



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:57 PM UTC

PDB ID : 9YC7 / pdb_00009yc7
Title : Plasmodium falciparum M17 aminopeptidase (PfA-M17) bound to inhibitor 3k (MIPS3415)
Authors : Mansouri, M.; McGowan, S.; Webb, C.T.
Deposited on : 2025-09-18
Resolution : 2.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

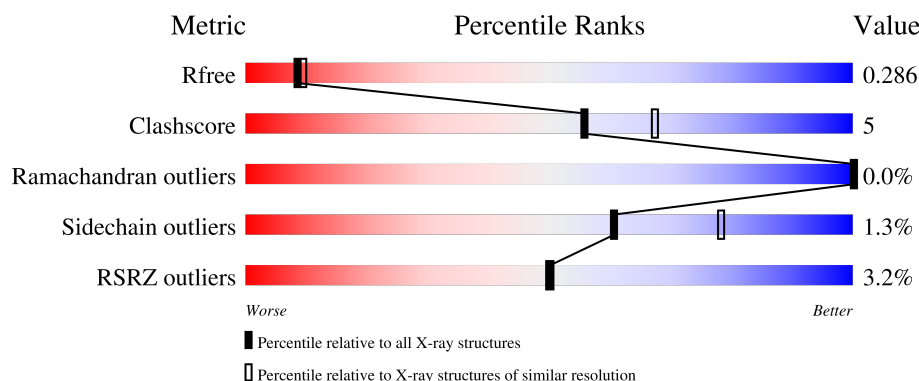
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 Å.

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



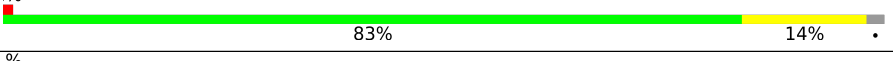
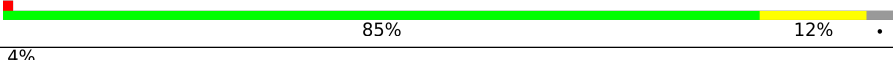
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	% 85% 13% .
1	B	527	9% 86% 11% .
1	C	527	2% 84% 14% .
1	D	527	% 86% 12% .
1	E	527	% 85% 11% .

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Mol	Chain	Length	Quality of chain
1	F	527	 5% 84% 12% . .
1	G	527	 % 87% 11% .
1	H	527	 9% 84% 13% .
1	I	527	 3% 86% 13% .
1	J	527	 % 83% 14% .
1	K	527	 % 85% 12% .
1	L	527	 4% 84% 13% .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 50351 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	514	Total	C	N	O	S	0	0	0
			3978	2551	643	765	19			
1	B	514	Total	C	N	O	S	0	1	0
			3950	2536	642	753	19			
1	C	518	Total	C	N	O	S	0	0	0
			4006	2568	650	768	20			
1	D	514	Total	C	N	O	S	0	2	0
			3987	2560	648	759	20			
1	E	510	Total	C	N	O	S	0	0	0
			3965	2545	643	758	19			
1	F	509	Total	C	N	O	S	0	0	0
			3908	2512	634	744	18			
1	G	515	Total	C	N	O	S	0	0	0
			3998	2564	646	768	20			
1	H	510	Total	C	N	O	S	0	0	0
			3915	2514	638	744	19			
1	I	518	Total	C	N	O	S	0	0	0
			4016	2574	654	769	19			
1	J	514	Total	C	N	O	S	0	0	0
			3988	2559	647	762	20			
1	K	510	Total	C	N	O	S	0	0	0
			3954	2540	643	752	19			
1	L	509	Total	C	N	O	S	0	0	0
			3886	2496	629	742	19			

There are 108 discrepancies between the modelled and reference sequences:

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

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

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

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

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

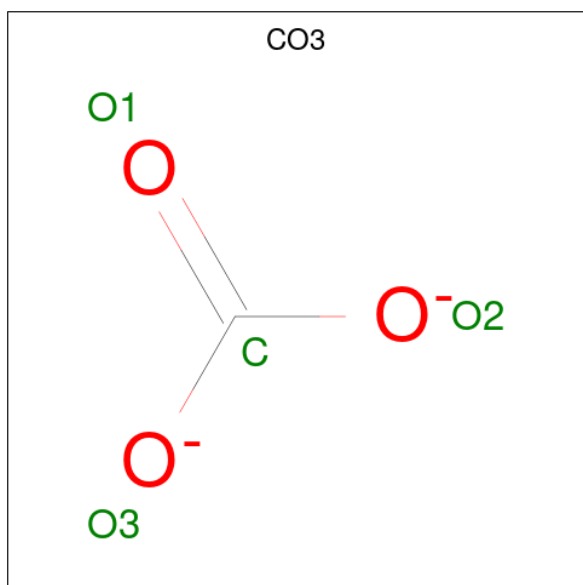
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0

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

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



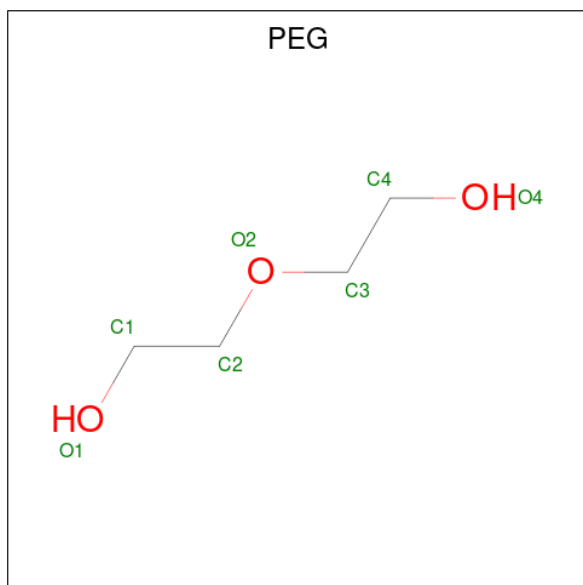
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	1	3		
3	B	1	Total	C	O	0	0
			4	1	3		
3	C	1	Total	C	O	0	0
			4	1	3		
3	D	1	Total	C	O	0	0
			4	1	3		
3	E	1	Total	C	O	0	0
			4	1	3		
3	F	1	Total	C	O	0	0
			4	1	3		
3	G	1	Total	C	O	0	0
			4	1	3		
3	H	1	Total	C	O	0	0
			4	1	3		
3	I	1	Total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

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

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



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

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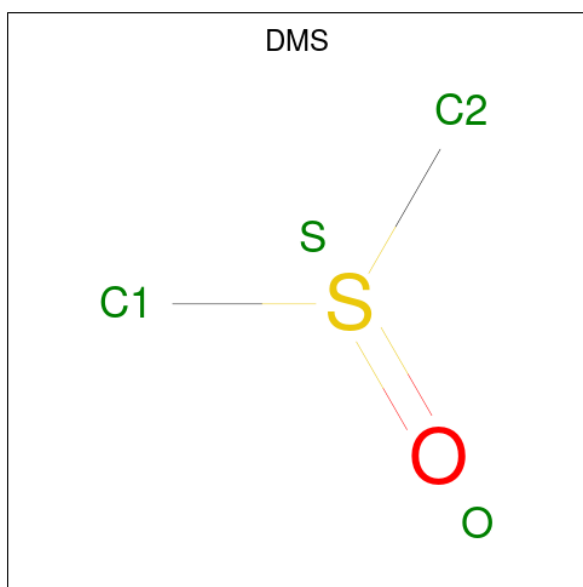
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		
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 DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



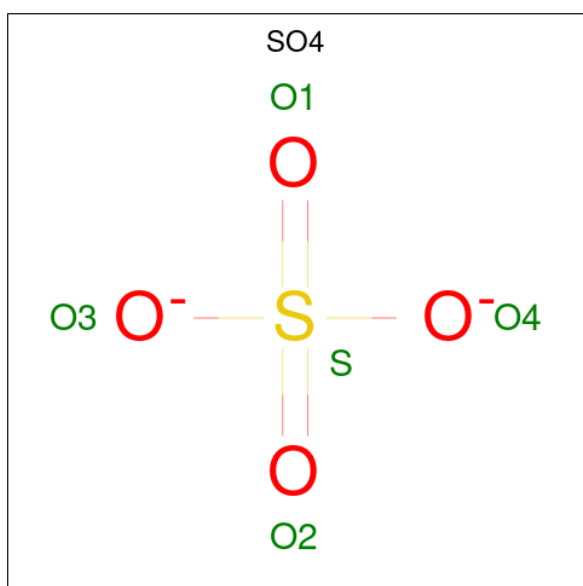
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	F	1	Total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

