



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:06 pm BST

PDB ID : 5IVH
Title : The alpha-esterase-7 carboxylesterase, E3, from the blowfly *Lucilia cuprina*:
apo-enzyme ensemble refinement
Authors : Correy, G.J.; Jackson, C.J.
Deposited on : 2016-03-20
Resolution : 1.71 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

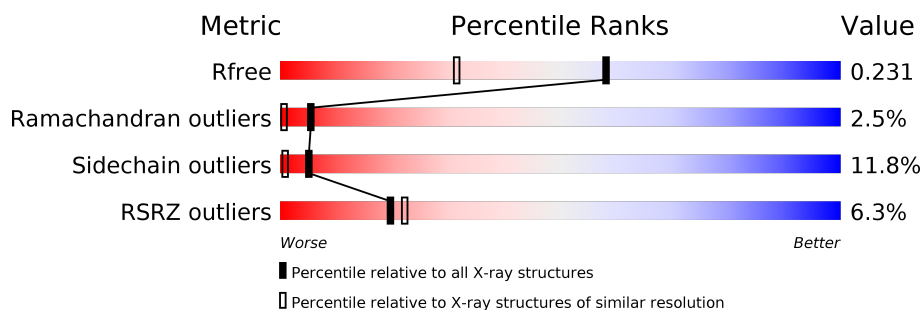
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5722 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 on 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	1-A	577	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
1	10-A	577	<div> <div>7%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	11-A	577	<div> <div>7%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	12-A	577	<div> <div>7%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	13-A	577	<div> <div>7%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	14-A	577	<div> <div>7%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	15-A	577	<div> <div>7%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	16-A	577	7% 85% 11% ..
1	17-A	577	7% 84% 13% .
1	18-A	577	7% 84% 13% ..
1	19-A	577	7% 86% 11% ..
1	2-A	577	7% 86% 10% ..
1	20-A	577	7% 86% 11% ...
1	21-A	577	7% 87% 9% ..
1	22-A	577	7% 84% 12% ..
1	23-A	577	7% 83% 13% ..
1	24-A	577	7% 82% 15% ..
1	25-A	577	7% 84% 12% ..
1	26-A	577	7% 86% 10% ..
1	27-A	577	7% 83% 12% ..
1	28-A	577	7% 86% 11% ..
1	29-A	577	7% 85% 12% ..
1	3-A	577	7% 85% 12% ..
1	30-A	577	7% 86% 10% ..
1	31-A	577	7% 86% 11% ..
1	32-A	577	7% 84% 12% ..
1	33-A	577	7% 86% 10% ..
1	34-A	577	7% 85% 11% ..
1	35-A	577	7% 86% 11% ..
1	36-A	577	7% 86% 10% ..
1	37-A	577	7% 85% 11% ..
1	38-A	577	7% 83% 14% ..

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Mol	Chain	Length	Quality of chain
1	39-A	577	
1	4-A	577	
1	40-A	577	
1	41-A	577	
1	42-A	577	
1	43-A	577	
1	44-A	577	
1	5-A	577	
1	6-A	577	
1	7-A	577	
1	8-A	577	
1	9-A	577	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 407711 atoms, of which 197120 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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	2-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	3-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	4-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	5-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	6-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	7-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	8-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	9-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	10-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	11-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	12-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	13-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	14-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	15-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	16-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	18-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	19-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	20-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	21-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	22-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	23-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	24-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	25-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	26-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	27-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	28-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	29-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	30-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	31-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	32-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	33-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	34-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	35-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	36-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0
1	37-A	566	Total 9037	C 2911	H 4480	N 766	O 846	S 34	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	39-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	40-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	41-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	42-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	43-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			
1	44-A	566	Total	C	H	N	O	S	0	0	0
			9037	2911	4480	766	846	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q25252
A	-5	HIS	-	expression tag	UNP Q25252
A	-4	HIS	-	expression tag	UNP Q25252
A	-3	HIS	-	expression tag	UNP Q25252
A	-2	HIS	-	expression tag	UNP Q25252
A	-1	HIS	-	expression tag	UNP Q25252
A	0	HIS	-	expression tag	UNP Q25252
A	83	ALA	ASP	conflict	UNP Q25252
A	364	LEU	MET	conflict	UNP Q25252
A	419	PHE	ILE	conflict	UNP Q25252
A	472	THR	ALA	conflict	UNP Q25252
A	505	THR	ILE	conflict	UNP Q25252
A	530	GLU	LYS	conflict	UNP Q25252
A	554	GLY	ASP	conflict	UNP Q25252

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	234	Total	O	0	0
			234	234		
2	2-A	234	Total	O	0	0
			234	234		
2	3-A	224	Total	O	0	0
			224	224		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	4-A	222	Total 222	O 222	0	0
2	5-A	230	Total 230	O 230	0	0
2	6-A	233	Total 233	O 233	0	0
2	7-A	241	Total 241	O 241	0	0
2	8-A	238	Total 238	O 238	0	0
2	9-A	218	Total 218	O 218	0	0
2	10-A	217	Total 217	O 217	0	0
2	11-A	219	Total 219	O 219	0	0
2	12-A	231	Total 231	O 231	0	0
2	13-A	231	Total 231	O 231	0	0
2	14-A	235	Total 235	O 235	0	0
2	15-A	226	Total 226	O 226	0	0
2	16-A	230	Total 230	O 230	0	0
2	17-A	211	Total 211	O 211	0	0
2	18-A	228	Total 228	O 228	0	0
2	19-A	228	Total 228	O 228	0	0
2	20-A	236	Total 236	O 236	0	0
2	21-A	234	Total 234	O 234	0	0
2	22-A	225	Total 225	O 225	0	0
2	23-A	206	Total 206	O 206	0	0
2	24-A	218	Total 218	O 218	0	0

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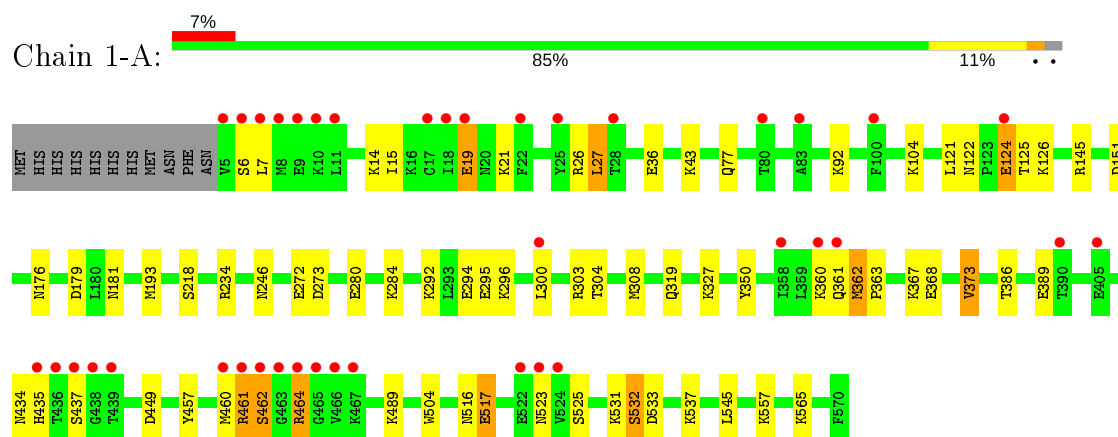
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	25-A	227	Total 227	O 227	0	0
2	26-A	227	Total 227	O 227	0	0
2	27-A	214	Total 214	O 214	0	0
2	28-A	237	Total 237	O 237	0	0
2	29-A	238	Total 238	O 238	0	0
2	30-A	237	Total 237	O 237	0	0
2	31-A	224	Total 224	O 224	0	0
2	32-A	224	Total 224	O 224	0	0
2	33-A	224	Total 224	O 224	0	0
2	34-A	235	Total 235	O 235	0	0
2	35-A	227	Total 227	O 227	0	0
2	36-A	236	Total 236	O 236	0	0
2	37-A	234	Total 234	O 234	0	0
2	38-A	244	Total 244	O 244	0	0
2	39-A	231	Total 231	O 231	0	0
2	40-A	231	Total 231	O 231	0	0
2	41-A	242	Total 242	O 242	0	0
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2	43-A	233	Total 233	O 233	0	0
2	44-A	223	Total 223	O 223	0	0

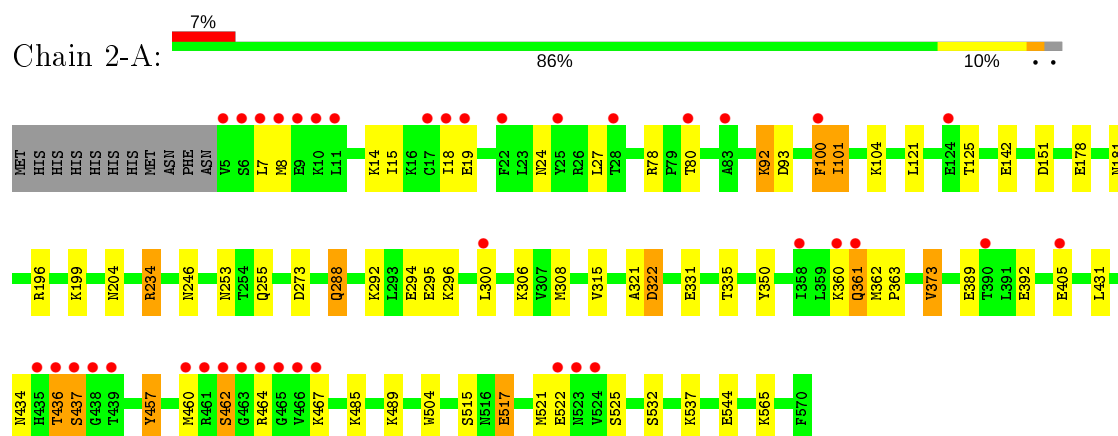
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

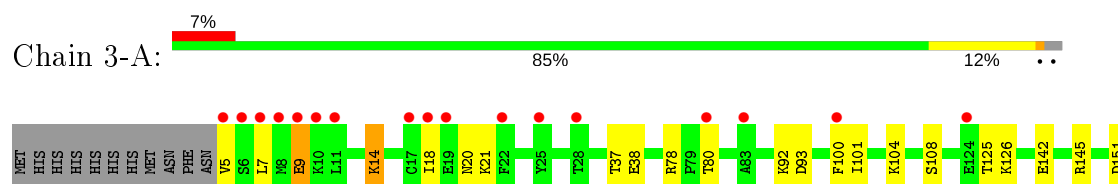
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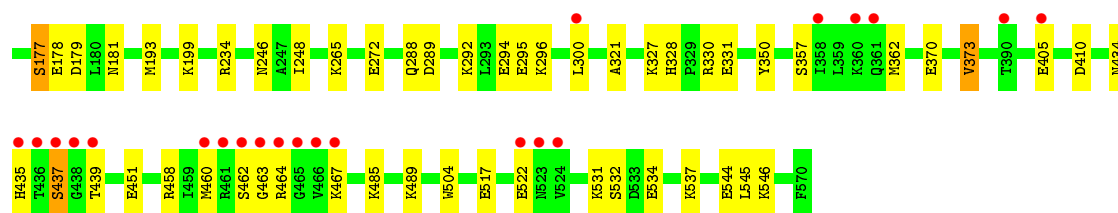


