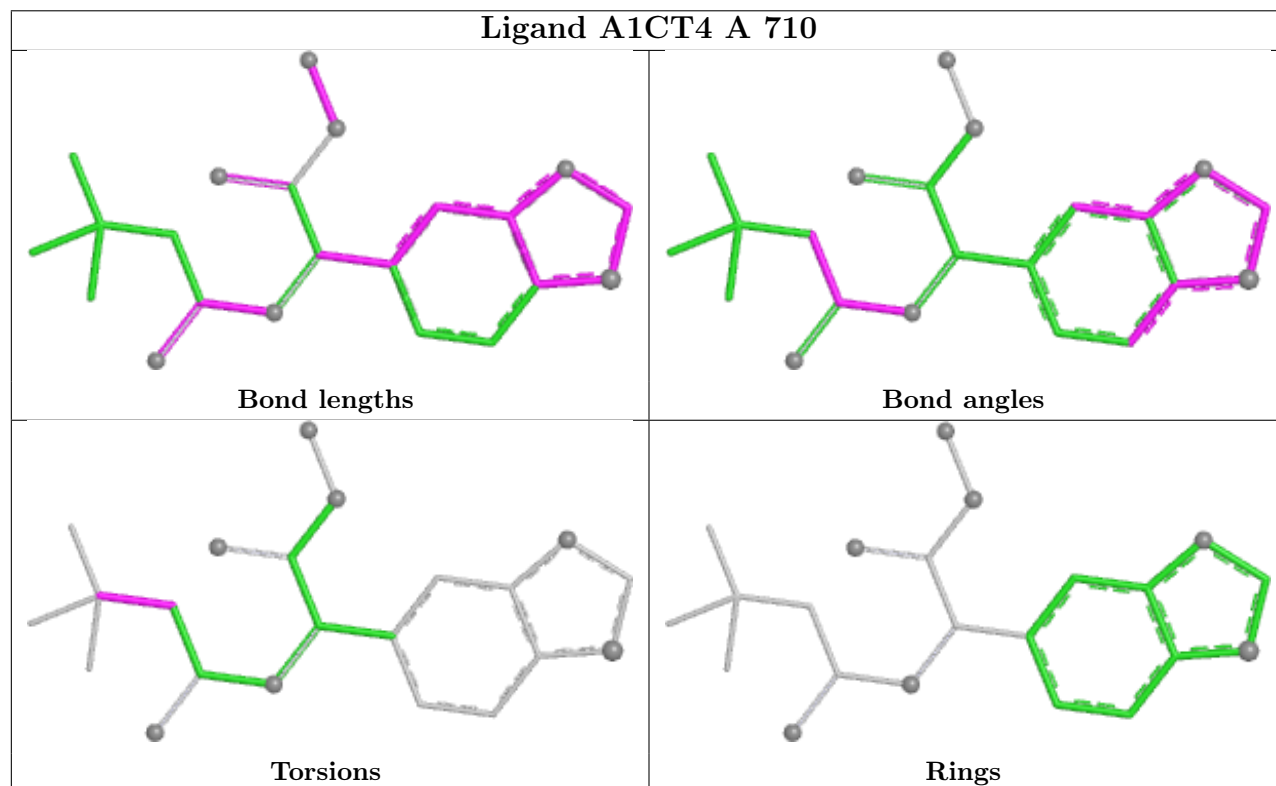
Ligand A1CT4 I 708



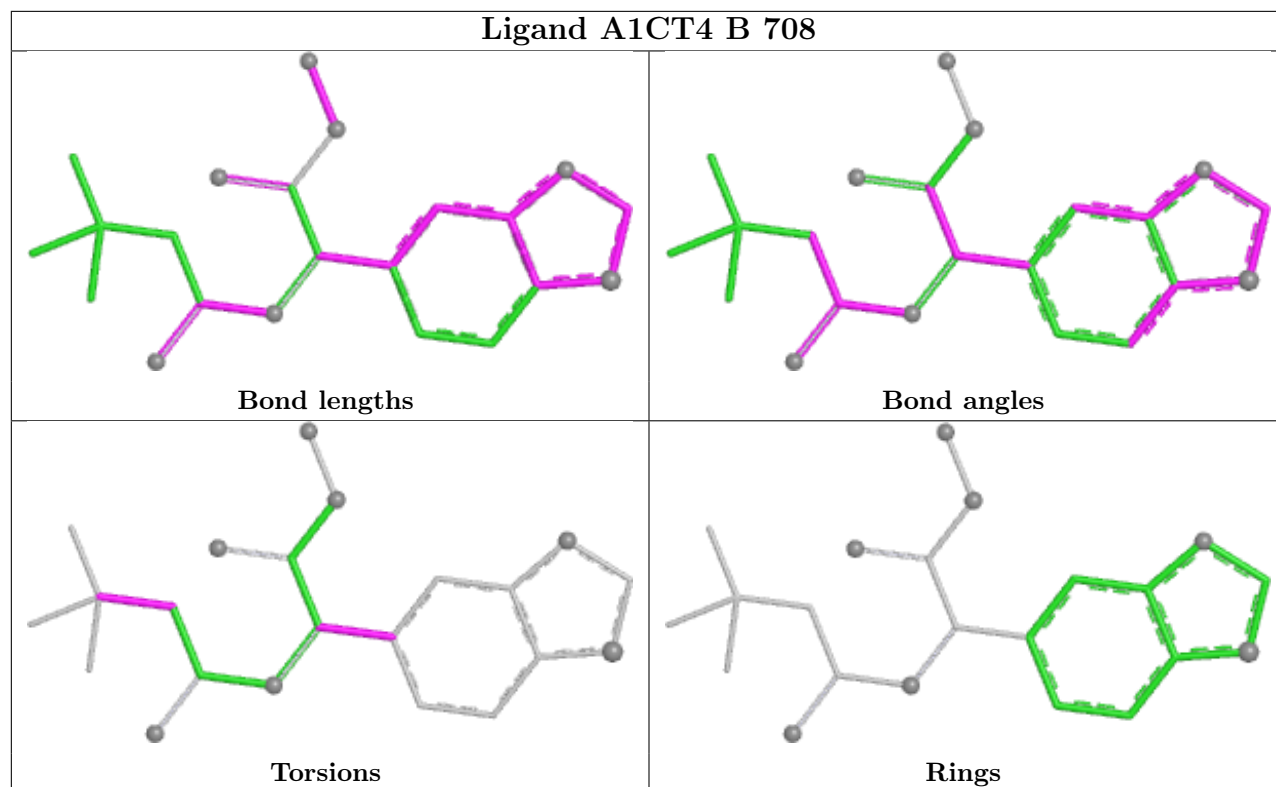
Ligand A1CT4 F 707



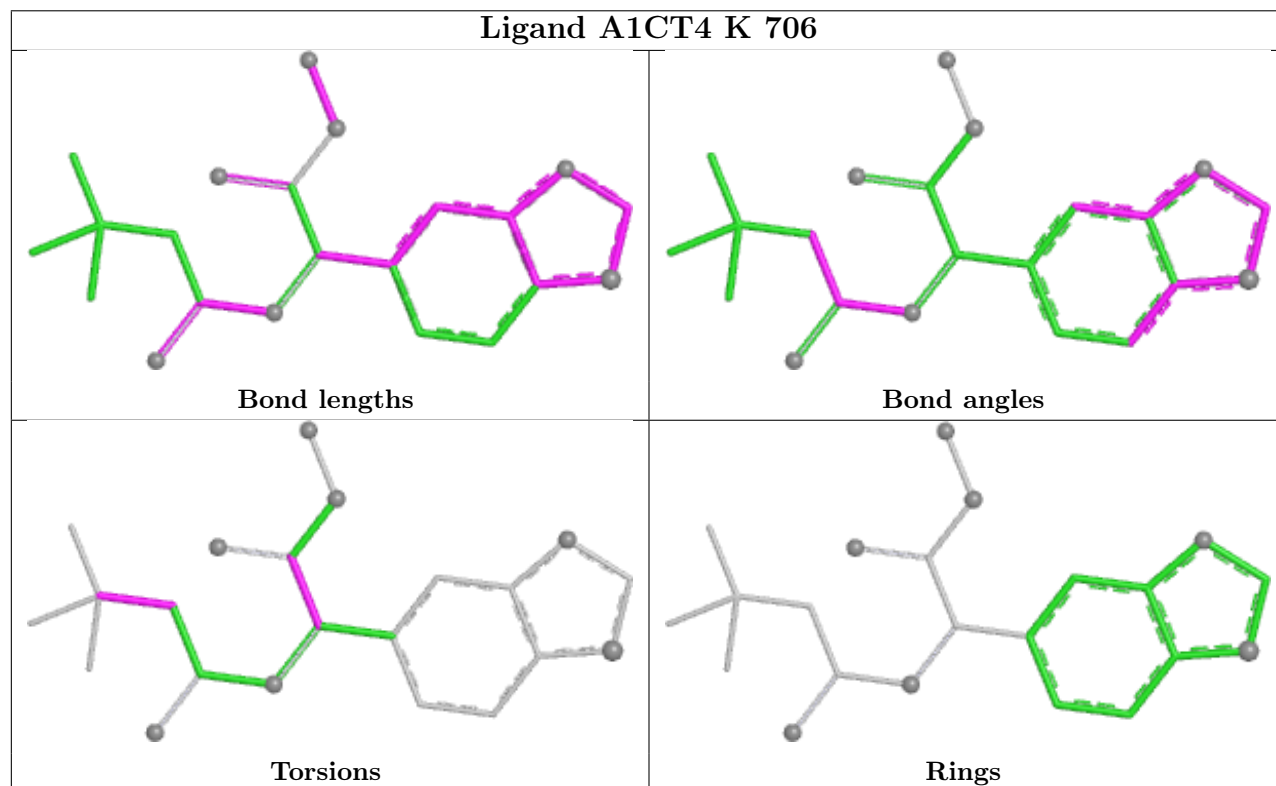
Ligand A1CT4 A 710

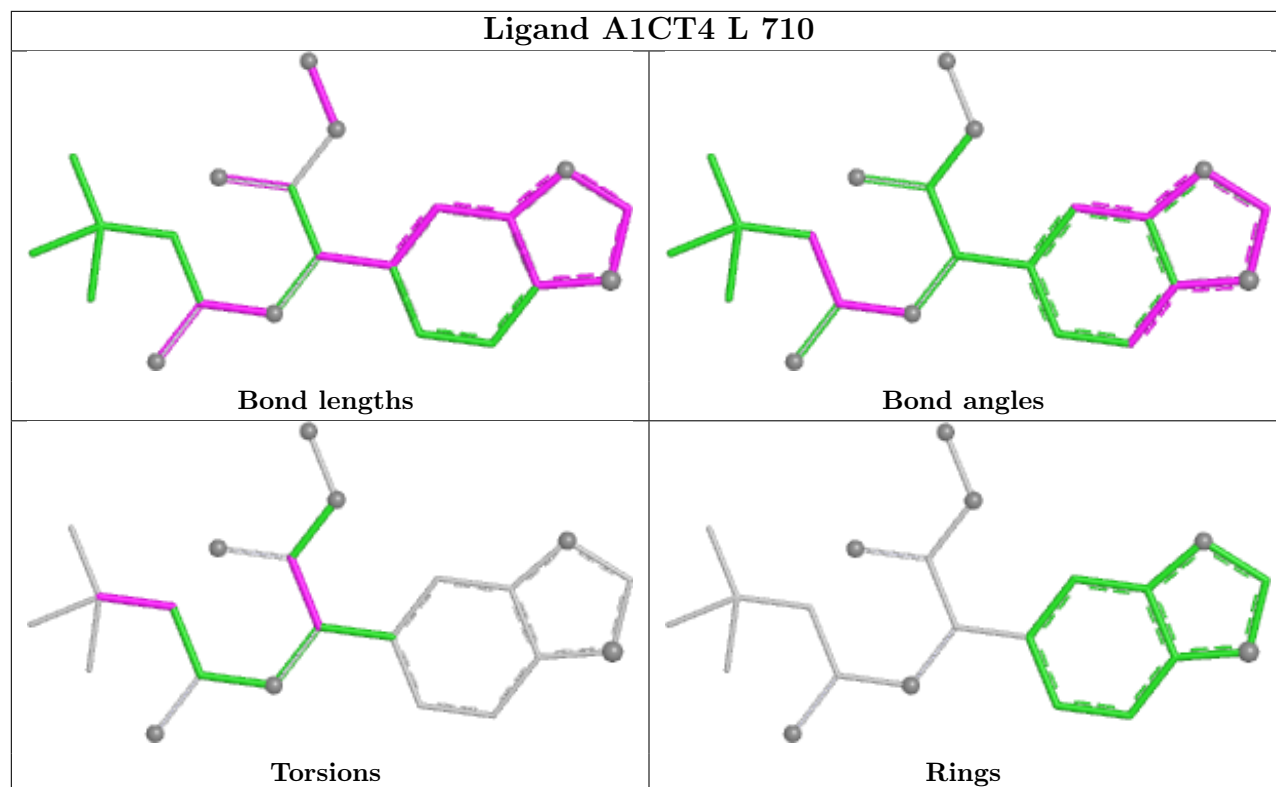


Ligand A1CT4 B 708



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)

All (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
1	H	119	GLY	3.2
1	B	135	PRO	3.2
1	B	175	PHE	3.2
1	H	192	CYS	3.1
1	J	364	ASP	3.1
1	H	255	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	104[A]	ASN	3.1
1	H	142	VAL	2.9
1	B	162	MET	2.9
1	A	260	ASN	2.9
1	H	167	VAL	2.9
1	H	144	ILE	2.9
1	F	121	CYS	2.8
1	F	196	ALA	2.8