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



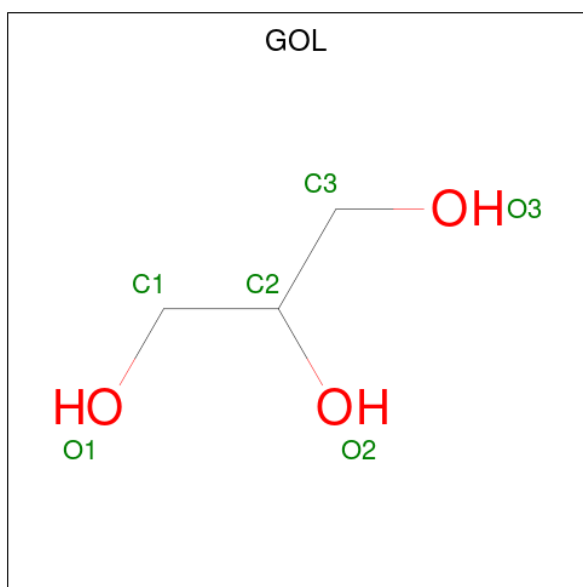
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

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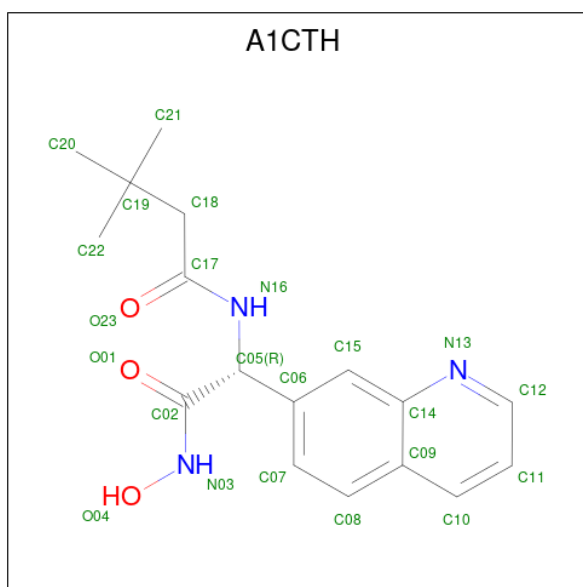
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



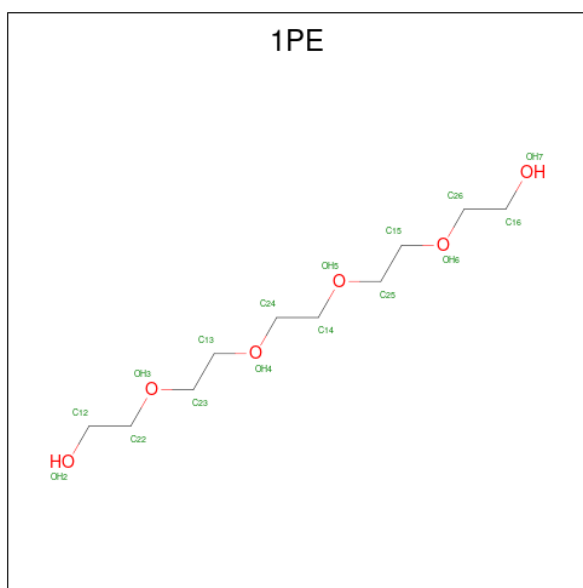
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	G	1	Total C O 6 3 3	0	0

- Molecule 8 is N-[(1R)-2-(hydroxyamino)-2-oxo-1-(quinolin-7-yl)ethyl]-3,3-dimethylbutanamide (CCD ID: A1CTH) (formula: C₁₇H₂₁N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			23	17	3	3		

- Molecule 9 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			16	10	6		
9	D	1	Total	C	O	0	0
			16	10	6		
9	E	1	Total	C	O	0	0
			13	8	5		
9	H	1	Total	C	O	0	0
			16	10	6		
9	I	1	Total	C	O	0	0
			16	10	6		
9	I	1	Total	C	O	0	0
			16	10	6		
9	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	226	Total	O	0	0
			226	226		
10	B	171	Total	O	0	0
			171	171		
10	C	188	Total	O	0	0
			188	188		
10	D	208	Total	O	0	0
			208	208		

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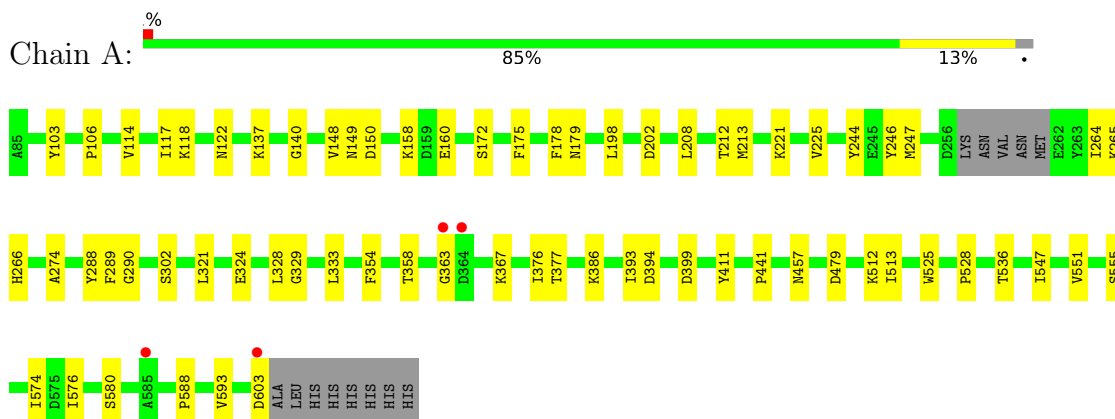
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	192	Total 192	O 192	0	0
10	F	170	Total 170	O 170	0	0
10	G	146	Total 146	O 146	0	0
10	H	140	Total 140	O 140	0	0
10	I	193	Total 193	O 193	0	0
10	J	181	Total 181	O 181	0	0
10	K	157	Total 157	O 157	0	0
10	L	126	Total 126	O 126	0	0

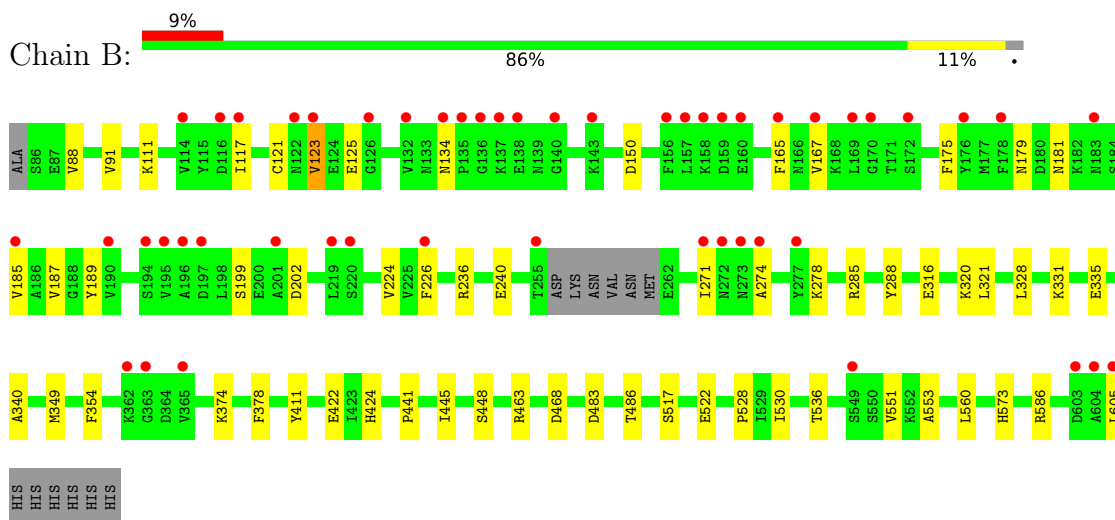
3 Residue-property plots [i](#)