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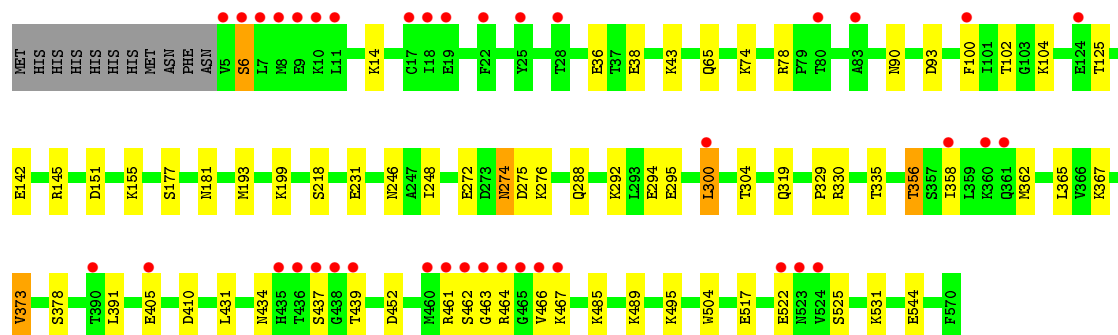
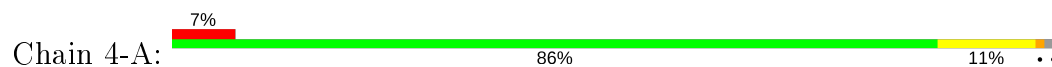


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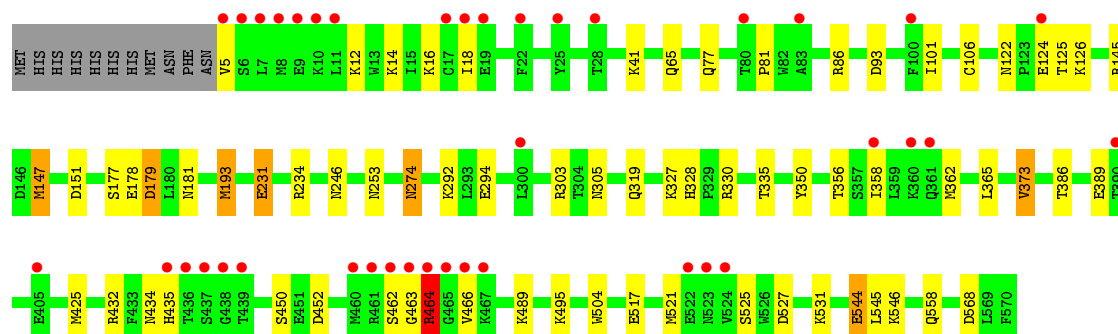
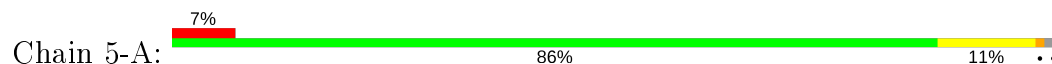




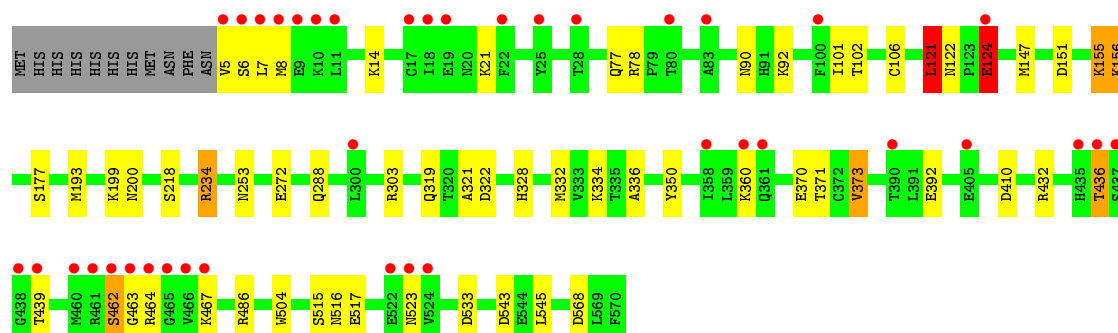
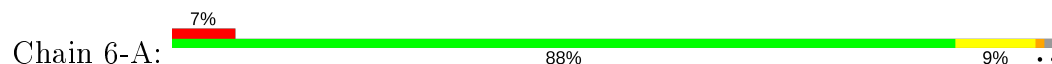
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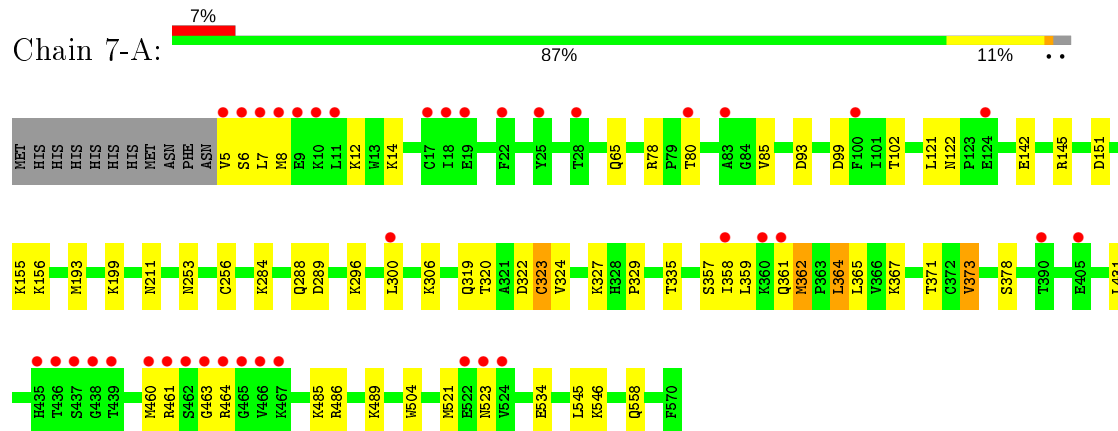
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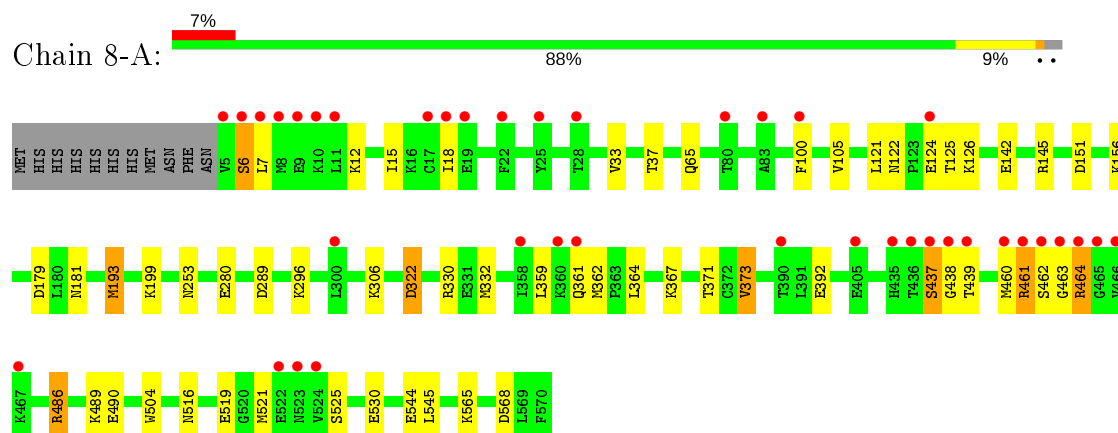
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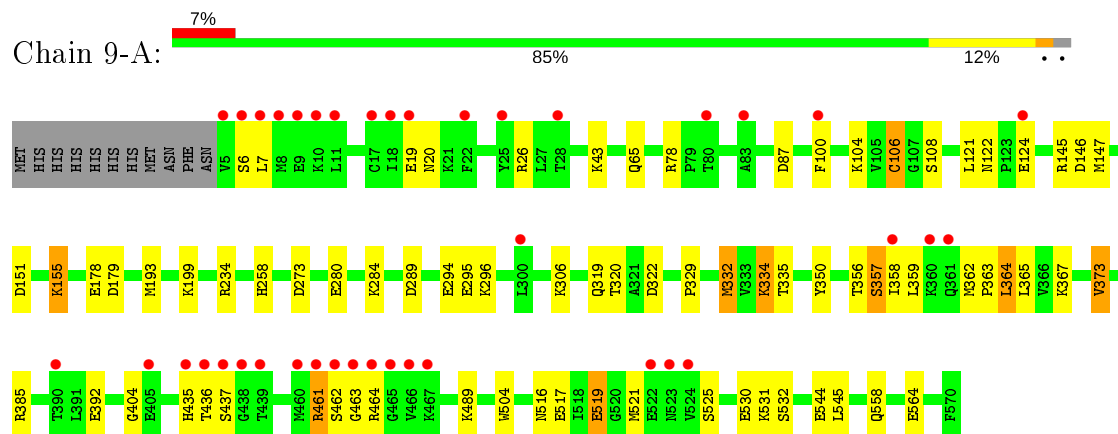
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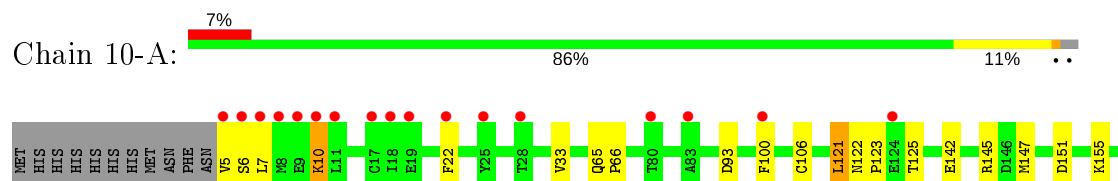
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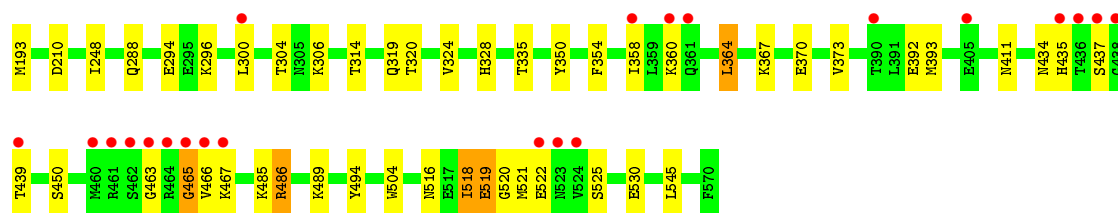