1	B	272	ASN	2.8
1	I	259	VAL	2.8
1	B	176	TYR	2.7
1	L	175	PHE	2.7
1	J	603	ASP	2.7
1	G	85	ALA	2.6
1	H	183	ASN	2.6
1	D	259	VAL	2.6
1	B	169	LEU	2.6
1	L	161	ASN	2.6
1	I	261	MET	2.6
1	B	123	VAL	2.6
1	G	257	LYS	2.5
1	I	200	GLU	2.5
1	B	229	ASN	2.5
1	G	258	ASN	2.5
1	A	364	ASP	2.5
1	B	185	VAL	2.5
1	F	161	ASN	2.4
1	H	273	ASN	2.4
1	H	194	SER	2.4
1	C	259	VAL	2.4
1	H	159	ASP	2.4
1	B	178	PHE	2.4
1	H	134	ASN	2.3
1	B	274	ALA	2.3
1	B	144	ILE	2.3
1	H	178	PHE	2.2
1	H	141	PRO	2.2
1	L	178	PHE	2.2
1	C	258	ASN	2.2
1	H	135	PRO	2.2
1	H	196	ALA	2.2
1	I	260	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	136	GLY	2.2
1	F	178	PHE	2.2
1	H	180	ASP	2.2
1	I	258	ASN	2.2
1	J	363	GLY	2.2
1	I	549	SER	2.2
1	A	602	ASN	2.1
1	L	195	VAL	2.1
1	F	177	MET	2.1
1	H	157	LEU	2.1
1	F	197	ASP	2.1
1	H	175	PHE	2.1
1	I	257	LYS	2.1
1	B	262	GLU	2.1
1	A	176	TYR	2.1
1	A	256	ASP	2.1
1	H	185	VAL	2.1
1	B	156	PHE	2.1
1	H	117	ILE	2.1
1	F	153	VAL	2.1
1	L	262	GLU	2.0
1	B	275	ASP	2.0
1	C	149	ASN	2.0
1	L	181	ASN	2.0
1	F	184	SER	2.0
1	F	198	LEU	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

Continued on next page...

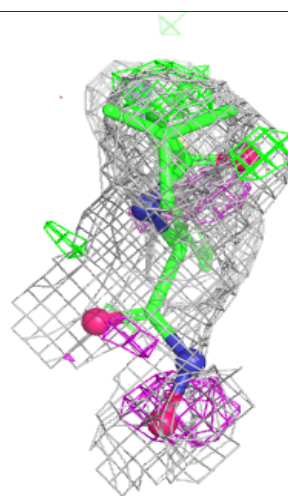
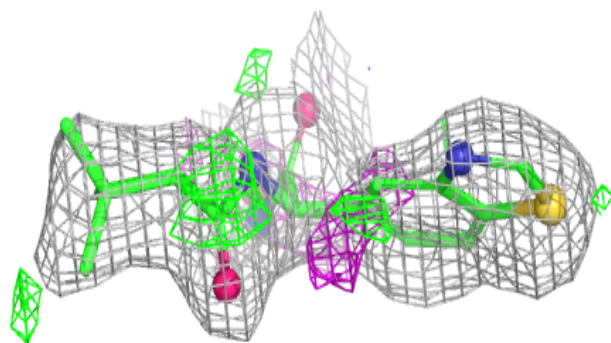
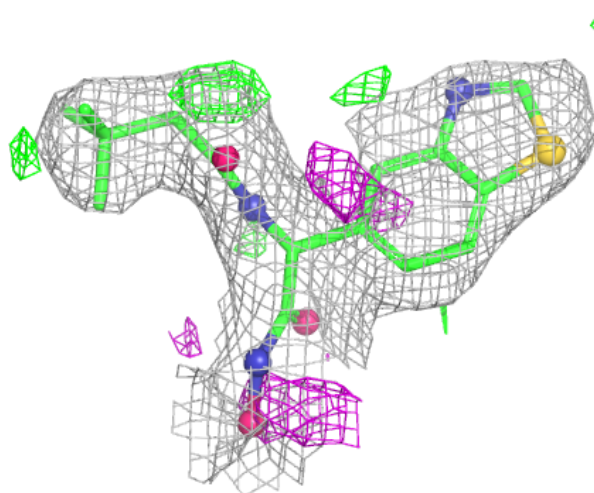
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.