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

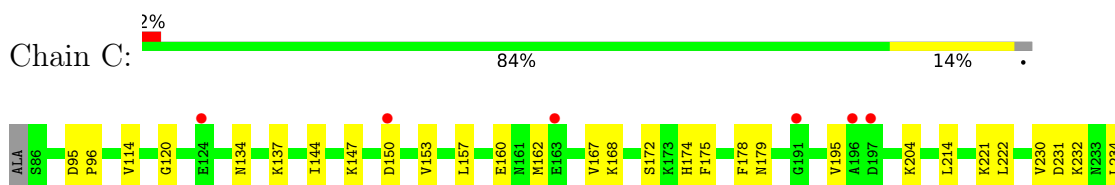
- Molecule 1: M17 leucyl aminopeptidase

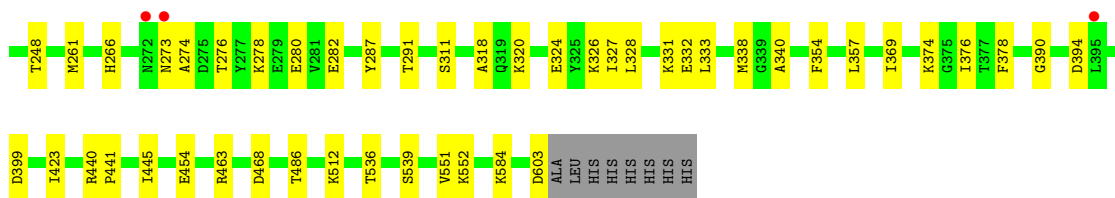


- Molecule 1: M17 leucyl aminopeptidase

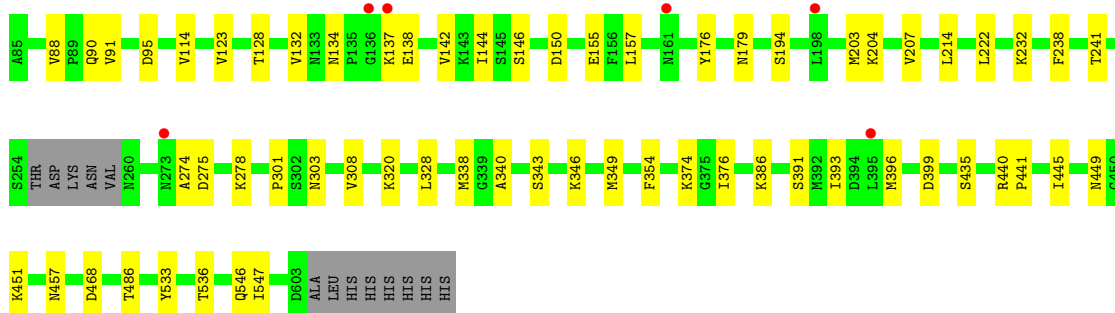
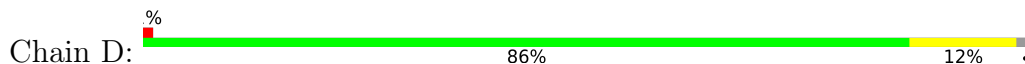


- Molecule 1: M17 leucyl aminopeptidase

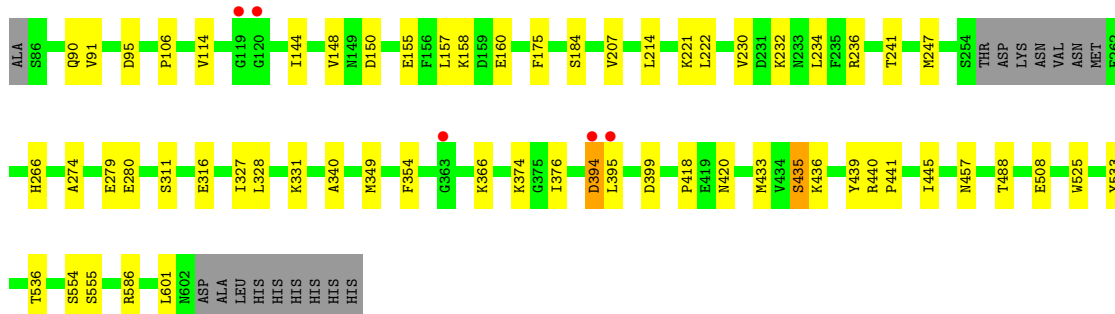
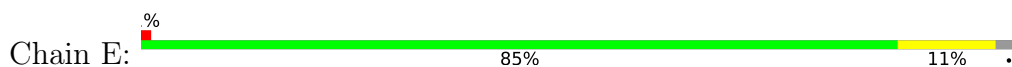




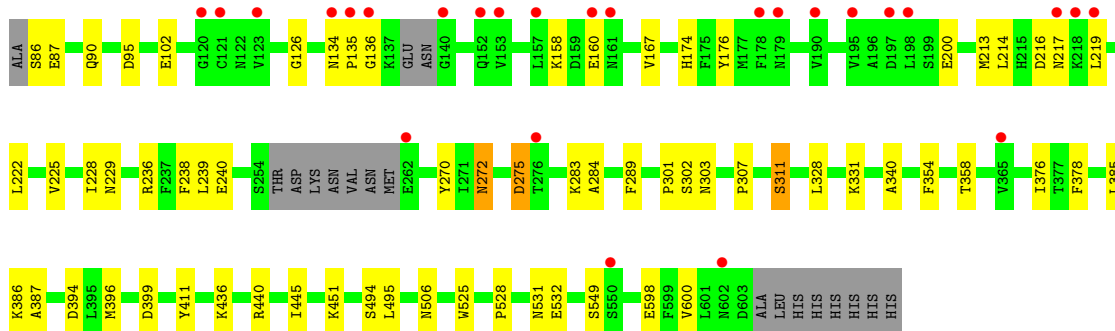
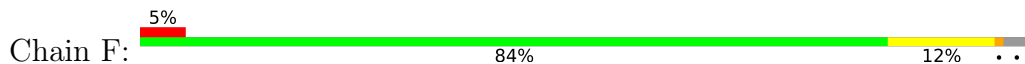
● Molecule 1: M17 leucyl aminopeptidase