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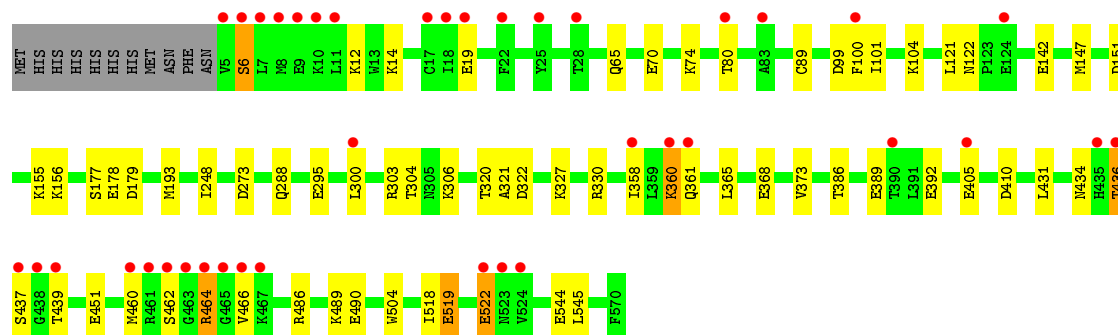
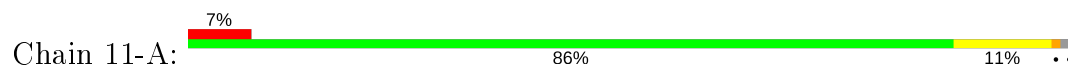


- Molecule 1: Carboxylic ester hydrolase

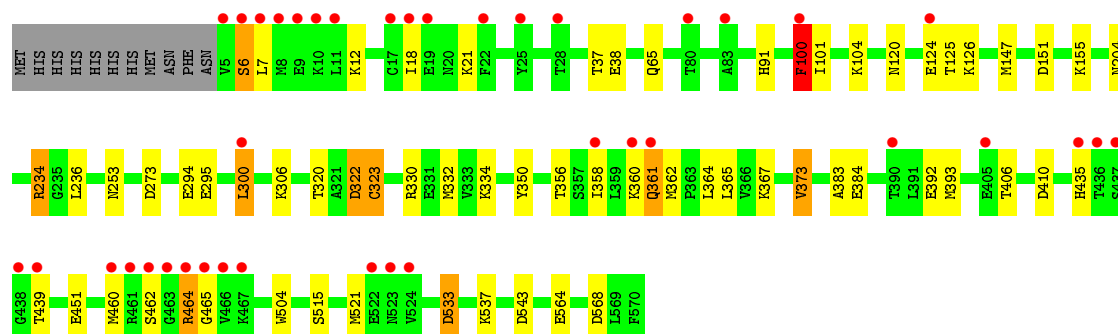
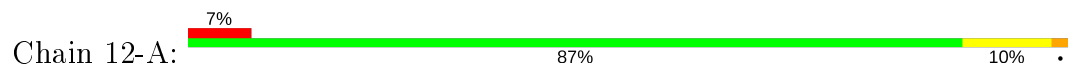




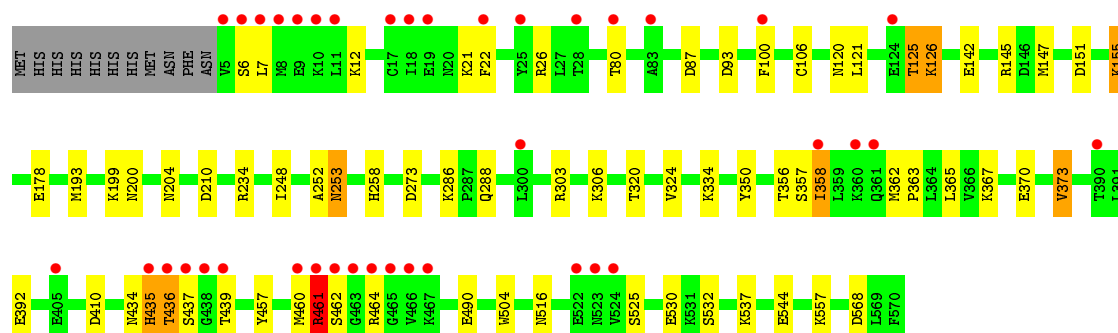
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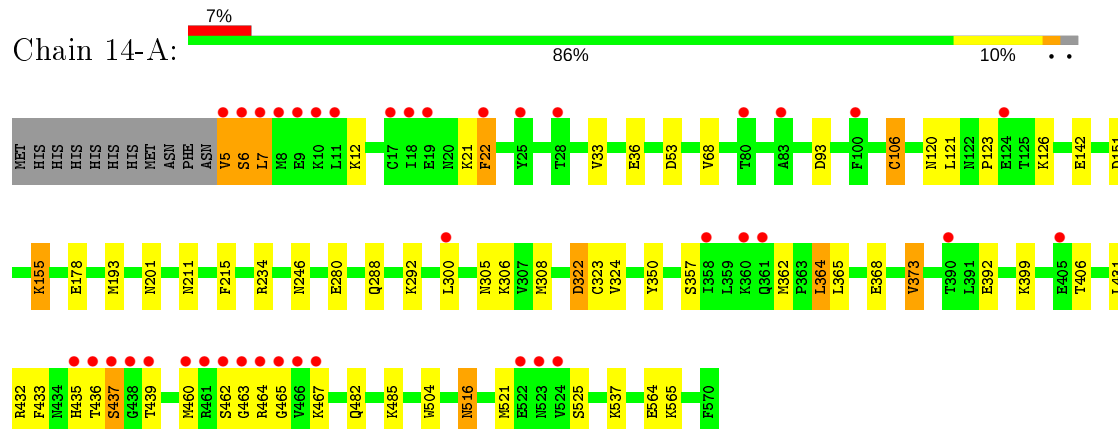
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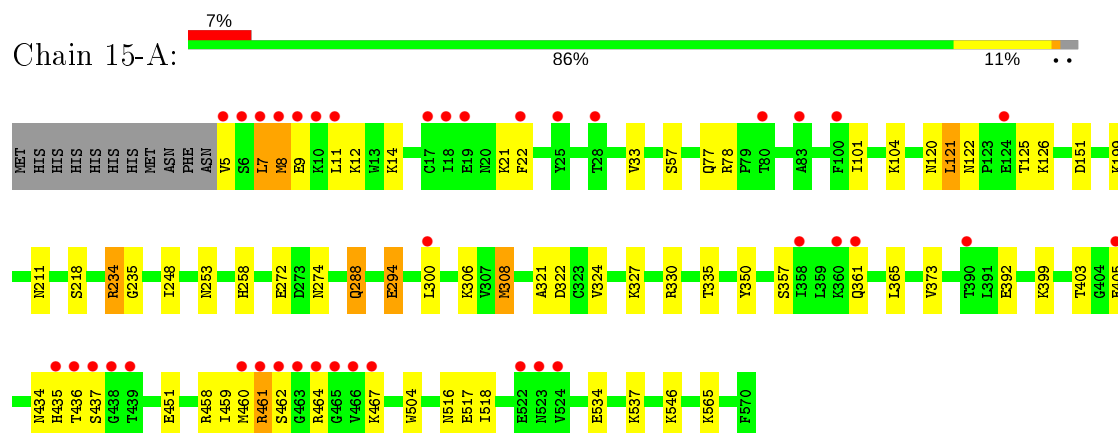
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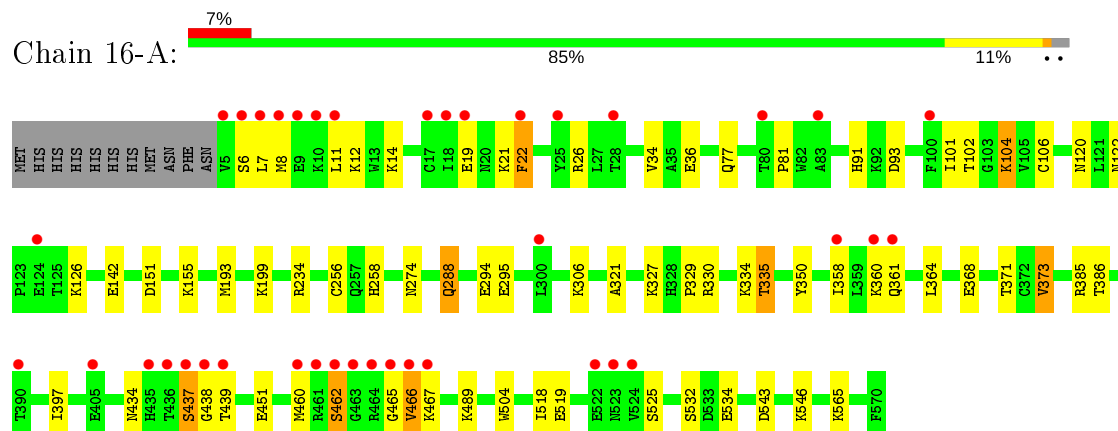
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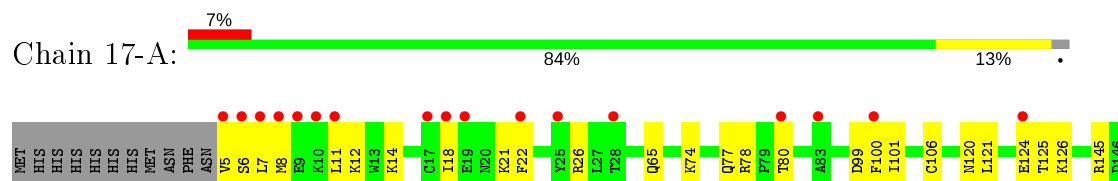
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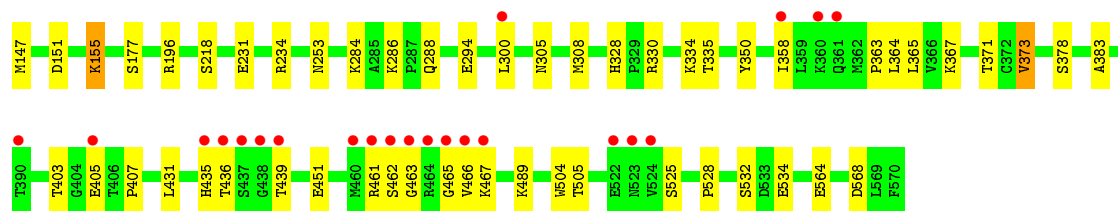


• Molecule 1: Carboxylic ester hydrolase

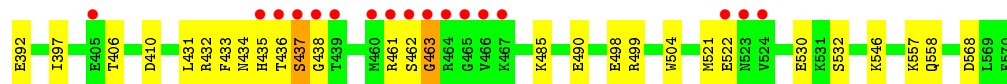
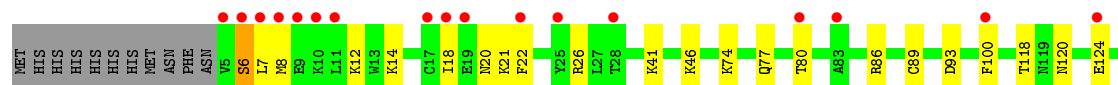
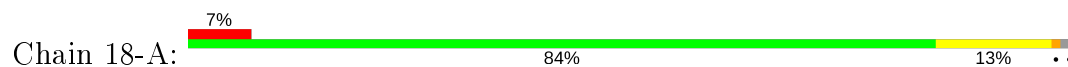