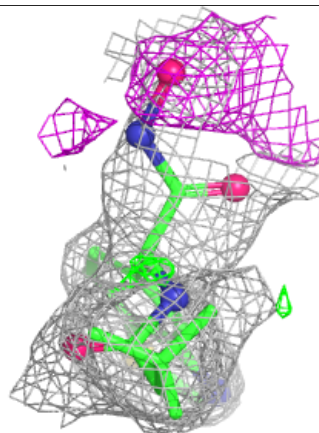
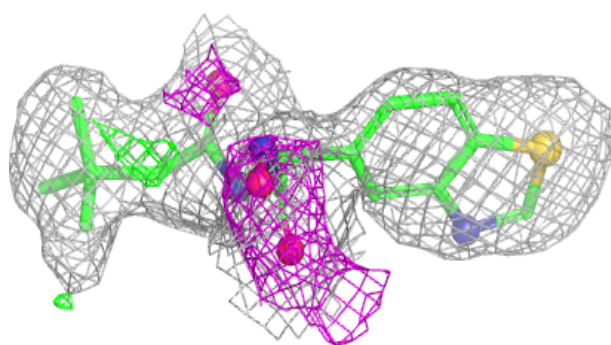
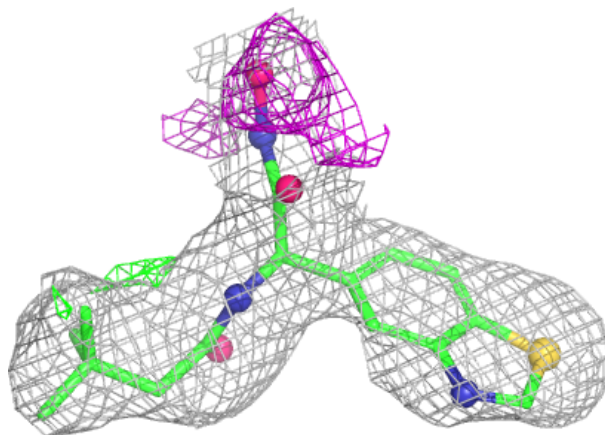
Electron density around A1CT4 L 710:

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



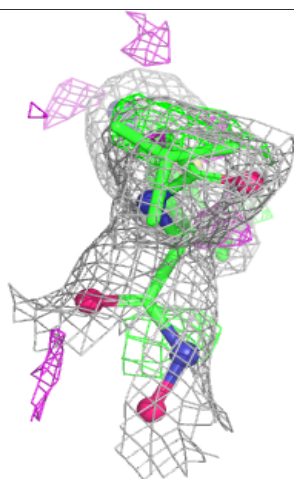
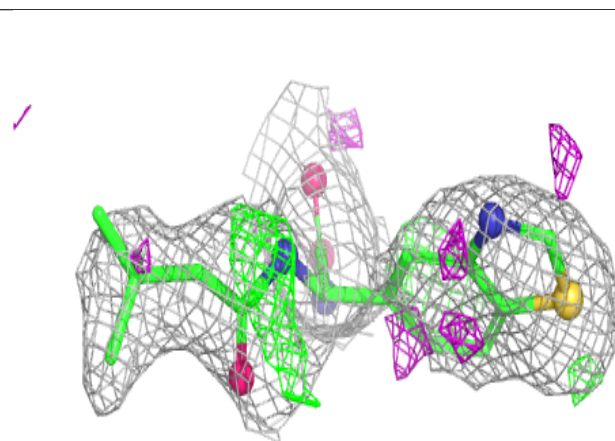
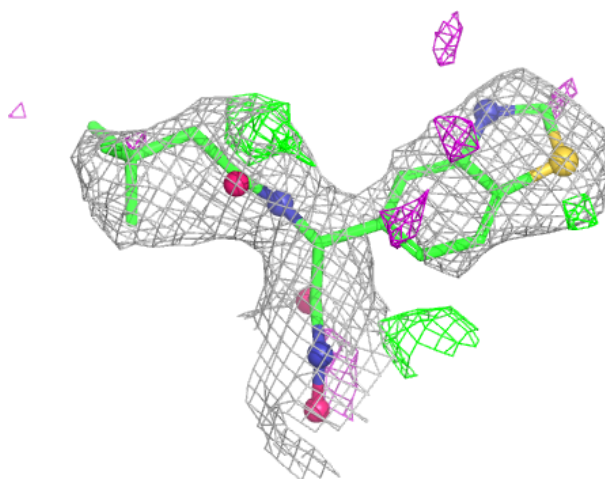
Electron density around A1CT4 D 707:

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



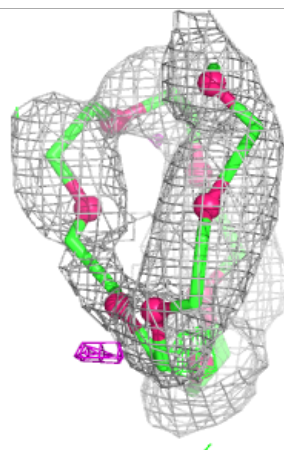
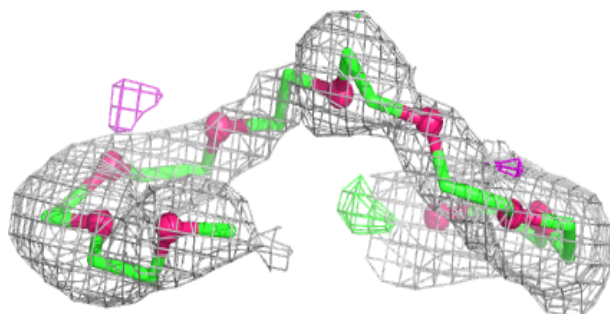
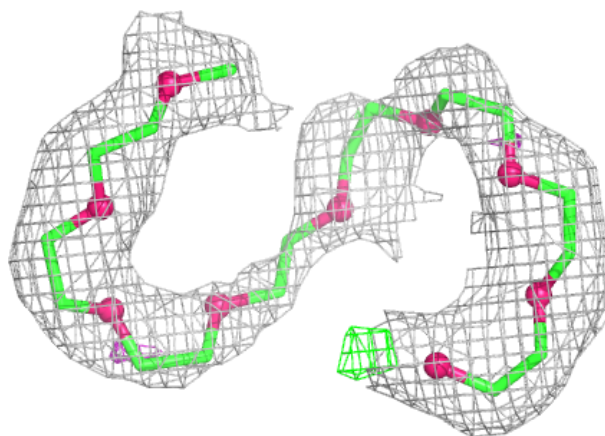
Electron density around A1CT4 I 708:

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



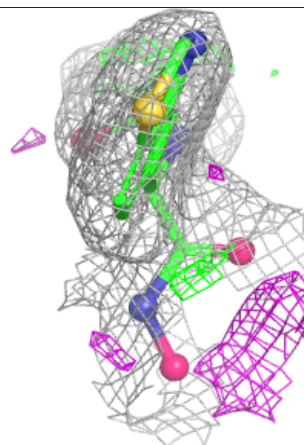
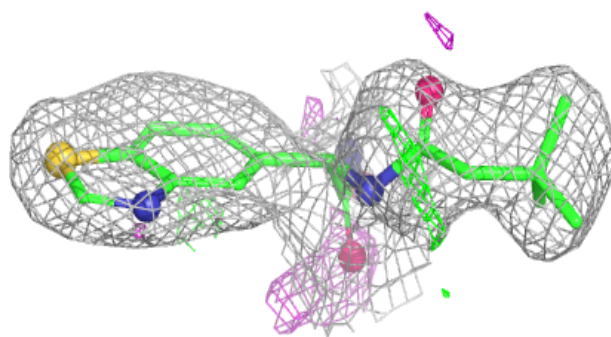
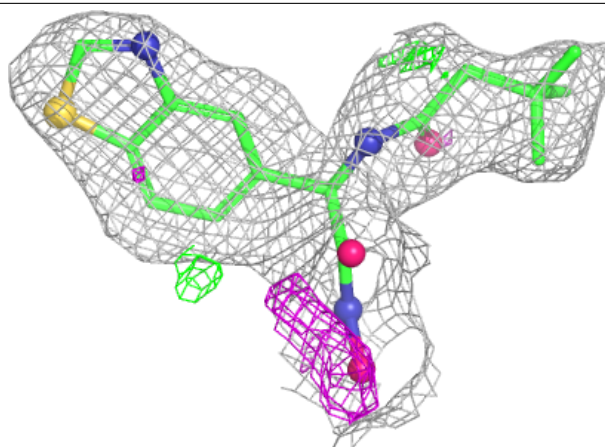
Electron density around 2PE B 714:

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



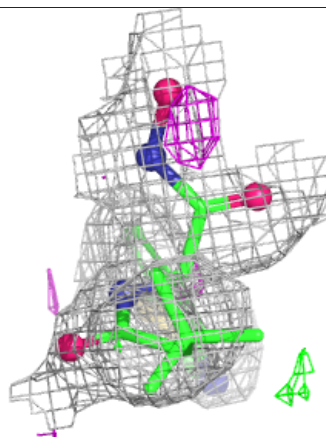
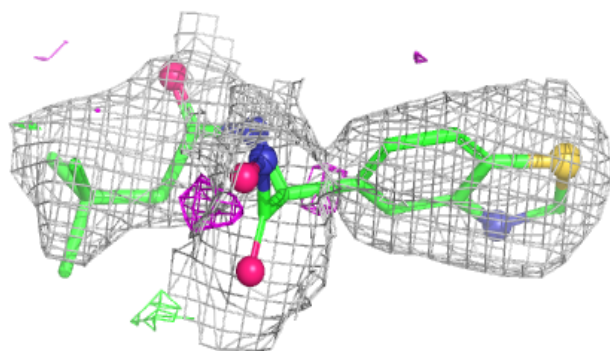
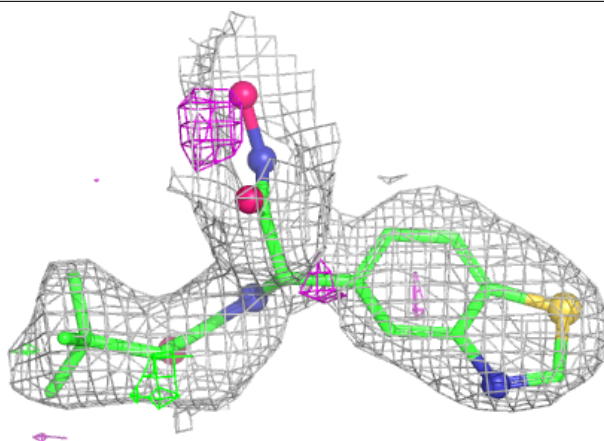
Electron density around A1CT4 B 708:

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



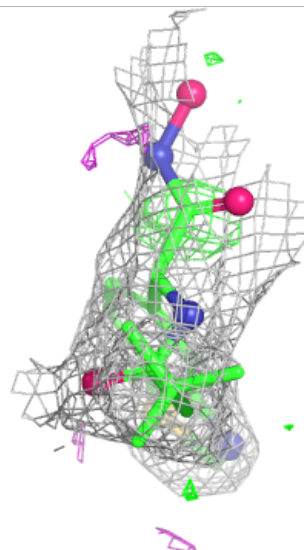
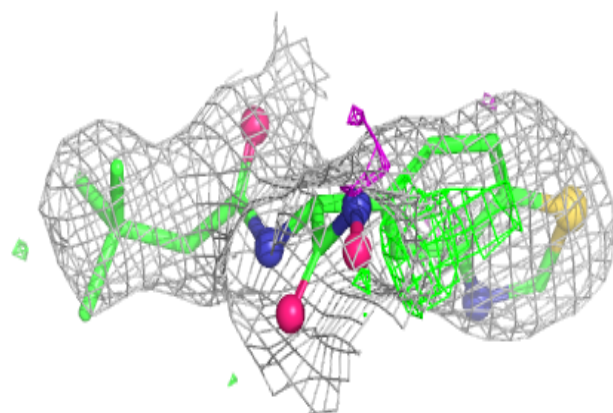
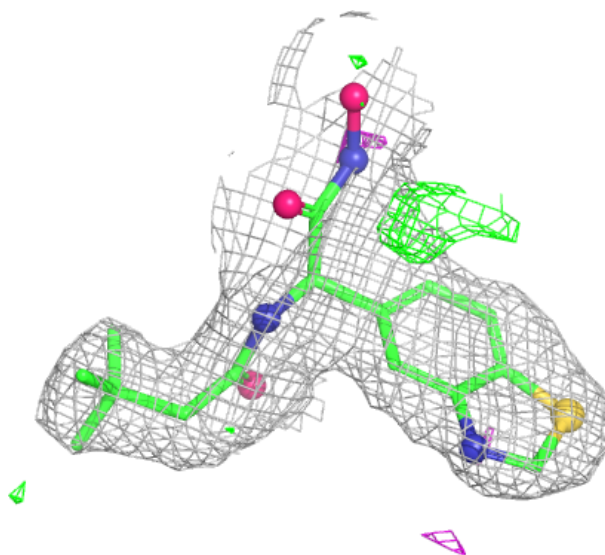
Electron density around A1CT5 G 705:

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



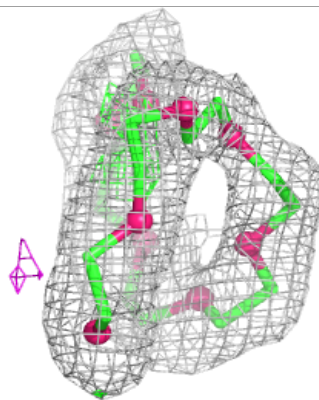
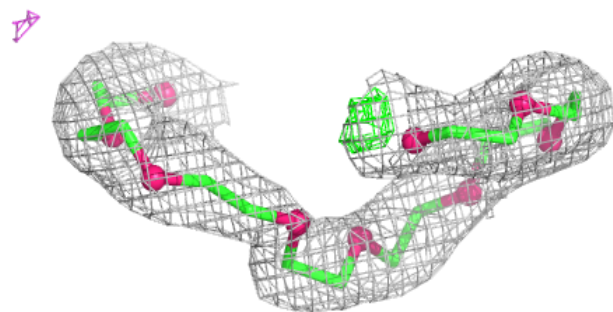
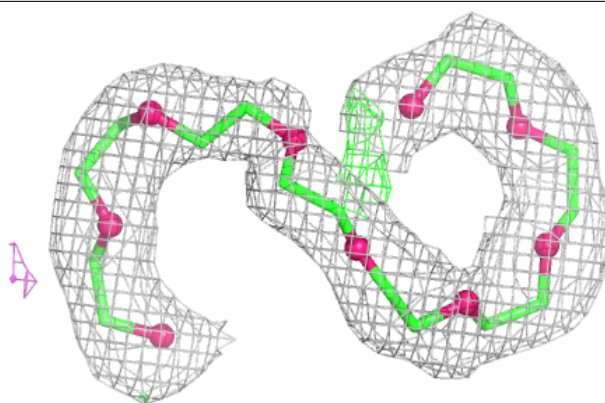
Electron density around A1CT4 K 706:

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



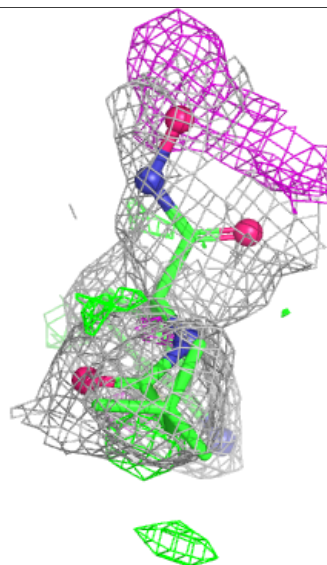
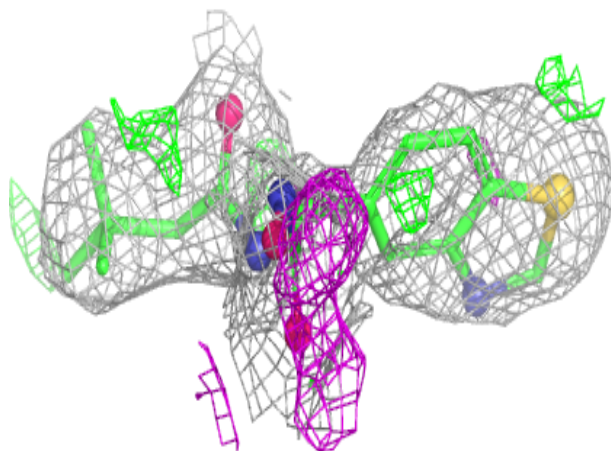
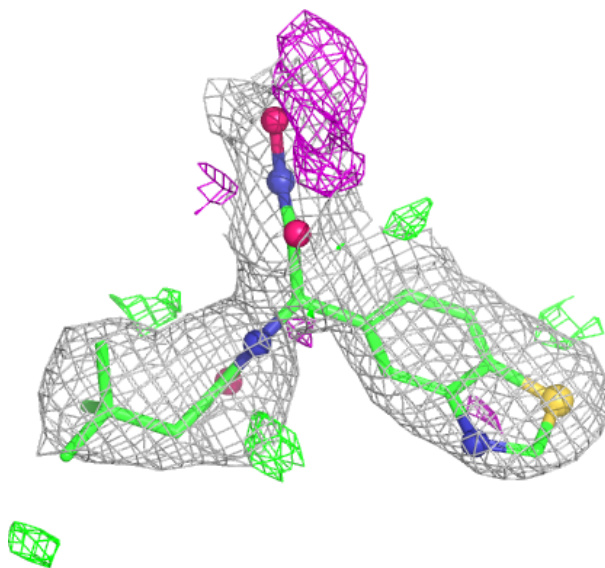
Electron density around 2PE H 712:

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



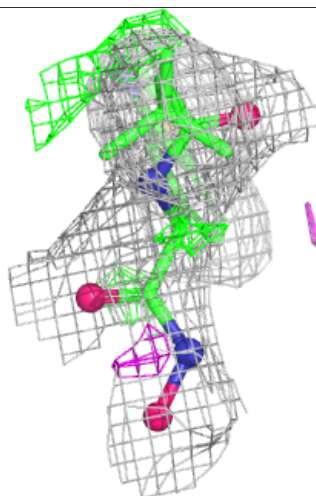
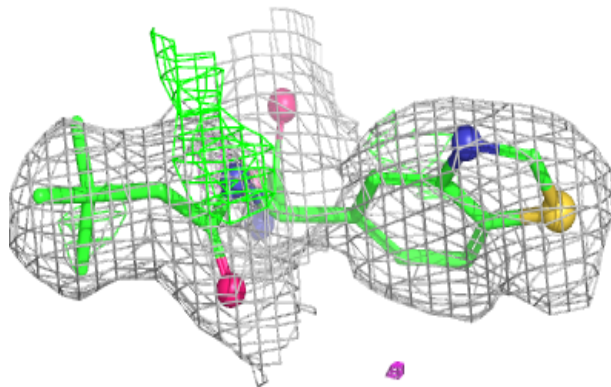
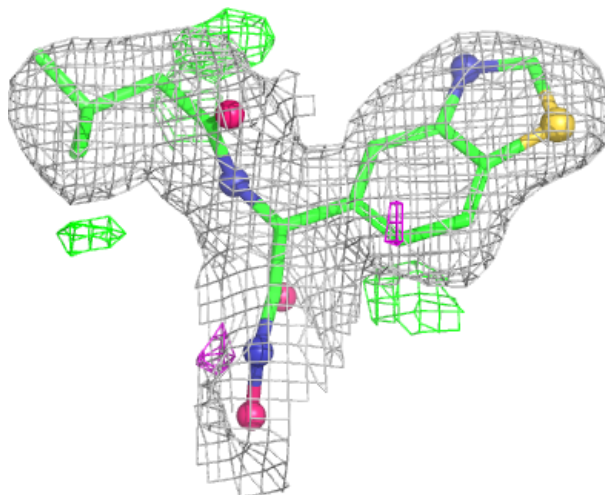
Electron density around A1CT4 C 710:

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



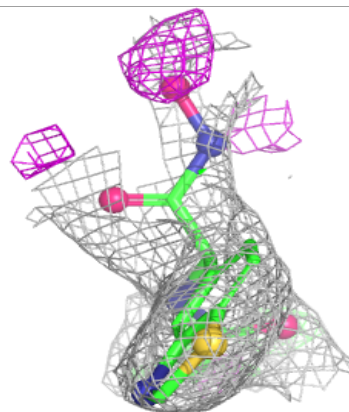
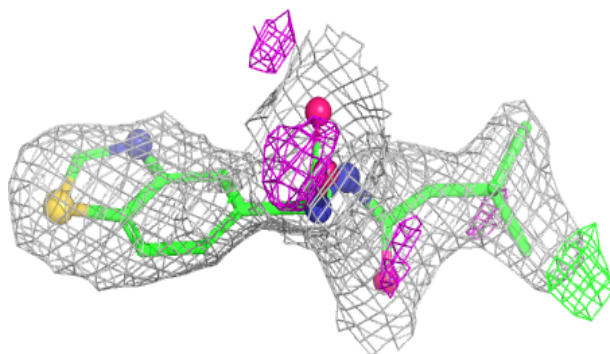
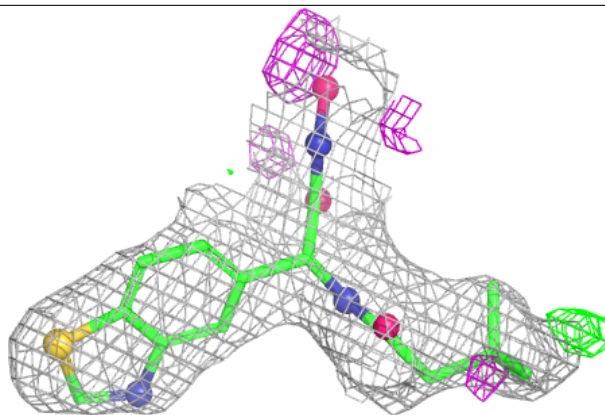
Electron density around A1CT4 A 710:

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



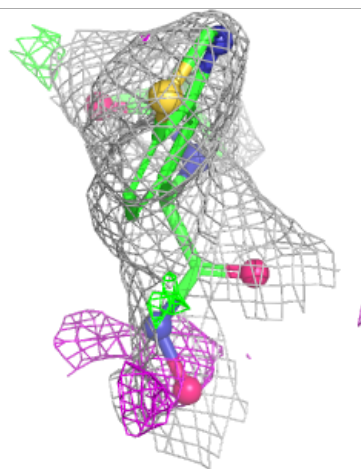
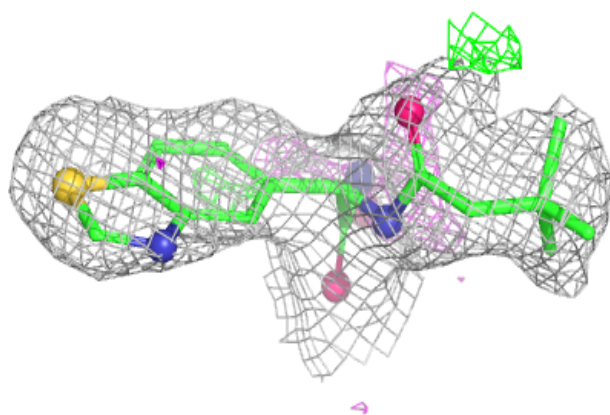
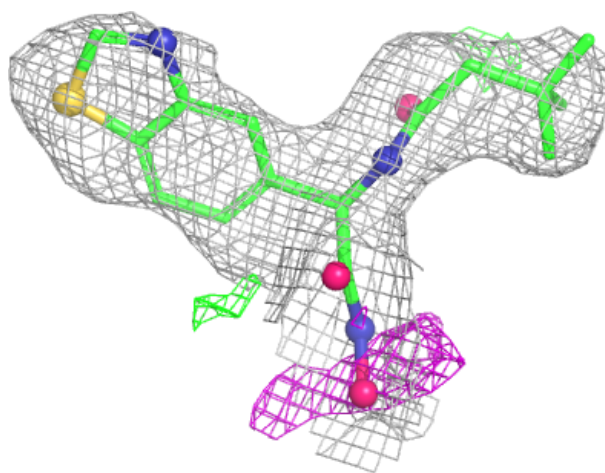
Electron density around A1CT4 J 707:

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



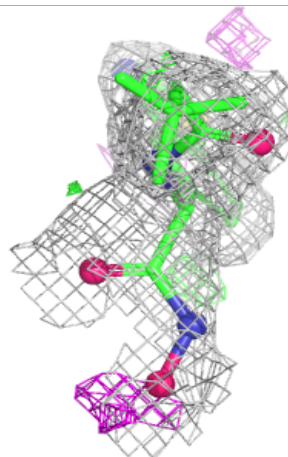
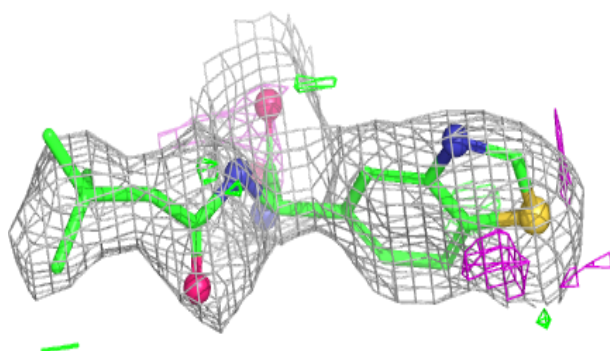
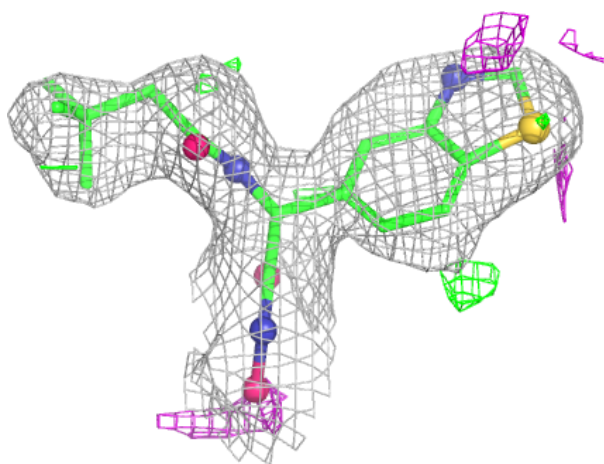
Electron density around A1CT4 E 708:

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



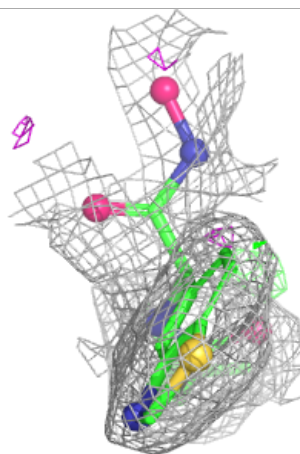
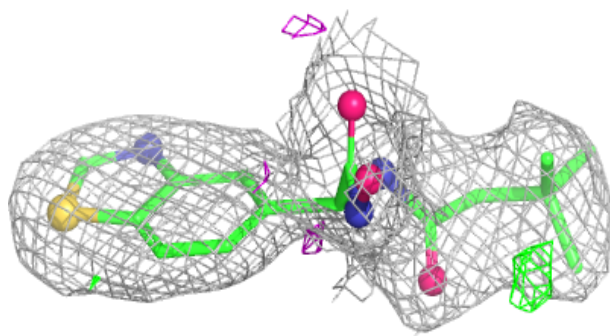
Electron density around A1CT4 F 707:

$2mF_o-DF_c$ (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.