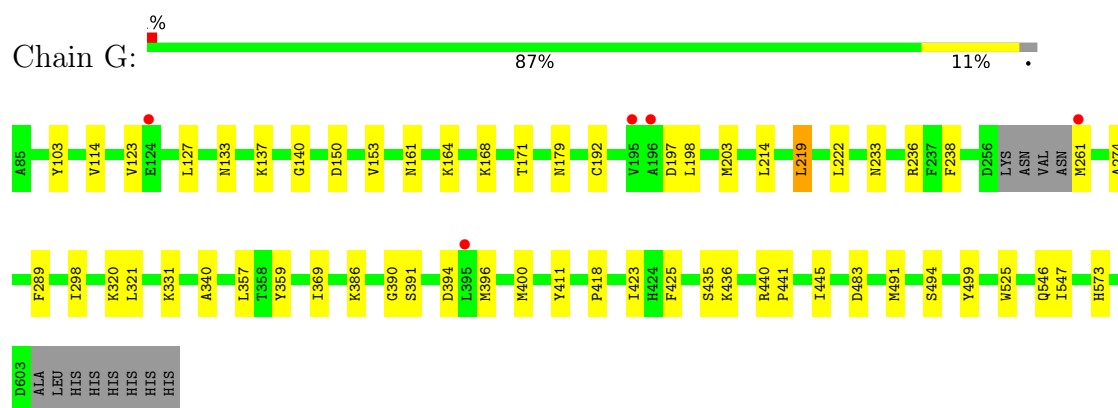
● Molecule 1: M17 leucyl aminopeptidase



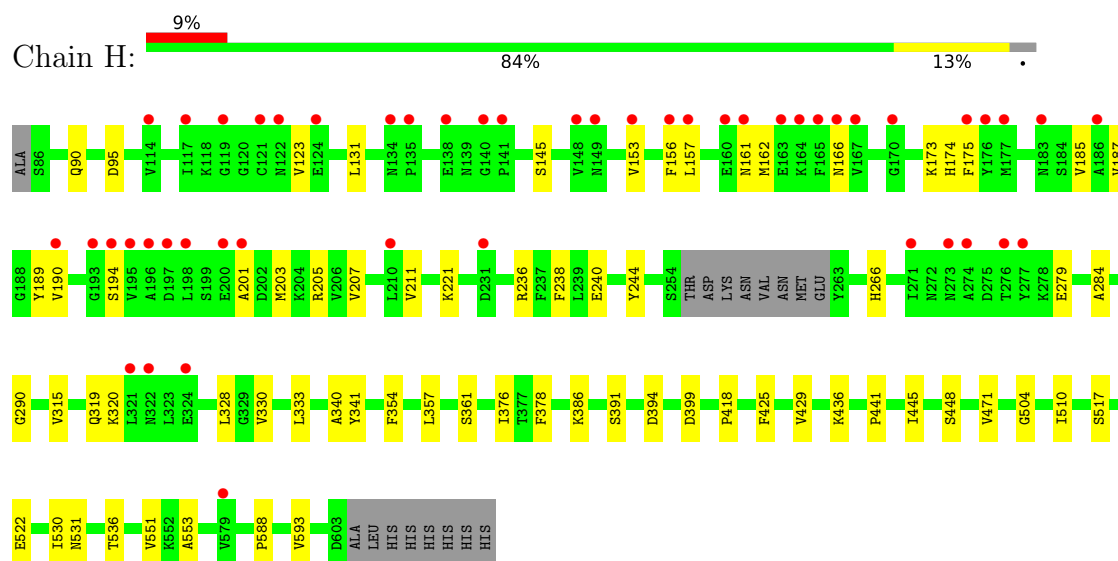
● Molecule 1: M17 leucyl aminopeptidase



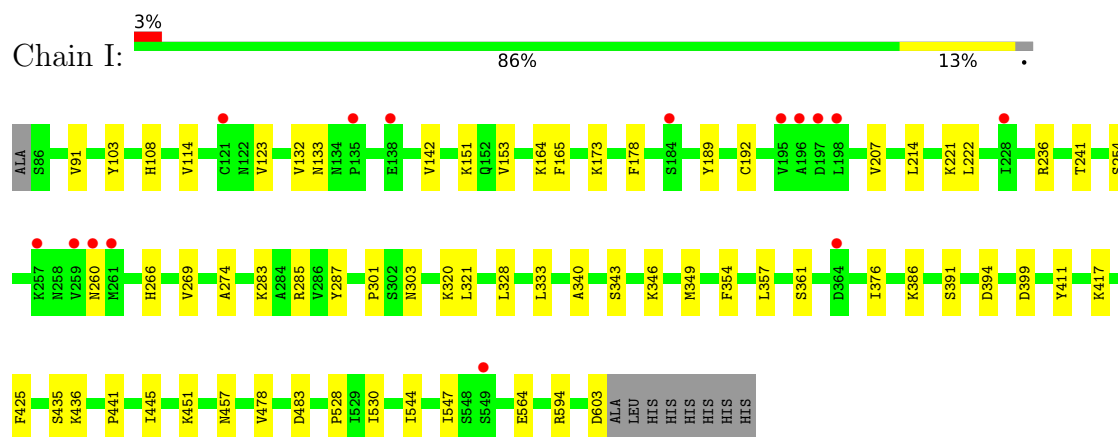
● Molecule 1: M17 leucyl aminopeptidase



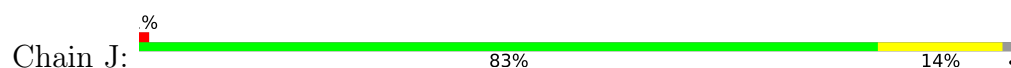
- Molecule 1: M17 leucyl aminopeptidase

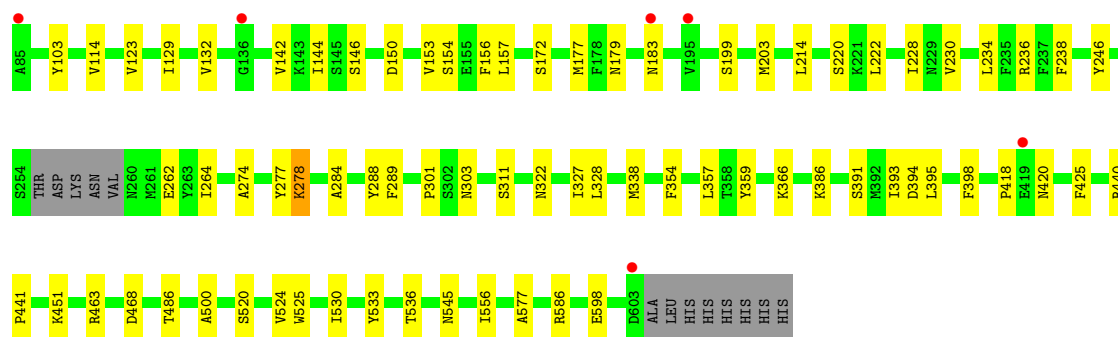


- Molecule 1: M17 leucyl aminopeptidase

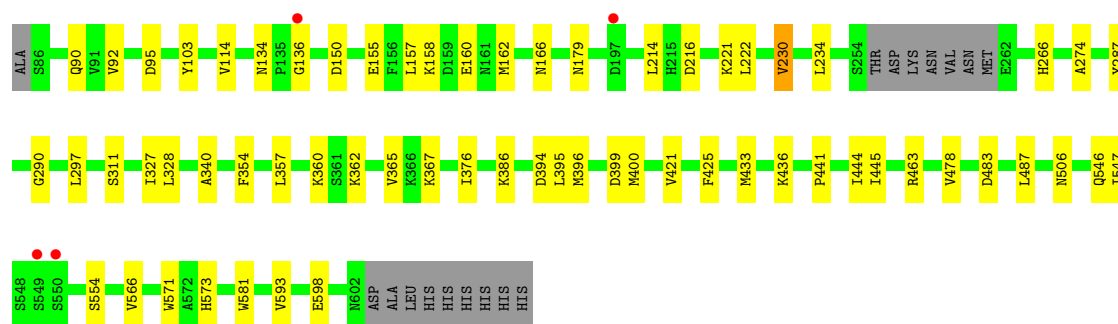
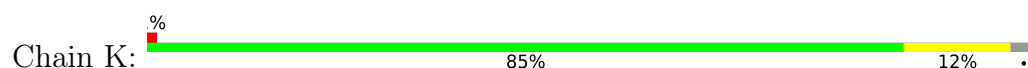


- Molecule 1: M17 leucyl aminopeptidase

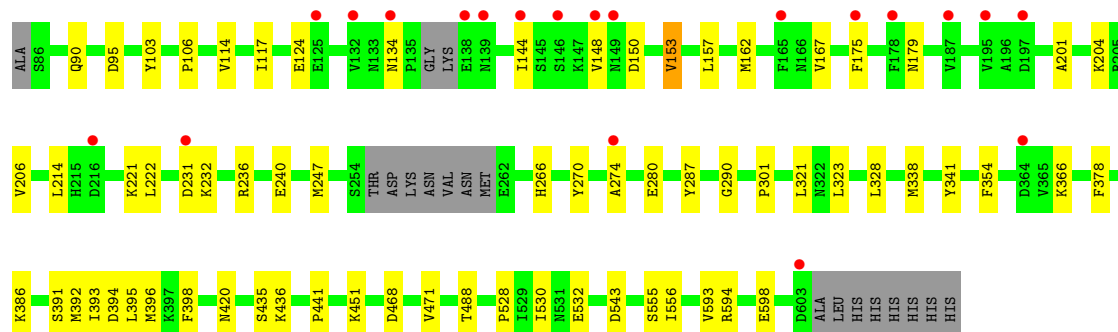
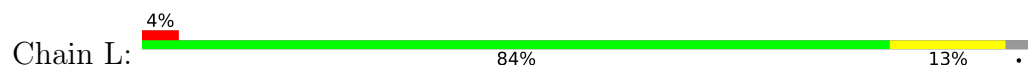




● Molecule 1: M17 leucyl aminopeptidase



● 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	173.84Å 177.51Å 230.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.37 48.30 – 2.37	Depositor EDS
% Data completeness (in resolution range)	83.1 (48.30-2.37) 86.0 (48.30-2.37)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.248 , 0.287 0.249 , 0.286	Depositor DCC
R_{free} test set	13813 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50351	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 48.57 % 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 8.4453e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, CO3, SO4, PEG, ZN, GOL, DMS, A1CTH

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	0.06	0/4055	0.22	0/5492
1	B	0.07	0/4031	0.23	0/5465
1	C	0.07	0/4084	0.22	0/5533
1	D	0.07	0/4064	0.23	0/5503
1	E	0.06	0/4042	0.23	0/5470
1	F	0.06	0/3984	0.22	0/5399
1	G	0.06	0/4075	0.22	0/5515
1	H	0.06	0/3991	0.22	0/5408
1	I	0.06	0/4094	0.21	0/5543
1	J	0.07	0/4065	0.22	0/5501
1	K	0.06	0/4031	0.22	0/5456
1	L	0.06	0/3961	0.22	0/5374
All	All	0.07	0/48477	0.22	0/65659

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3978	0	3955	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3950	0	3904	35	0
1	C	4006	0	3982	51	0
1	D	3987	0	3971	39	0
1	E	3965	0	3966	38	0
1	F	3908	0	3867	41	0
1	G	3998	0	3990	38	0
1	H	3915	0	3887	39	0
1	I	4016	0	4005	39	0
1	J	3988	0	3984	45	0
1	K	3954	0	3956	39	0
1	L	3886	0	3818	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	1	0
3	D	4	0	0	1	0
3	E	4	0	0	0	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	1	0
3	K	4	0	0	1	0
3	L	4	0	0	0	0
4	A	35	0	50	4	0
4	B	28	0	40	0	0
4	C	7	0	10	1	0
4	D	14	0	20	1	0
4	E	42	0	60	1	0
4	F	35	0	50	2	0
4	G	21	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	7	0	10	0	0
4	I	21	0	30	1	0
4	J	28	0	40	1	0
4	K	35	0	50	4	0
4	L	28	0	40	6	0
5	A	8	0	12	1	0
5	B	8	0	12	1	0
5	C	4	0	6	0	0
5	E	8	0	12	0	0
5	F	12	0	18	3	0
5	G	4	0	6	2	0
5	H	4	0	6	0	0
5	I	4	0	6	0	0
5	J	16	0	24	5	0
5	K	4	0	6	1	0
5	L	4	0	6	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	1	0
6	D	5	0	0	0	0
6	E	10	0	0	0	0
6	F	15	0	0	0	0
6	G	5	0	0	1	0
6	I	10	0	0	1	0
6	J	20	0	0	0	0
6	K	15	0	0	0	0
6	L	5	0	0	0	0
7	A	6	0	8	0	0
7	G	6	0	8	0	0
8	A	23	0	0	0	0
9	C	16	0	22	0	0
9	D	16	0	22	0	0
9	E	13	0	17	1	0
9	H	16	0	22	2	0
9	I	32	0	44	4	0
9	L	10	0	12	0	0
10	A	226	0	0	1	0
10	B	171	0	0	0	0
10	C	188	0	0	1	0
10	D	208	0	0	1	0
10	E	192	0	0	1	0
10	F	170	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	G	146	0	0	3	0
10	H	140	0	0	0	0
10	I	193	0	0	1	0
10	J	181	0	0	1	0
10	K	157	0	0	0	0
10	L	126	0	0	0	0
All	All	50351	0	47984	453	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 453 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:D:338:MET:HE3	1:D:468:ASP:HB3	1.62	0.80
1:H:531:ASN:HB2	4:K:701:PEG:H11	1.64	0.78
1:G:298:ILE:HA	1:G:400:MET:HE1	1.66	0.78
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.67	0.77
1:L:392:MET:HB3	1:L:395:LEU:HD23	1.71	0.73