• Molecule 1: Carboxylic ester hydrolase

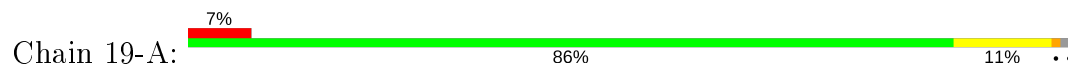




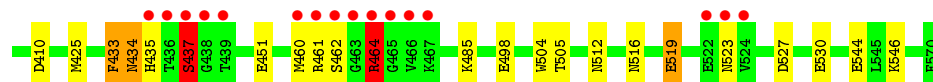
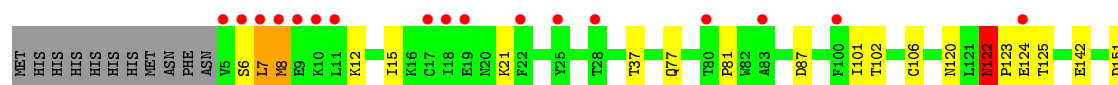
● Molecule 1: Carboxylic ester hydrolase



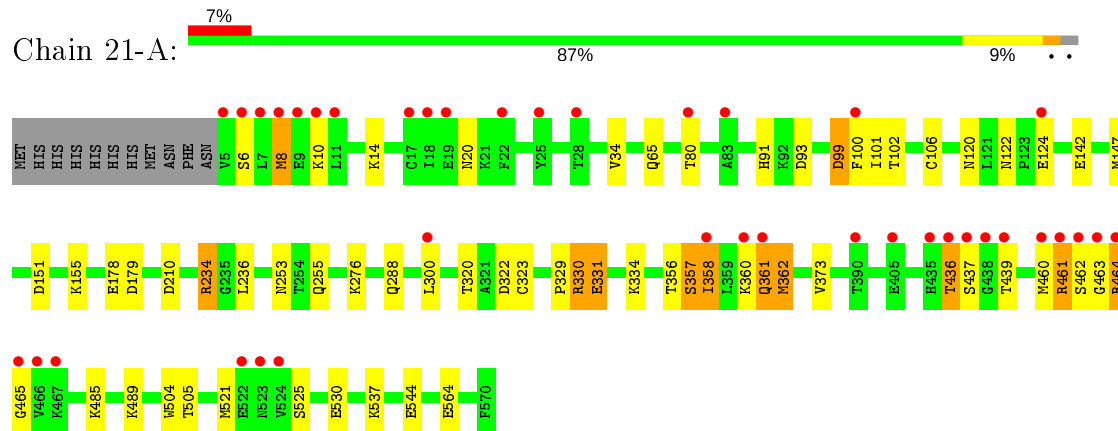
● Molecule 1: Carboxylic ester hydrolase



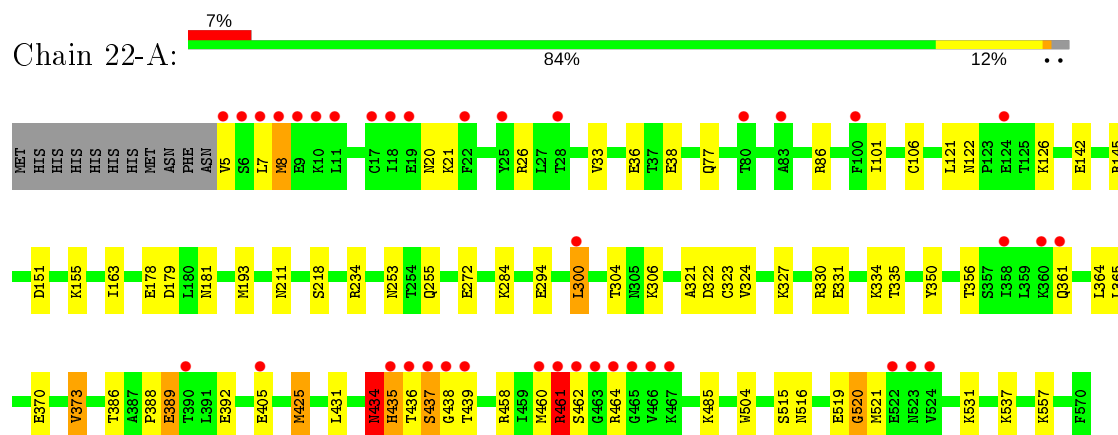
● Molecule 1: Carboxylic ester hydrolase



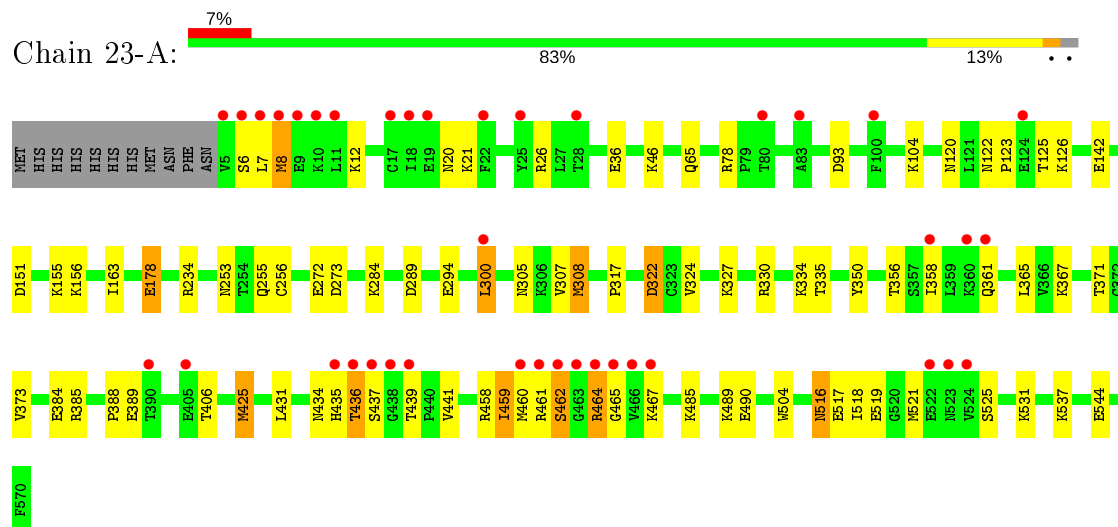
- Molecule 1: Carboxylic ester hydrolase



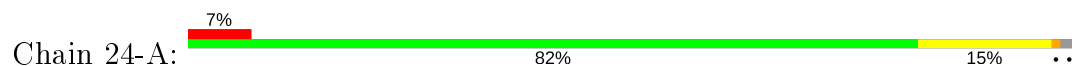
- Molecule 1: Carboxylic ester hydrolase

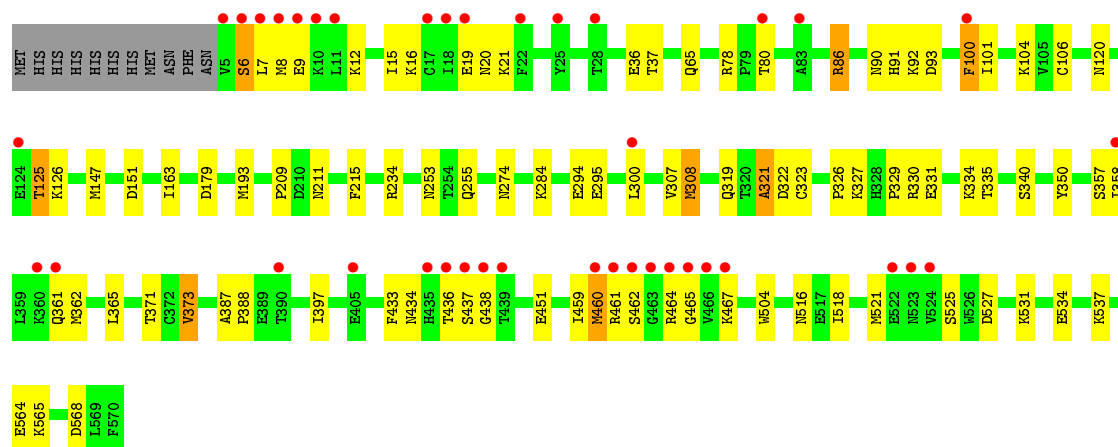


- Molecule 1: Carboxylic ester hydrolase

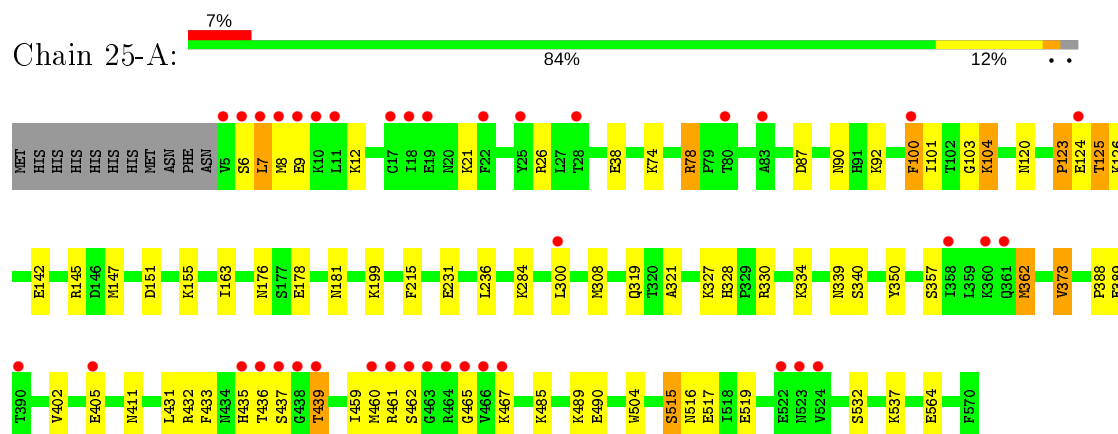


- Molecule 1: Carboxylic ester hydrolase

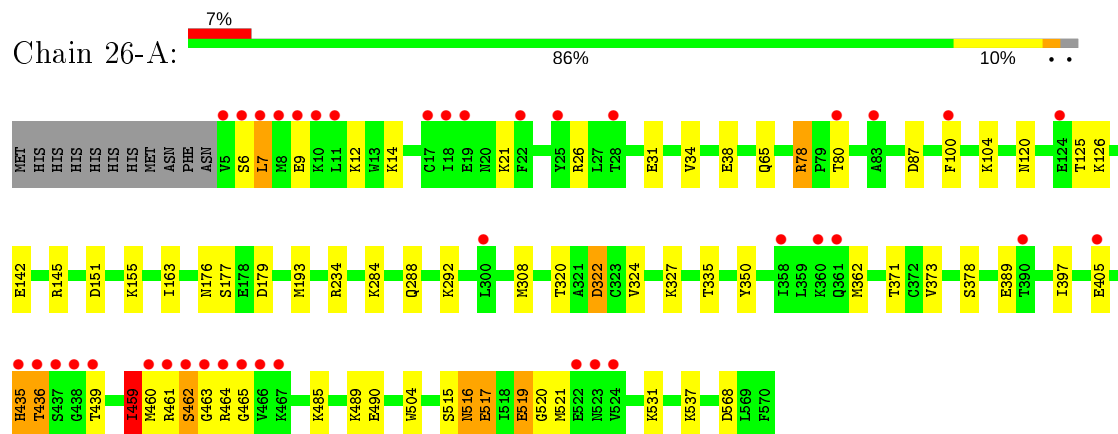




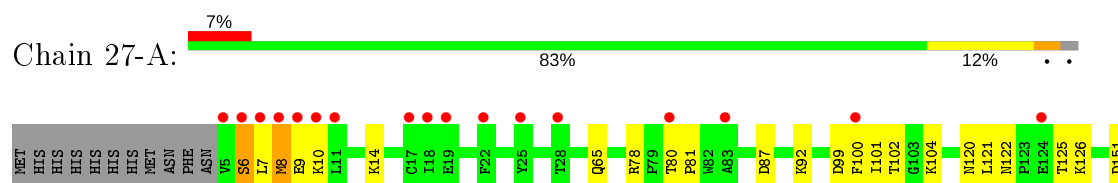
- Molecule 1: Carboxylic ester hydrolase