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/527 (97%)	493 (97%)	17 (3%)	0	100	100
1	B	511/527 (97%)	492 (96%)	19 (4%)	0	100	100
1	C	516/527 (98%)	504 (98%)	12 (2%)	0	100	100
1	D	512/527 (97%)	497 (97%)	14 (3%)	1 (0%)	43	56
1	E	506/527 (96%)	495 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	503/527 (95%)	485 (96%)	16 (3%)	2 (0%)	30	40
1	G	511/527 (97%)	495 (97%)	16 (3%)	0	100	100
1	H	506/527 (96%)	492 (97%)	14 (3%)	0	100	100
1	I	516/527 (98%)	504 (98%)	12 (2%)	0	100	100
1	J	510/527 (97%)	497 (98%)	13 (2%)	0	100	100
1	K	506/527 (96%)	489 (97%)	17 (3%)	0	100	100
1	L	503/527 (95%)	487 (97%)	16 (3%)	0	100	100
All	All	6110/6324 (97%)	5930 (97%)	177 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	396	MET
1	F	136	GLY
1	F	135	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	435/454 (96%)	433 (100%)	2 (0%)	81	90
1	B	426/454 (94%)	420 (99%)	6 (1%)	59	77
1	C	438/454 (96%)	435 (99%)	3 (1%)	76	87
1	D	434/454 (96%)	433 (100%)	1 (0%)	87	94
1	E	436/454 (96%)	430 (99%)	6 (1%)	59	77
1	F	421/454 (93%)	411 (98%)	10 (2%)	43	63
1	G	439/454 (97%)	435 (99%)	4 (1%)	70	84
1	H	423/454 (93%)	416 (98%)	7 (2%)	53	72
1	I	440/454 (97%)	433 (98%)	7 (2%)	55	74
1	J	437/454 (96%)	427 (98%)	10 (2%)	44	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	433/454 (95%)	429 (99%)	4 (1%)	70	84
1	L	416/454 (92%)	410 (99%)	6 (1%)	59	77
All	All	5178/5448 (95%)	5112 (99%)	66 (1%)	61	78