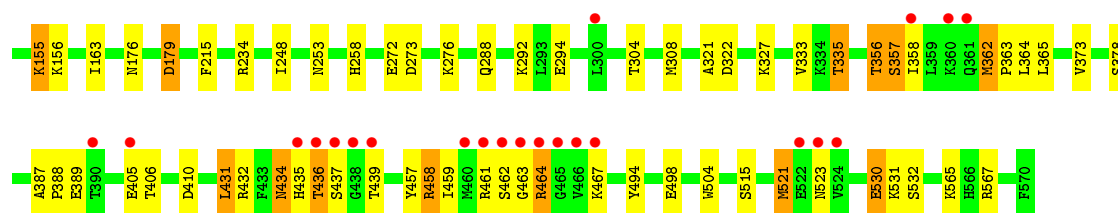


- Molecule 1: Carboxylic ester hydrolase

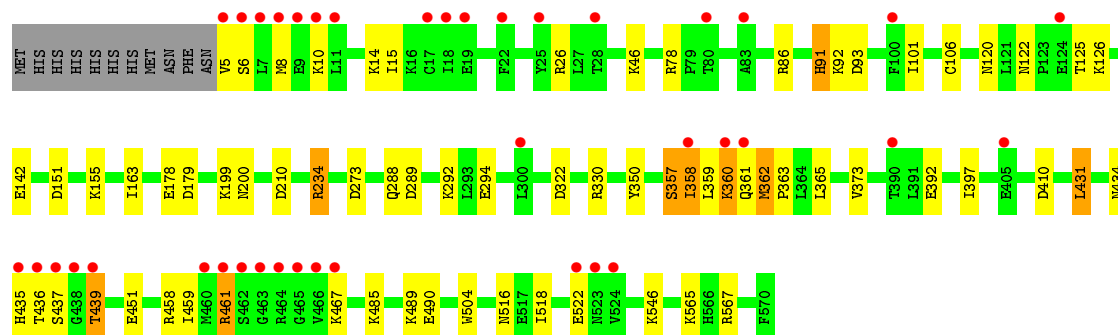
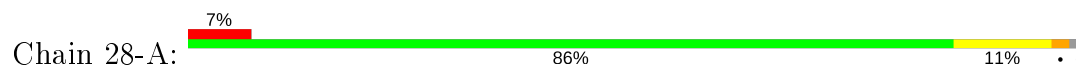


- Molecule 1: Carboxylic ester hydrolase

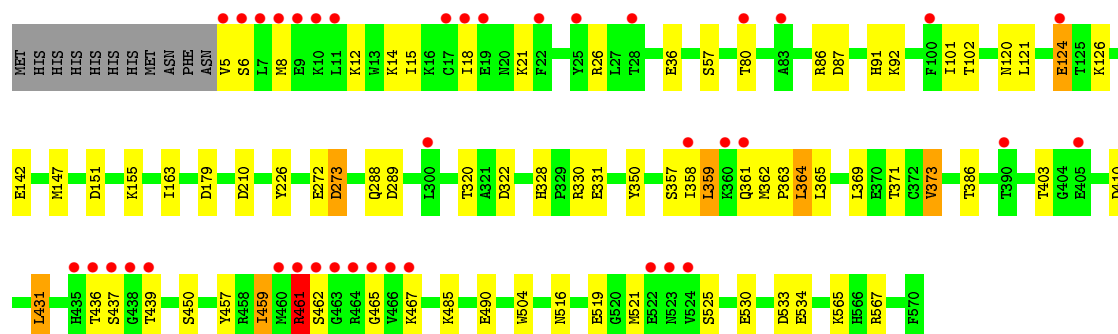
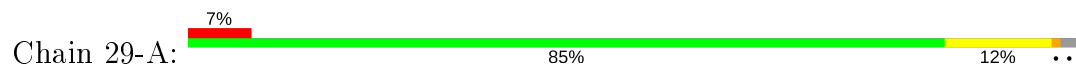




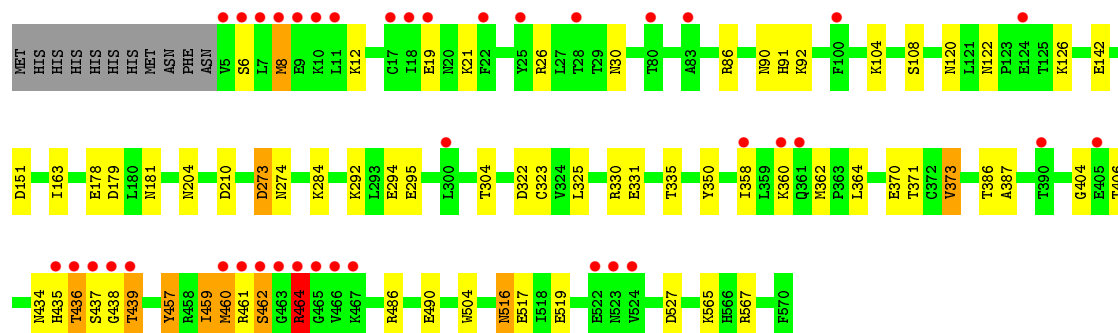
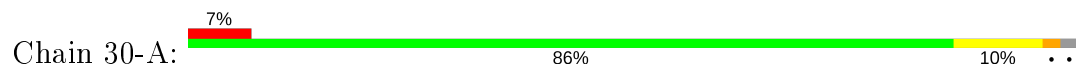
• Molecule 1: Carboxylic ester hydrolase



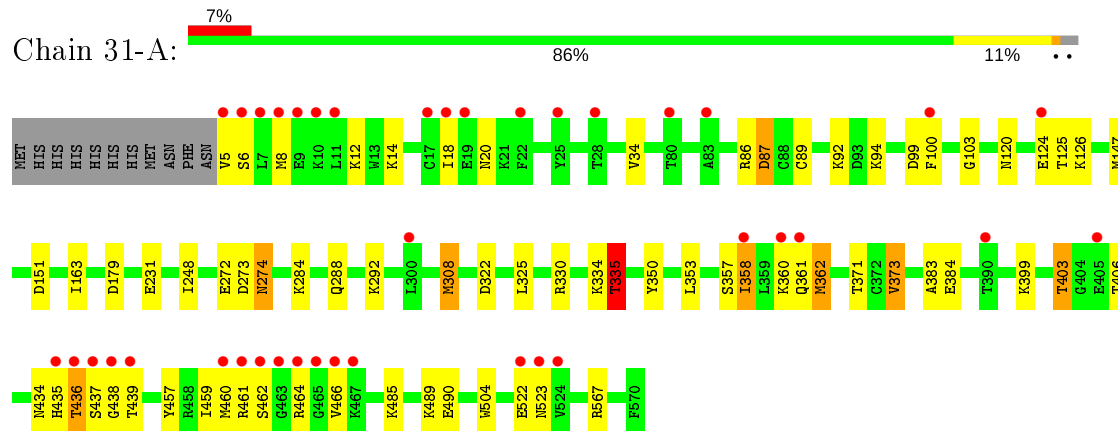
• Molecule 1: Carboxylic ester hydrolase



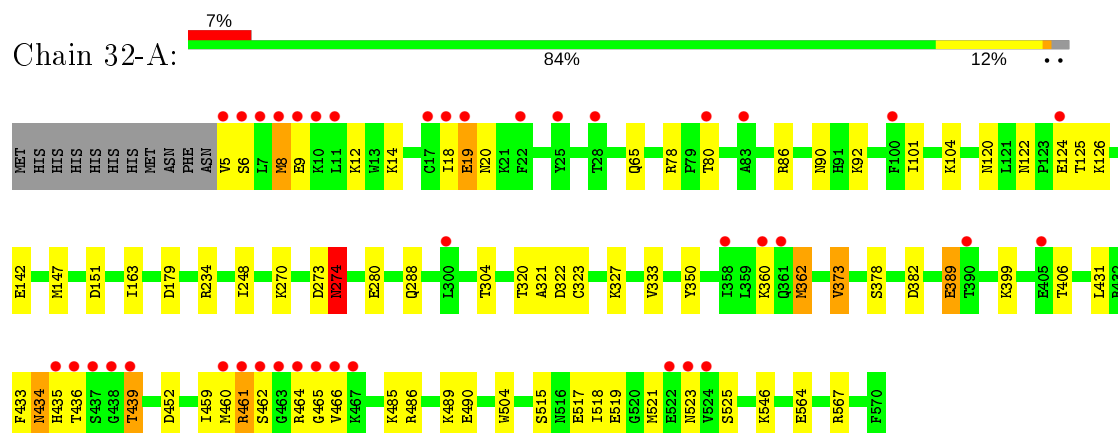
• Molecule 1: Carboxylic ester hydrolase



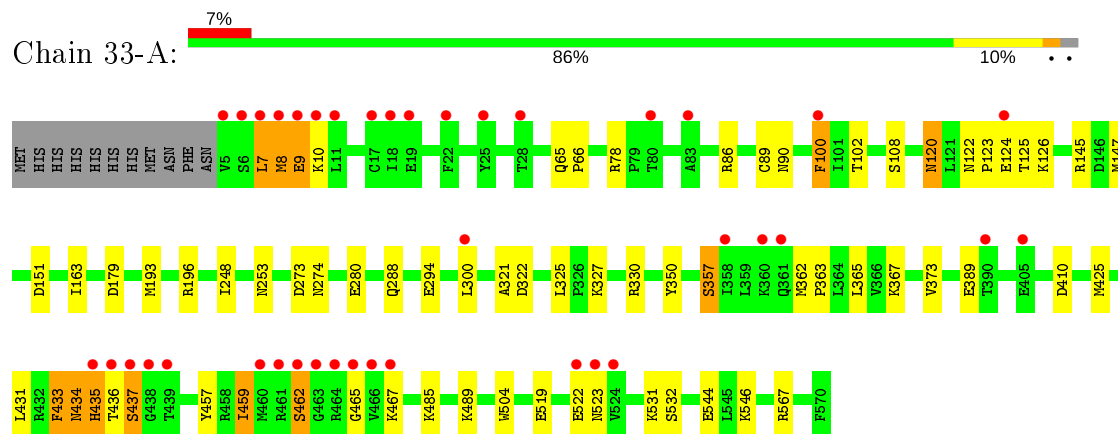
- Molecule 1: Carboxylic ester hydrolase



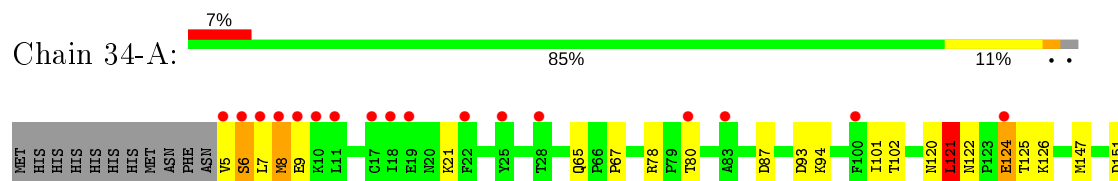
- Molecule 1: Carboxylic ester hydrolase

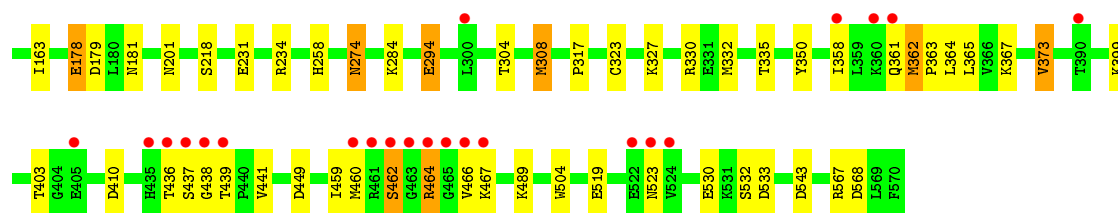


- Molecule 1: Carboxylic ester hydrolase

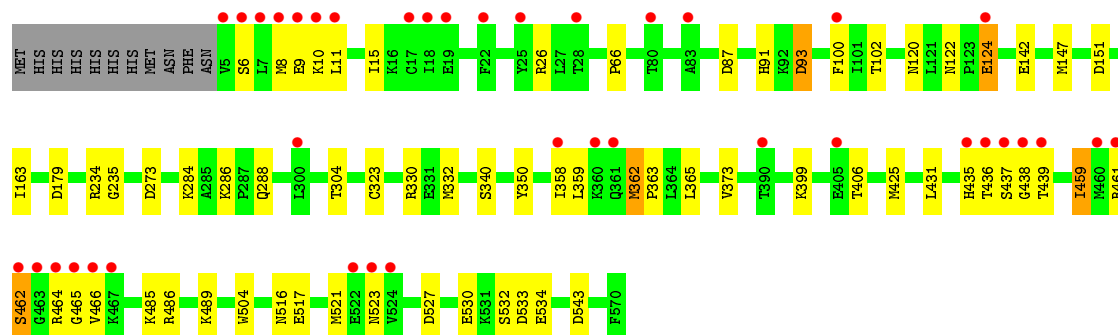
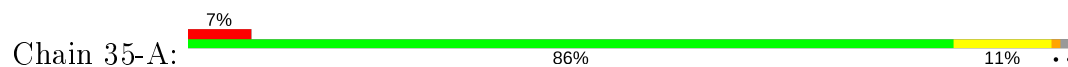


- Molecule 1: Carboxylic ester hydrolase

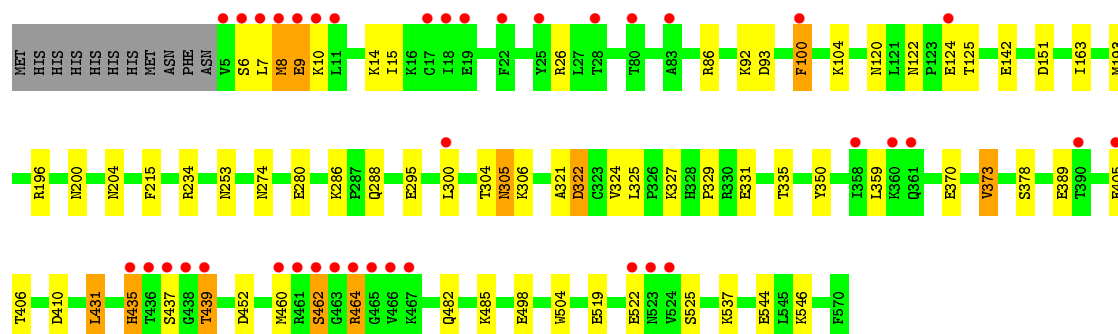
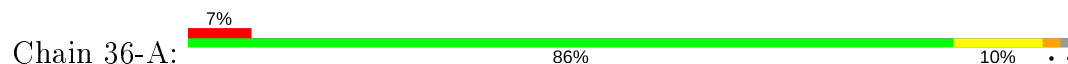




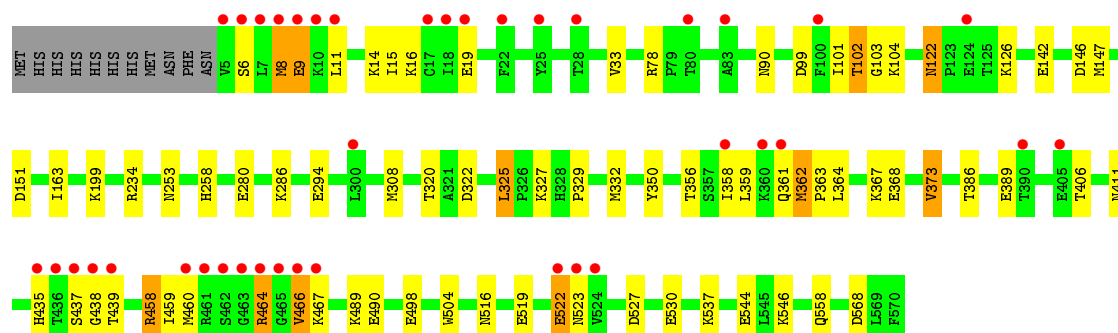
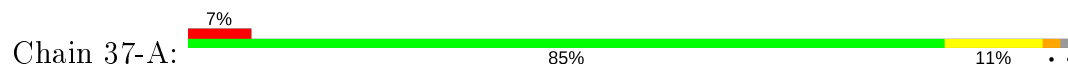
• Molecule 1: Carboxylic ester hydrolase



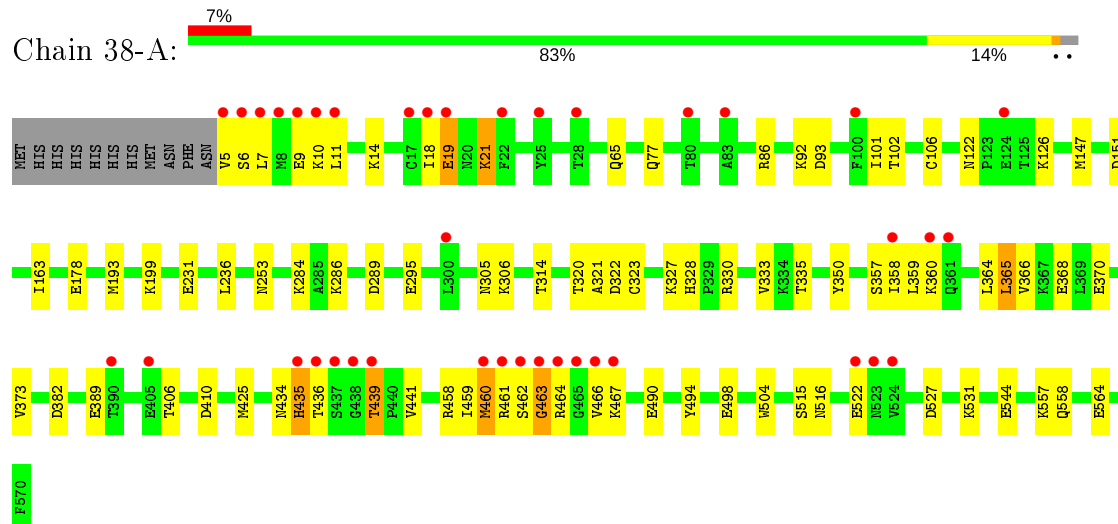
• Molecule 1: Carboxylic ester hydrolase



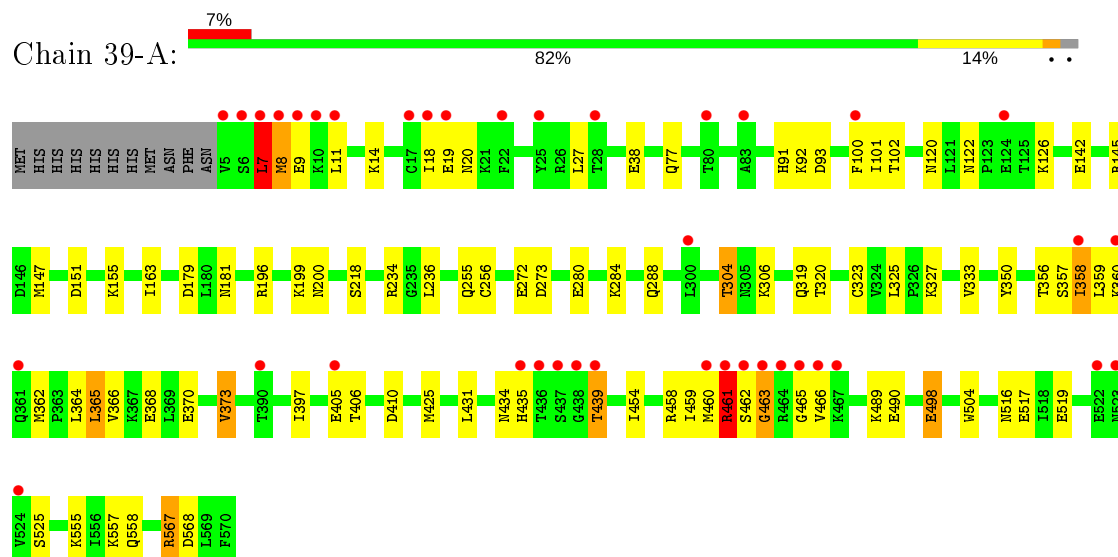
• Molecule 1: Carboxylic ester hydrolase



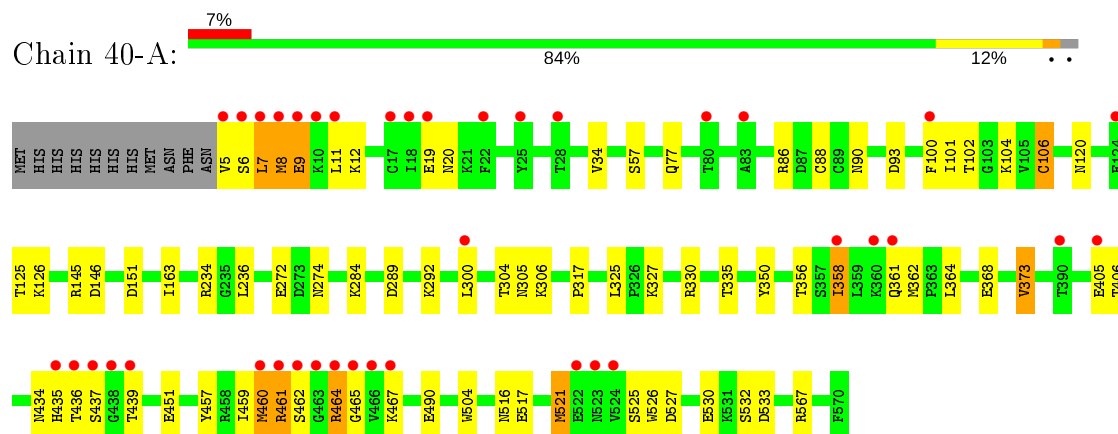
- Molecule 1: Carboxylic ester hydrolase