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	230	VAL
1	K	554	SER
1	L	471	VAL
1	F	311	SER
1	F	275	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	545	ASN
1	I	260	ASN
1	K	602	ASN
1	G	602	ASN
1	H	161	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 131 ligands modelled in this entry, 24 are monoatomic - leaving 107 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$
4	PEG	K	701	-	6,6,6	0.10	0	5,5,5	0.10	0
6	SO4	J	1013	-	4,4,4	0.22	0	6,6,6	0.08	0
4	PEG	K	712	-	6,6,6	0.11	0	5,5,5	0.07	0
5	DMS	E	1011	-	3,3,3	0.67	0	3,3,3	0.52	0
4	PEG	J	1004	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	B	1005	-	6,6,6	0.11	0	5,5,5	0.10	0
5	DMS	J	1010	-	3,3,3	0.66	0	3,3,3	0.51	0
8	A1CTH	A	1010	2	23,24,24	2.46	8 (34%)	29,34,34	1.24	2 (6%)
4	PEG	A	1004	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	H	1006	-	6,6,6	0.11	0	5,5,5	0.09	0
6	SO4	K	708	-	4,4,4	0.24	0	6,6,6	0.08	0
4	PEG	F	704	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	E	1013	-	6,6,6	0.12	0	5,5,5	0.09	0
4	PEG	B	1011	-	6,6,6	0.11	0	5,5,5	0.10	0
6	SO4	C	706	-	4,4,4	0.23	0	6,6,6	0.08	0
4	PEG	G	1003	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	E	1007	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	L	1010	-	6,6,6	0.10	0	5,5,5	0.12	0
6	SO4	J	1006	-	4,4,4	0.23	0	6,6,6	0.08	0
5	DMS	J	1012	-	3,3,3	0.67	0	3,3,3	0.57	0
5	DMS	F	708	-	3,3,3	0.67	0	3,3,3	0.52	0
5	DMS	J	1011	-	3,3,3	0.65	0	3,3,3	0.50	0
4	PEG	E	1006	-	6,6,6	0.11	0	5,5,5	0.09	0
4	PEG	J	1014	-	6,6,6	0.11	0	5,5,5	0.11	0
4	PEG	L	1009	-	6,6,6	0.11	0	5,5,5	0.08	0
4	PEG	K	705	-	6,6,6	0.11	0	5,5,5	0.09	0
9	1PE	I	1005	-	15,15,15	0.11	0	14,14,14	0.09	0
5	DMS	E	1012	-	3,3,3	0.67	0	3,3,3	0.51	0
4	PEG	E	1005	-	6,6,6	0.12	0	5,5,5	0.08	0
4	PEG	F	714	-	6,6,6	0.11	0	5,5,5	0.08	0
3	CO3	F	710	-	3,3,3	0.79	0	2,3,3	0.09	0
4	PEG	K	711	-	6,6,6	0.11	0	5,5,5	0.10	0
5	DMS	I	1008	-	3,3,3	0.66	0	3,3,3	0.49	0
4	PEG	J	1015	-	6,6,6	0.12	0	5,5,5	0.07	0
3	CO3	K	710	-	3,3,3	0.84	0	2,3,3	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	D	1007	-	6,6,6	0.11	0	5,5,5	0.10	0
6	SO4	I	1003	-	4,4,4	0.24	0	6,6,6	0.07	0
7	GOL	G	1008	-	5,5,5	0.92	0	5,5,5	1.09	0
6	SO4	F	709	-	4,4,4	0.23	0	6,6,6	0.07	0
4	PEG	I	1009	-	6,6,6	0.13	0	5,5,5	0.03	0
4	PEG	B	1009	-	6,6,6	0.11	0	5,5,5	0.09	0
9	1PE	H	1003	-	15,15,15	0.12	0	14,14,14	0.10	0
3	CO3	L	1006	-	3,3,3	0.83	0	2,3,3	0.17	0
5	DMS	C	701	-	3,3,3	0.67	0	3,3,3	0.49	0
4	PEG	A	1011	-	6,6,6	0.10	0	5,5,5	0.09	0
6	SO4	F	701	-	4,4,4	0.22	0	6,6,6	0.08	0
3	CO3	A	1002	-	3,3,3	0.81	0	2,3,3	0.09	0
4	PEG	E	1004	-	6,6,6	0.11	0	5,5,5	0.10	0
6	SO4	D	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
4	PEG	G	1009	-	6,6,6	0.12	0	5,5,5	0.07	0
5	DMS	B	1007	-	3,3,3	0.66	0	3,3,3	0.50	0
4	PEG	G	1005	-	6,6,6	0.11	0	5,5,5	0.10	0
6	SO4	E	1008	-	4,4,4	0.23	0	6,6,6	0.08	0
5	DMS	B	1008	-	3,3,3	0.67	0	3,3,3	0.53	0
6	SO4	E	1010	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	B	1006	-	4,4,4	0.24	0	6,6,6	0.08	0
5	DMS	H	1005	-	3,3,3	0.67	0	3,3,3	0.54	0
4	PEG	L	1004	-	6,6,6	0.10	0	5,5,5	0.10	0
5	DMS	A	1008	-	3,3,3	0.67	0	3,3,3	0.52	0
4	PEG	I	1010	-	6,6,6	0.11	0	5,5,5	0.10	0
4	PEG	F	713	-	6,6,6	0.11	0	5,5,5	0.10	0
9	1PE	E	1009	-	12,12,15	0.11	0	11,11,14	0.13	0
6	SO4	G	1006	-	4,4,4	0.24	0	6,6,6	0.07	0
4	PEG	K	706	-	6,6,6	0.12	0	5,5,5	0.08	0
3	CO3	J	1009	-	3,3,3	0.83	0	2,3,3	0.13	0
4	PEG	F	706	-	6,6,6	0.10	0	5,5,5	0.09	0
4	PEG	J	1003	-	6,6,6	0.11	0	5,5,5	0.10	0
5	DMS	L	1007	-	3,3,3	0.67	0	3,3,3	0.52	0
3	CO3	B	1002	-	3,3,3	0.85	0	2,3,3	0.23	0
5	DMS	J	1008	-	3,3,3	0.67	0	3,3,3	0.52	0
4	PEG	L	1008	-	6,6,6	0.11	0	5,5,5	0.09	0
5	DMS	K	709	-	3,3,3	0.66	0	3,3,3	0.51	0
6	SO4	K	707	-	4,4,4	0.23	0	6,6,6	0.08	0
9	1PE	D	1006	-	15,15,15	0.11	0	14,14,14	0.09	0
4	PEG	A	1013	-	6,6,6	0.11	0	5,5,5	0.10	0
4	PEG	I	1011	-	6,6,6	0.10	0	5,5,5	0.11	0
3	CO3	C	708	-	3,3,3	0.87	0	2,3,3	0.17	0
6	SO4	A	1006	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	A	1012	-	6,6,6	0.11	0	5,5,5	0.08	0
6	SO4	J	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
4	PEG	F	707	-	6,6,6	0.12	0	5,5,5	0.09	0
3	CO3	G	1007	-	3,3,3	0.81	0	2,3,3	0.13	0
6	SO4	J	1007	-	4,4,4	0.23	0	6,6,6	0.08	0
9	1PE	L	1005	-	9,9,15	0.09	0	8,8,14	0.17	0
5	DMS	F	712	-	3,3,3	0.67	0	3,3,3	0.54	0
7	GOL	A	1009	-	5,5,5	0.96	0	5,5,5	1.06	0
5	DMS	A	1005	-	3,3,3	0.67	0	3,3,3	0.53	0
4	PEG	E	1014	-	6,6,6	0.10	0	5,5,5	0.11	0
6	SO4	K	704	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	I	1004	-	4,4,4	0.24	0	6,6,6	0.07	0
3	CO3	I	1007	-	3,3,3	0.83	0	2,3,3	0.12	0
3	CO3	D	1002	-	3,3,3	0.86	0	2,3,3	0.11	0
3	CO3	H	1004	-	3,3,3	0.80	0	2,3,3	0.05	0
6	SO4	C	705	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	F	705	-	4,4,4	0.24	0	6,6,6	0.08	0
5	DMS	F	711	-	3,3,3	0.67	0	3,3,3	0.50	0
6	SO4	B	1004	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	L	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
4	PEG	C	704	-	6,6,6	0.12	0	5,5,5	0.06	0
9	1PE	I	1006	-	15,15,15	0.11	0	14,14,14	0.08	0
9	1PE	C	707	-	15,15,15	0.11	0	14,14,14	0.10	0
5	DMS	G	1004	-	3,3,3	0.67	0	3,3,3	0.54	0
4	PEG	A	1014	-	6,6,6	0.11	0	5,5,5	0.09	0
3	CO3	E	1002	-	3,3,3	0.81	0	2,3,3	0.09	0
4	PEG	B	1010	-	6,6,6	0.12	0	5,5,5	0.07	0
4	PEG	D	1004	-	6,6,6	0.12	0	5,5,5	0.08	0
6	SO4	A	1007	-	4,4,4	0.24	0	6,6,6	0.07	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
4	PEG	E	1005	-	-	4/4/4/4	-
4	PEG	K	701	-	-	2/4/4/4	-
7	GOL	A	1009	-	-	0/4/4/4	-
4	PEG	F	714	-	-	2/4/4/4	-
4	PEG	E	1014	-	-	1/4/4/4	-
4	PEG	K	712	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	K	711	-	-	3/4/4/4	-
4	PEG	J	1004	-	-	1/4/4/4	-
4	PEG	B	1005	-	-	1/4/4/4	-
4	PEG	J	1015	-	-	0/4/4/4	-
4	PEG	L	1004	-	-	3/4/4/4	-
4	PEG	D	1007	-	-	1/4/4/4	-
4	PEG	F	713	-	-	2/4/4/4	-
4	PEG	I	1010	-	-	2/4/4/4	-
7	GOL	G	1008	-	-	0/4/4/4	-
8	A1CTH	A	1010	2	-	3/19/19/19	0/2/2/2
9	1PE	E	1009	-	-	4/10/10/13	-
4	PEG	A	1004	-	-	2/4/4/4	-
4	PEG	H	1006	-	-	1/4/4/4	-
4	PEG	K	706	-	-	1/4/4/4	-
4	PEG	F	704	-	-	1/4/4/4	-
4	PEG	I	1009	-	-	2/4/4/4	-
4	PEG	B	1009	-	-	3/4/4/4	-
9	1PE	H	1003	-	-	7/13/13/13	-
4	PEG	E	1013	-	-	2/4/4/4	-
4	PEG	F	706	-	-	2/4/4/4	-
4	PEG	J	1003	-	-	0/4/4/4	-
4	PEG	B	1011	-	-	3/4/4/4	-
4	PEG	L	1008	-	-	3/4/4/4	-
4	PEG	G	1003	-	-	1/4/4/4	-
4	PEG	E	1007	-	-	2/4/4/4	-
4	PEG	L	1010	-	-	2/4/4/4	-
9	1PE	D	1006	-	-	4/13/13/13	-
4	PEG	A	1013	-	-	1/4/4/4	-
4	PEG	I	1011	-	-	1/4/4/4	-
4	PEG	A	1011	-	-	1/4/4/4	-
4	PEG	C	704	-	-	3/4/4/4	-
4	PEG	E	1006	-	-	0/4/4/4	-
4	PEG	J	1014	-	-	2/4/4/4	-
9	1PE	I	1006	-	-	4/13/13/13	-
4	PEG	A	1012	-	-	3/4/4/4	-
4	PEG	E	1004	-	-	3/4/4/4	-
9	1PE	C	707	-	-	8/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	L	1009	-	-	2/4/4/4	-
4	PEG	A	1014	-	-	1/4/4/4	-
4	PEG	F	707	-	-	4/4/4/4	-
9	1PE	L	1005	-	-	3/7/7/13	-
4	PEG	K	705	-	-	2/4/4/4	-
4	PEG	G	1009	-	-	0/4/4/4	-
9	1PE	I	1005	-	-	7/13/13/13	-
4	PEG	B	1010	-	-	3/4/4/4	-
4	PEG	G	1005	-	-	2/4/4/4	-
4	PEG	D	1004	-	-	2/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1010	A1CTH	C17-N16	7.53	1.50	1.34
8	A	1010	A1CTH	C09-C14	-3.80	1.36	1.42
8	A	1010	A1CTH	C07-C06	3.53	1.44	1.39
8	A	1010	A1CTH	O04-N03	3.53	1.48	1.40
8	A	1010	A1CTH	C12-N13	3.28	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1010	A1CTH	C18-C17-N16	2.65	120.07	115.65
8	A	1010	A1CTH	C11-C12-N13	-2.55	120.23	123.97

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	1006	1PE	OH6-C15-C25-OH5
9	H	1003	1PE	C12-C22-OH3-C23
4	A	1004	PEG	O2-C3-C4-O4
4	E	1005	PEG	O2-C3-C4-O4
4	E	1007	PEG	O1-C1-C2-O2

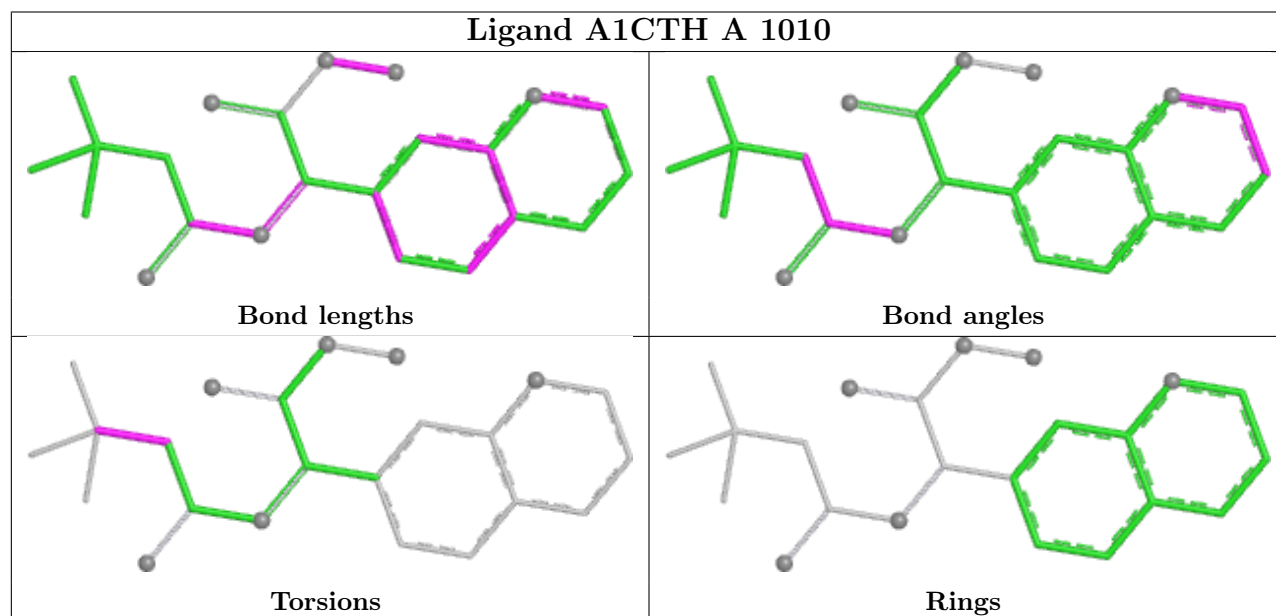
There are no ring outliers.

39 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	701	PEG	2	0
4	K	712	PEG	1	0
4	J	1004	PEG	1	0
5	J	1010	DMS	1	0
4	A	1004	PEG	1	0
6	C	706	SO4	1	0
4	L	1010	PEG	1	0
5	J	1012	DMS	1	0
5	F	708	DMS	1	0
5	J	1011	DMS	1	0
4	L	1009	PEG	2	0
4	K	705	PEG	1	0
9	I	1005	1PE	1	0
4	E	1005	PEG	1	0
3	K	710	CO3	1	0
4	I	1009	PEG	1	0
9	H	1003	1PE	2	0
4	A	1011	PEG	2	0
5	B	1007	DMS	1	0
5	A	1008	DMS	1	0
4	F	713	PEG	1	0
9	E	1009	1PE	1	0
6	G	1006	SO4	1	0
3	J	1009	CO3	1	0
4	F	706	PEG	1	0
3	B	1002	CO3	1	0
5	J	1008	DMS	2	0
4	L	1008	PEG	3	0
5	K	709	DMS	1	0
4	A	1013	PEG	1	0
3	C	708	CO3	1	0
5	F	712	DMS	1	0
6	I	1004	SO4	1	0
3	D	1002	CO3	1	0
5	F	711	DMS	1	0
4	C	704	PEG	1	0
9	I	1006	1PE	3	0
5	G	1004	DMS	2	0
4	D	1004	PEG	1	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.



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	514/527 (97%)	0.25	4 (0%)	82 82	15, 22, 39, 75	1 (0%)
1	B	514/527 (97%)	0.59	50 (9%)	13 12	14, 25, 59, 81	1 (0%)
1	C	518/527 (98%)	0.31	9 (1%)	69 68	14, 22, 48, 69	0
1	D	514/527 (97%)	0.24	6 (1%)	76 76	14, 22, 39, 56	2 (0%)
1	E	510/527 (96%)	0.19	5 (0%)	79 78	15, 21, 38, 58	0
1	F	509/527 (96%)	0.48	26 (5%)	33 33	15, 24, 54, 72	0
1	G	515/527 (97%)	0.25	5 (0%)	79 78	15, 22, 41, 66	0
1	H	510/527 (96%)	0.56	49 (9%)	13 12	14, 24, 61, 82	1 (0%)
1	I	518/527 (98%)	0.37	15 (2%)	53 53	15, 23, 50, 72	0
1	J	514/527 (97%)	0.22	6 (1%)	76 76	14, 22, 41, 63	0
1	K	510/527 (96%)	0.19	4 (0%)	82 82	15, 21, 37, 61	0
1	L	509/527 (96%)	0.41	20 (3%)	43 43	15, 23, 53, 77	0
All	All	6155/6324 (97%)	0.34	199 (3%)	50 50	14, 22, 50, 82	5 (0%)

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	196	ALA	5.6
1	C	395	LEU	5.1
1	B	176	TYR	4.9
1	H	322	ASN	4.8
1	K	136	GLY	4.4

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	F	702	1/1	0.63	0.17	121,121,121,121	0
2	ZN	L	1001	1/1	0.68	0.17	112,112,112,112	0
4	PEG	E	1006	7/7	0.68	0.18	29,35,39,41	0
4	PEG	I	1011	7/7	0.69	0.21	32,34,41,44	0
5	DMS	F	711	4/4	0.69	0.20	35,46,57,65	0
5	DMS	J	1011	4/4	0.70	0.22	36,37,45,60	0
2	ZN	J	1002	1/1	0.74	0.15	69,69,69,69	0
2	ZN	B	1001	1/1	0.74	0.14	61,61,61,61	0
2	ZN	G	1002	1/1	0.74	0.14	94,94,94,94	0
4	PEG	L	1009	7/7	0.75	0.16	29,38,41,54	0
4	PEG	G	1009	7/7	0.75	0.20	29,31,42,51	0
4	PEG	K	711	7/7	0.75	0.17	30,31,45,47	0
5	DMS	E	1011	4/4	0.76	0.19	50,50,58,60	0
6	SO4	E	1008	5/5	0.76	0.19	57,64,76,80	0
6	SO4	K	707	5/5	0.76	0.17	48,56,67,70	0
9	1PE	L	1005	10/16	0.76	0.14	37,41,51,52	0
8	A1CTH	A	1010	23/23	0.77	0.19	36,40,54,59	0
2	ZN	H	1002	1/1	0.78	0.15	92,92,92,92	0
5	DMS	L	1007	4/4	0.79	0.18	29,44,60,81	0
4	PEG	F	713	7/7	0.80	0.18	27,32,43,44	0
6	SO4	F	709	5/5	0.80	0.15	70,72,83,98	0
4	PEG	B	1011	7/7	0.80	0.16	39,41,48,59	0
5	DMS	J	1012	4/4	0.80	0.19	28,46,46,71	0
2	ZN	I	1001	1/1	0.80	0.18	107,107,107,107	0
2	ZN	L	1002	1/1	0.81	0.12	68,68,68,68	0
4	PEG	G	1005	7/7	0.81	0.14	22,30,31,45	0
2	ZN	C	702	1/1	0.82	0.15	58,58,58,58	0
5	DMS	B	1008	4/4	0.82	0.20	49,49,53,57	0
4	PEG	B	1010	7/7	0.82	0.17	36,39,46,47	0
2	ZN	K	702	1/1	0.82	0.16	98,98,98,98	0
7	GOL	G	1008	6/6	0.82	0.13	22,28,35,37	0
4	PEG	E	1005	7/7	0.82	0.18	23,26,38,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	1001	1/1	0.82	0.11	75,75,75,75	0
6	SO4	B	1006	5/5	0.83	0.18	40,41,65,75	0
4	PEG	E	1014	7/7	0.83	0.14	33,34,43,45	0
5	DMS	H	1005	4/4	0.83	0.15	28,35,37,62	0
5	DMS	J	1008	4/4	0.83	0.16	44,52,57,66	0
2	ZN	H	1001	1/1	0.83	0.12	73,73,73,73	0
4	PEG	C	704	7/7	0.83	0.14	27,35,43,44	0
9	1PE	D	1006	16/16	0.83	0.12	27,41,52,59	0
5	DMS	F	708	4/4	0.83	0.17	29,50,59,61	0
2	ZN	E	1003	1/1	0.84	0.12	72,72,72,72	0
4	PEG	K	712	7/7	0.84	0.22	32,33,36,38	0
4	PEG	I	1009	7/7	0.84	0.14	17,21,22,28	0
4	PEG	L	1010	7/7	0.84	0.17	32,39,48,48	0
5	DMS	A	1008	4/4	0.84	0.17	41,44,55,73	0
3	CO3	J	1009	4/4	0.84	0.16	27,29,32,32	0
4	PEG	J	1014	7/7	0.84	0.12	28,37,43,50	0
9	1PE	I	1005	16/16	0.84	0.15	24,41,59,60	0
9	1PE	I	1006	16/16	0.84	0.15	25,35,49,50	0
6	SO4	A	1006	5/5	0.84	0.15	42,51,64,66	0
4	PEG	A	1013	7/7	0.85	0.13	23,33,37,51	0
4	PEG	F	714	7/7	0.85	0.12	25,26,31,40	0
4	PEG	A	1011	7/7	0.85	0.14	23,33,38,41	0
4	PEG	D	1004	7/7	0.85	0.13	19,29,36,40	0
4	PEG	A	1012	7/7	0.86	0.10	22,28,30,35	0
2	ZN	E	1001	1/1	0.86	0.12	77,77,77,77	0
6	SO4	C	706	5/5	0.86	0.11	40,56,58,76	0
9	1PE	H	1003	16/16	0.86	0.13	34,38,45,54	0
3	CO3	F	710	4/4	0.86	0.16	15,17,18,22	0
4	PEG	F	707	7/7	0.86	0.13	18,23,28,30	0
5	DMS	F	712	4/4	0.86	0.11	21,25,43,63	0
6	SO4	J	1007	5/5	0.87	0.16	44,48,54,69	0
4	PEG	J	1004	7/7	0.87	0.15	23,28,36,41	0
4	PEG	J	1015	7/7	0.87	0.12	19,27,33,36	0
6	SO4	K	708	5/5	0.88	0.16	54,62,74,80	0
5	DMS	I	1008	4/4	0.88	0.14	41,42,48,62	0
4	PEG	L	1004	7/7	0.88	0.13	27,33,38,42	0
9	1PE	C	707	16/16	0.88	0.12	25,37,61,64	0
4	PEG	E	1013	7/7	0.88	0.11	18,21,27,32	0
4	PEG	K	706	7/7	0.88	0.11	24,32,36,37	0
6	SO4	J	1006	5/5	0.88	0.13	43,43,61,63	0
4	PEG	H	1006	7/7	0.88	0.10	22,27,34,38	0
3	CO3	D	1002	4/4	0.88	0.16	26,27,31,31	0