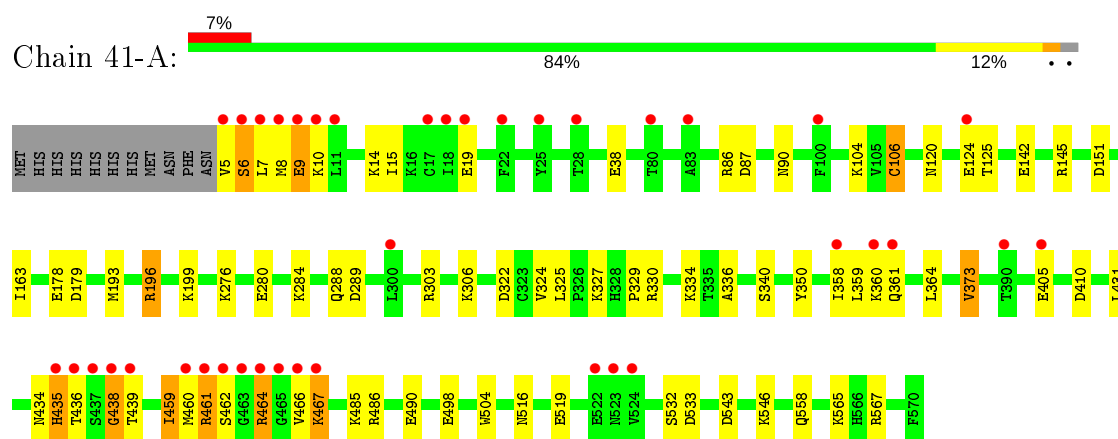
- Molecule 1: Carboxylic ester hydrolase



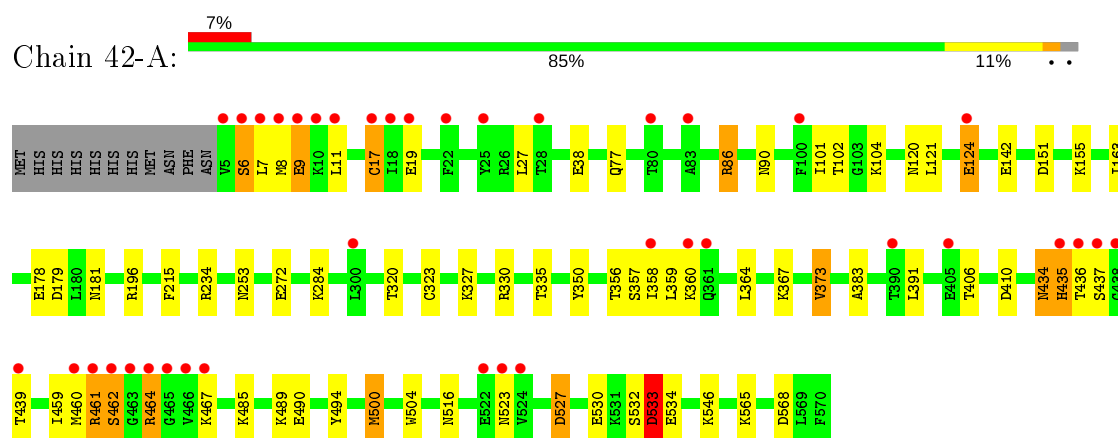
- Molecule 1: Carboxylic ester hydrolase



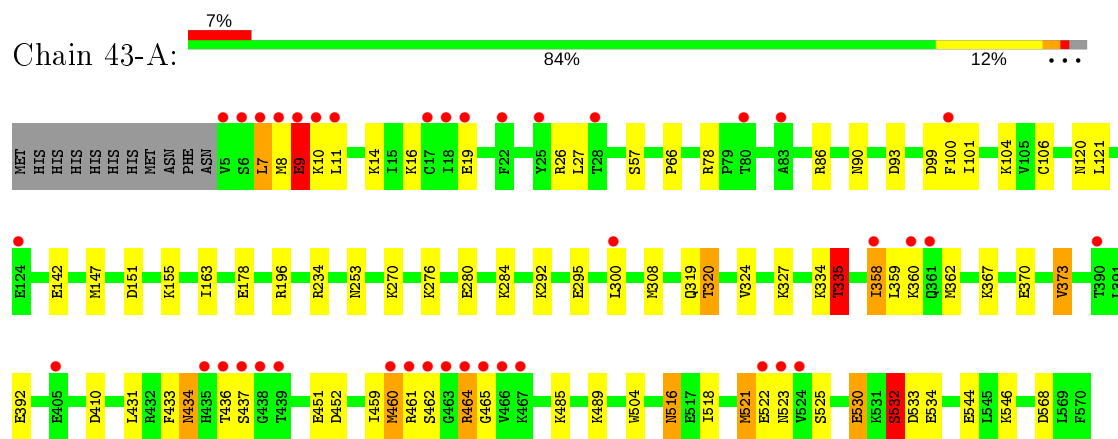
- Molecule 1: Carboxylic ester hydrolase



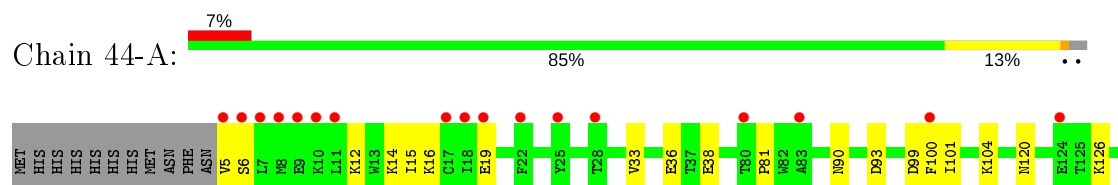
- Molecule 1: Carboxylic ester hydrolase

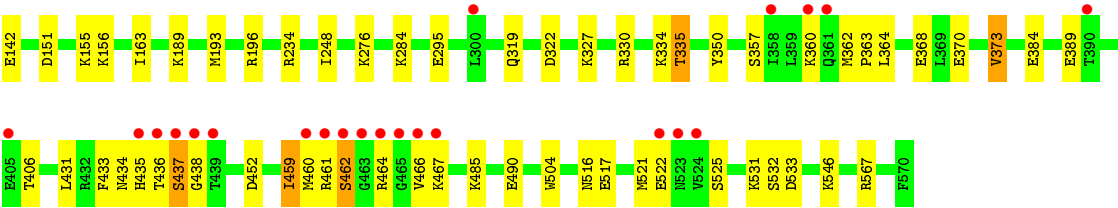


- Molecule 1: Carboxylic ester hydrolase



- Molecule 1: Carboxylic ester hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	48.57Å 100.47Å 221.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.76 – 1.71 45.76 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.76-1.71) 91.5 (45.76-1.71)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.167 , 0.208 0.188 , 0.231	Depositor DCC
R_{free} test set	3002 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 237.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	407711	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1-A	0.63	4/4672 (0.1%)	0.79	5/6320 (0.1%)
1	2-A	0.65	3/4672 (0.1%)	0.76	6/6320 (0.1%)
1	3-A	0.60	0/4672	0.75	3/6320 (0.0%)
1	4-A	0.64	0/4672	0.77	4/6320 (0.1%)
1	5-A	0.65	3/4672 (0.1%)	0.78	8/6320 (0.1%)
1	6-A	0.62	2/4672 (0.0%)	0.75	3/6320 (0.0%)
1	7-A	0.62	2/4672 (0.0%)	0.77	4/6320 (0.1%)
1	8-A	0.65	1/4672 (0.0%)	0.78	6/6320 (0.1%)
1	9-A	0.67	4/4672 (0.1%)	0.76	5/6320 (0.1%)
1	10-A	0.63	3/4672 (0.1%)	0.77	5/6320 (0.1%)
1	11-A	0.64	1/4672 (0.0%)	0.75	3/6320 (0.0%)
1	12-A	0.67	2/4672 (0.0%)	0.78	6/6320 (0.1%)
1	13-A	0.64	1/4672 (0.0%)	0.77	6/6320 (0.1%)
1	14-A	0.65	4/4672 (0.1%)	0.78	6/6320 (0.1%)
1	15-A	0.66	1/4672 (0.0%)	0.80	7/6320 (0.1%)
1	16-A	0.66	2/4672 (0.0%)	0.79	6/6320 (0.1%)
1	17-A	0.62	2/4672 (0.0%)	0.78	5/6320 (0.1%)
1	18-A	0.64	4/4672 (0.1%)	0.78	6/6320 (0.1%)
1	19-A	0.69	3/4672 (0.1%)	0.78	4/6320 (0.1%)
1	20-A	0.66	3/4672 (0.1%)	0.77	7/6320 (0.1%)
1	21-A	0.65	2/4672 (0.0%)	0.76	3/6320 (0.0%)
1	22-A	0.64	1/4672 (0.0%)	0.78	6/6320 (0.1%)
1	23-A	0.65	0/4672	0.79	9/6320 (0.1%)
1	24-A	0.65	2/4672 (0.0%)	0.80	6/6320 (0.1%)
1	25-A	0.63	0/4672	0.76	5/6320 (0.1%)
1	26-A	0.64	0/4672	0.79	5/6320 (0.1%)
1	27-A	0.66	2/4672 (0.0%)	0.80	10/6320 (0.2%)
1	28-A	0.63	1/4672 (0.0%)	0.77	5/6320 (0.1%)
1	29-A	0.67	2/4672 (0.0%)	0.82	10/6320 (0.2%)
1	30-A	0.65	3/4672 (0.1%)	0.81	8/6320 (0.1%)
1	31-A	0.65	3/4672 (0.1%)	0.78	3/6320 (0.0%)
1	32-A	0.62	2/4672 (0.0%)	0.77	4/6320 (0.1%)
1	33-A	0.68	4/4672 (0.1%)	0.82	10/6320 (0.2%)
1	34-A	0.62	2/4672 (0.0%)	0.79	5/6320 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	35-A	0.64	3/4672 (0.1%)	0.78	3/6320 (0.0%)
1	36-A	0.62	0/4672	0.79	7/6320 (0.1%)
1	37-A	0.64	0/4672	0.79	4/6320 (0.1%)
1	38-A	0.64	2/4672 (0.0%)	0.79	5/6320 (0.1%)
1	39-A	0.65	1/4672 (0.0%)	0.79	6/6320 (0.1%)
1	40-A	0.69	4/4672 (0.1%)	0.80	9/6320 (0.1%)
1	41-A	0.64	1/4672 (0.0%)	0.78	10/6320 (0.2%)
1	42-A	0.66	4/4672 (0.1%)	0.79	8/6320 (0.1%)
1	43-A	0.67	5/4672 (0.1%)	0.78	8/6320 (0.1%)
1	44-A	0.65	0/4672	0.77	3/6320 (0.0%)
All	All	0.65	89/205568 (0.0%)	0.78	257/278080 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	3
1	2-A	0	4
1	3-A	0	6
1	4-A	0	2
1	6-A	0	4
1	7-A	0	1
1	8-A	0	2
1	9-A	0	5
1	10-A	0	3
1	11-A	0	3
1	12-A	0	3
1	13-A	0	6
1	14-A	0	5
1	15-A	0	1
1	16-A	0	3
1	17-A	0	4
1	18-A	0	7
1	19-A	0	3
1	20-A	0	4
1	21-A	0	6
1	22-A	0	5
1	23-A	0	11
1	24-A	0	10
1	25-A	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	26-A	0	8
1	27-A	0	9
1	28-A	0	5
1	29-A	0	5
1	30-A	0	7
1	31-A	0	10
1	32-A	0	8
1	33-A	0	7
1	34-A	0	5
1	35-A	0	3
1	36-A	0	2
1	37-A	0	1
1	38-A	0	5
1	39-A	0	8
1	40-A	0	7
1	41-A	0	7
1	42-A	0	5
1	43-A	0	5
1	44-A	0	4
All	All	0	219