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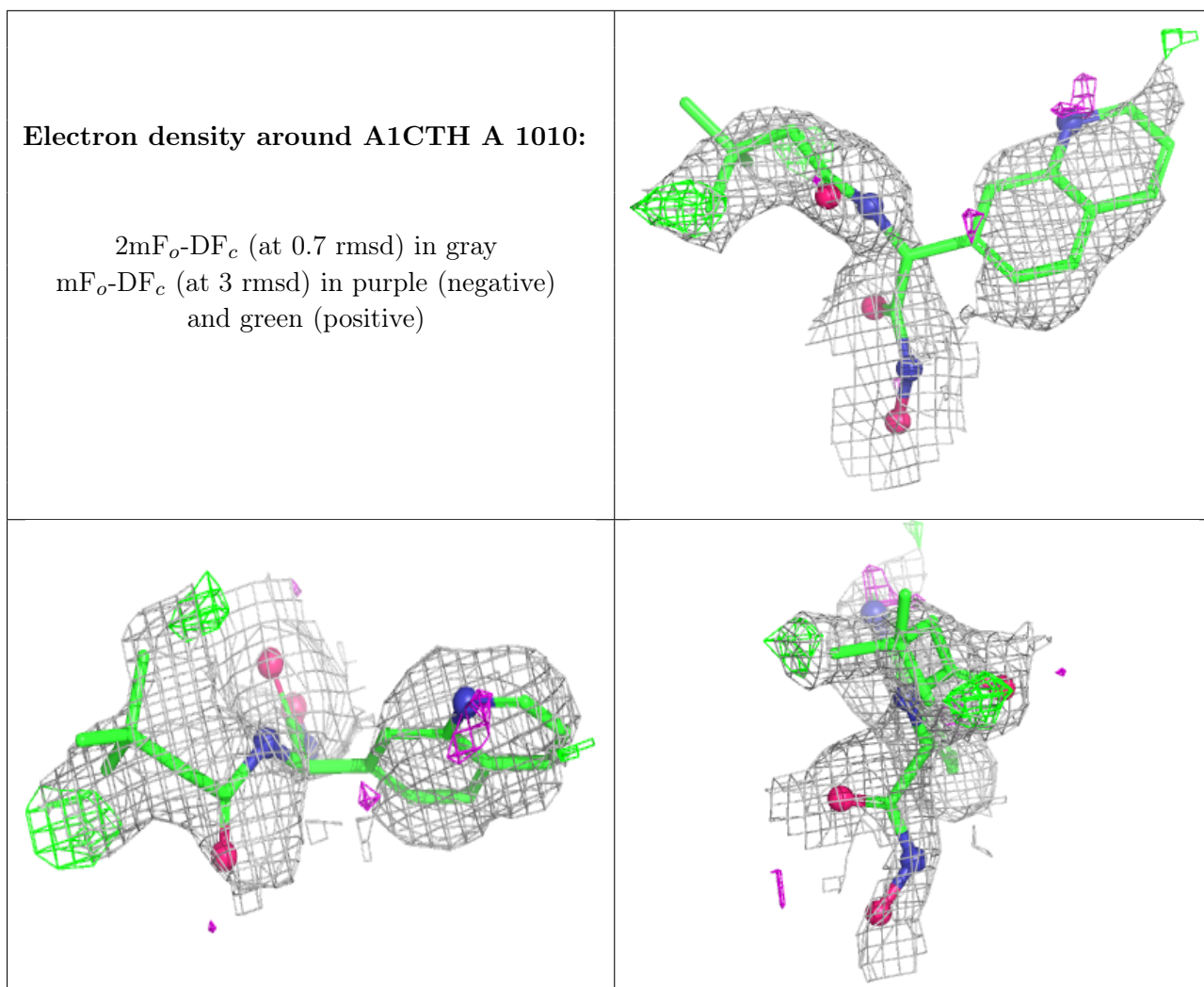
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	E	1010	5/5	0.89	0.15	40,46,54,55	0
4	PEG	I	1010	7/7	0.89	0.13	19,33,45,50	0
3	CO3	L	1006	4/4	0.89	0.15	36,36,37,43	0
9	1PE	E	1009	13/16	0.89	0.11	26,31,36,41	0
5	DMS	B	1007	4/4	0.89	0.15	45,52,63,66	0
3	CO3	A	1002	4/4	0.89	0.15	13,20,21,28	0
2	ZN	G	1001	1/1	0.89	0.10	64,64,64,64	0
4	PEG	G	1003	7/7	0.89	0.10	24,31,33,34	0
3	CO3	E	1002	4/4	0.90	0.10	14,21,24,24	0
5	DMS	C	701	4/4	0.90	0.17	40,41,51,56	0
7	GOL	A	1009	6/6	0.90	0.16	22,28,33,34	0
4	PEG	A	1014	7/7	0.90	0.11	20,27,32,38	0
2	ZN	I	1002	1/1	0.90	0.12	73,73,73,73	0
4	PEG	L	1008	7/7	0.90	0.10	21,21,33,33	0
4	PEG	K	701	7/7	0.91	0.16	18,26,27,32	0
6	SO4	K	704	5/5	0.91	0.12	36,43,59,60	0
3	CO3	C	708	4/4	0.91	0.20	14,23,26,28	0
3	CO3	H	1004	4/4	0.91	0.12	22,24,26,26	0
5	DMS	K	709	4/4	0.91	0.16	33,35,43,46	0
2	ZN	D	1003	1/1	0.91	0.09	64,64,64,64	0
5	DMS	E	1012	4/4	0.91	0.10	28,32,40,48	0
4	PEG	D	1007	7/7	0.91	0.10	13,27,33,41	0
4	PEG	J	1003	7/7	0.91	0.09	16,23,24,26	0
6	SO4	D	1005	5/5	0.91	0.13	47,50,61,64	0
3	CO3	K	710	4/4	0.91	0.19	36,36,39,41	0
5	DMS	G	1004	4/4	0.91	0.13	32,36,48,51	0
4	PEG	B	1005	7/7	0.91	0.09	26,30,38,41	0
3	CO3	B	1002	4/4	0.91	0.13	15,15,19,29	0
4	PEG	F	704	7/7	0.92	0.10	17,21,23,29	0
4	PEG	F	706	7/7	0.92	0.07	15,23,24,27	0
4	PEG	E	1007	7/7	0.92	0.09	22,23,26,27	0
6	SO4	L	1003	5/5	0.92	0.13	40,44,52,55	0
6	SO4	J	1005	5/5	0.92	0.11	40,41,66,68	0
3	CO3	G	1007	4/4	0.92	0.17	31,31,32,43	0
4	PEG	E	1004	7/7	0.92	0.08	15,19,27,31	0
2	ZN	B	1003	1/1	0.93	0.08	43,43,43,43	0
4	PEG	A	1004	7/7	0.94	0.08	16,19,26,26	0
5	DMS	A	1005	4/4	0.94	0.11	32,47,50,55	0
2	ZN	F	703	1/1	0.94	0.07	54,54,54,54	0
5	DMS	J	1010	4/4	0.94	0.15	36,43,48,53	0
6	SO4	F	705	5/5	0.94	0.12	30,42,52,58	0
4	PEG	K	705	7/7	0.94	0.08	14,18,22,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	G	1006	5/5	0.94	0.14	39,43,48,63	0
6	SO4	C	705	5/5	0.94	0.16	47,49,55,57	0
2	ZN	C	703	1/1	0.95	0.10	41,41,41,41	0
4	PEG	B	1009	7/7	0.95	0.07	18,26,33,33	0
6	SO4	A	1007	5/5	0.96	0.13	26,36,42,43	0
2	ZN	A	1001	1/1	0.96	0.12	76,76,76,76	0
2	ZN	K	703	1/1	0.96	0.05	65,65,65,65	0
6	SO4	I	1004	5/5	0.97	0.08	31,34,38,38	0
2	ZN	J	1001	1/1	0.97	0.12	66,66,66,66	0
3	CO3	I	1007	4/4	0.97	0.06	15,21,23,25	0
6	SO4	B	1004	5/5	0.98	0.06	19,19,21,22	0
6	SO4	J	1013	5/5	0.98	0.06	14,15,22,24	0
2	ZN	A	1003	1/1	0.98	0.07	43,43,43,43	0
6	SO4	I	1003	5/5	0.98	0.07	19,21,24,27	0
6	SO4	F	701	5/5	0.99	0.06	16,19,23,24	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.