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	40-A	106	CYS	CB-SG	13.00	2.04	1.82
1	21-A	106	CYS	CB-SG	10.02	1.99	1.82
1	42-A	17	CYS	CB-SG	8.87	1.97	1.82
1	40-A	526	TRP	C-N	8.79	1.54	1.34
1	43-A	530	GLU	CB-CG	8.34	1.68	1.52

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	30-A	322	ASP	CB-CG-OD1	13.73	130.66	118.30
1	29-A	461	ARG	NE-CZ-NH1	12.23	126.41	120.30
1	24-A	308	MET	CG-SD-CE	-10.92	82.73	100.20
1	22-A	461	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	8-A	373	VAL	CG1-CB-CG2	9.73	126.47	110.90

There are no chirality outliers.

5 of 219 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	435	HIS	Peptide
1	1-A	460	MET	Peptide
1	1-A	461	ARG	Peptide
1	2-A	101	ILE	Peptide
1	2-A	92	LYS	Peptide

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	1-A	4557	4480	4480	0	0
1	2-A	4557	4480	4480	0	0
1	3-A	4557	4480	4480	0	0
1	4-A	4557	4480	4480	0	0
1	5-A	4557	4480	4480	0	0
1	6-A	4557	4480	4480	0	0
1	7-A	4557	4480	4480	0	0
1	8-A	4557	4480	4480	0	0
1	9-A	4557	4480	4480	0	0
1	10-A	4557	4480	4480	0	0
1	11-A	4557	4480	4480	0	0
1	12-A	4557	4480	4480	0	0
1	13-A	4557	4480	4480	0	0
1	14-A	4557	4480	4480	0	0
1	15-A	4557	4480	4480	0	0
1	16-A	4557	4480	4480	0	0
1	17-A	4557	4480	4480	0	0
1	18-A	4557	4480	4480	0	0
1	19-A	4557	4480	4480	0	0
1	20-A	4557	4480	4480	0	0
1	21-A	4557	4480	4480	0	0
1	22-A	4557	4480	4480	0	0
1	23-A	4557	4480	4480	0	0
1	24-A	4557	4480	4480	0	0
1	25-A	4557	4480	4480	0	0
1	26-A	4557	4480	4480	0	0
1	27-A	4557	4480	4480	0	0
1	28-A	4557	4480	4480	0	0
1	29-A	4557	4480	4480	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	30-A	4557	4480	4480	0	0
1	31-A	4557	4480	4480	0	0
1	32-A	4557	4480	4480	0	0
1	33-A	4557	4480	4480	0	0
1	34-A	4557	4480	4480	0	0
1	35-A	4557	4480	4480	0	0
1	36-A	4557	4480	4480	0	0
1	37-A	4557	4480	4480	0	0
1	38-A	4557	4480	4480	0	0
1	39-A	4557	4480	4480	0	0
1	40-A	4557	4480	4480	0	0
1	41-A	4557	4480	4480	0	0
1	42-A	4557	4480	4480	0	0
1	43-A	4557	4480	4480	0	0
1	44-A	4557	4480	4480	0	0
2	1-A	234	0	0	0	0
2	2-A	234	0	0	0	0
2	3-A	224	0	0	0	0
2	4-A	222	0	0	0	0
2	5-A	230	0	0	0	0
2	6-A	233	0	0	0	0
2	7-A	241	0	0	0	0
2	8-A	238	0	0	0	0
2	9-A	218	0	0	0	0
2	10-A	217	0	0	0	0
2	11-A	219	0	0	0	0
2	12-A	231	0	0	0	0
2	13-A	231	0	0	0	0
2	14-A	235	0	0	0	0
2	15-A	226	0	0	0	0
2	16-A	230	0	0	0	0
2	17-A	211	0	0	0	0
2	18-A	228	0	0	0	0
2	19-A	228	0	0	0	0
2	20-A	236	0	0	0	0
2	21-A	234	0	0	0	0
2	22-A	225	0	0	0	0
2	23-A	206	0	0	0	0
2	24-A	218	0	0	0	0
2	25-A	227	0	0	0	0
2	26-A	227	0	0	0	0
2	27-A	214	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	28-A	237	0	0	0	0
2	29-A	238	0	0	0	0
2	30-A	237	0	0	0	0
2	31-A	224	0	0	0	0
2	32-A	224	0	0	0	0
2	33-A	224	0	0	0	0
2	34-A	235	0	0	0	0
2	35-A	227	0	0	0	0
2	36-A	236	0	0	0	0
2	37-A	234	0	0	0	0
2	38-A	244	0	0	0	0
2	39-A	231	0	0	0	0
2	40-A	231	0	0	0	0
2	41-A	242	0	0	0	0
2	42-A	246	0	0	0	0
2	43-A	233	0	0	0	0
2	44-A	223	0	0	0	0
All	All	210591	197120	197120	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	564/577 (98%)	514 (91%)	39 (7%)	11 (2%)	7 1
1	2-A	564/577 (98%)	523 (93%)	29 (5%)	12 (2%)	7 1
1	3-A	564/577 (98%)	518 (92%)	35 (6%)	11 (2%)	7 1
1	4-A	564/577 (98%)	527 (93%)	29 (5%)	8 (1%)	11 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	564/577 (98%)	518 (92%)	39 (7%)	7 (1%)	13	3
1	6-A	564/577 (98%)	521 (92%)	33 (6%)	10 (2%)	8	1
1	7-A	564/577 (98%)	521 (92%)	36 (6%)	7 (1%)	13	3
1	8-A	564/577 (98%)	521 (92%)	32 (6%)	11 (2%)	7	1
1	9-A	564/577 (98%)	507 (90%)	40 (7%)	17 (3%)	4	0
1	10-A	564/577 (98%)	511 (91%)	43 (8%)	10 (2%)	8	1
1	11-A	564/577 (98%)	513 (91%)	36 (6%)	15 (3%)	5	0
1	12-A	564/577 (98%)	528 (94%)	22 (4%)	14 (2%)	5	1
1	13-A	564/577 (98%)	524 (93%)	25 (4%)	15 (3%)	5	0
1	14-A	564/577 (98%)	514 (91%)	37 (7%)	13 (2%)	6	1
1	15-A	564/577 (98%)	518 (92%)	31 (6%)	15 (3%)	5	0
1	16-A	564/577 (98%)	516 (92%)	32 (6%)	16 (3%)	5	0
1	17-A	564/577 (98%)	521 (92%)	33 (6%)	10 (2%)	8	1
1	18-A	564/577 (98%)	522 (93%)	35 (6%)	7 (1%)	13	3
1	19-A	564/577 (98%)	518 (92%)	33 (6%)	13 (2%)	6	1
1	20-A	564/577 (98%)	515 (91%)	36 (6%)	13 (2%)	6	1
1	21-A	564/577 (98%)	516 (92%)	39 (7%)	9 (2%)	9	1
1	22-A	564/577 (98%)	513 (91%)	35 (6%)	16 (3%)	5	0
1	23-A	564/577 (98%)	510 (90%)	42 (7%)	12 (2%)	7	1
1	24-A	564/577 (98%)	510 (90%)	40 (7%)	14 (2%)	5	1
1	25-A	564/577 (98%)	507 (90%)	39 (7%)	18 (3%)	4	0
1	26-A	564/577 (98%)	508 (90%)	42 (7%)	14 (2%)	5	1
1	27-A	564/577 (98%)	511 (91%)	33 (6%)	20 (4%)	3	0
1	28-A	564/577 (98%)	513 (91%)	33 (6%)	18 (3%)	4	0
1	29-A	564/577 (98%)	515 (91%)	39 (7%)	10 (2%)	8	1
1	30-A	564/577 (98%)	512 (91%)	36 (6%)	16 (3%)	5	0
1	31-A	564/577 (98%)	511 (91%)	39 (7%)	14 (2%)	5	1
1	32-A	564/577 (98%)	511 (91%)	39 (7%)	14 (2%)	5	1
1	33-A	564/577 (98%)	515 (91%)	30 (5%)	19 (3%)	3	0
1	34-A	564/577 (98%)	514 (91%)	31 (6%)	19 (3%)	3	0
1	35-A	564/577 (98%)	513 (91%)	41 (7%)	10 (2%)	8	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	36-A	564/577 (98%)	515 (91%)	40 (7%)	9 (2%)	9	1
1	37-A	564/577 (98%)	513 (91%)	32 (6%)	19 (3%)	3	0
1	38-A	564/577 (98%)	505 (90%)	41 (7%)	18 (3%)	4	0
1	39-A	564/577 (98%)	509 (90%)	34 (6%)	21 (4%)	3	0
1	40-A	564/577 (98%)	514 (91%)	37 (7%)	13 (2%)	6	1
1	41-A	564/577 (98%)	509 (90%)	36 (6%)	19 (3%)	3	0
1	42-A	564/577 (98%)	509 (90%)	35 (6%)	20 (4%)	3	0
1	43-A	564/577 (98%)	516 (92%)	27 (5%)	21 (4%)	3	0
1	44-A	564/577 (98%)	512 (91%)	40 (7%)	12 (2%)	7	1
All	All	24816/25388 (98%)	22651 (91%)	1555 (6%)	610 (2%)	5	1

5 of 610 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	295	GLU
1	1-A	363	PRO
1	1-A	437	SER
1	1-A	464	ARG
1	2-A	100	PHE

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	1-A	500/511 (98%)	440 (88%)	60 (12%)	5	1
1	2-A	500/511 (98%)	436 (87%)	64 (13%)	4	1
1	3-A	500/511 (98%)	439 (88%)	61 (12%)	5	1
1	4-A	500/511 (98%)	439 (88%)	61 (12%)	5	1
1	5-A	500/511 (98%)	436 (87%)	64 (13%)	4	1
1	6-A	500/511 (98%)	448 (90%)	52 (10%)	7	1
1	7-A	500/511 (98%)	444 (89%)	56 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	500/511 (98%)	452 (90%)	48 (10%)	8	1
1	9-A	500/511 (98%)	443 (89%)	57 (11%)	5	1
1	10-A	500/511 (98%)	444 (89%)	56 (11%)	6	1
1	11-A	500/511 (98%)	449 (90%)	51 (10%)	7	1
1	12-A	500/511 (98%)	448 (90%)	52 (10%)	7	1
1	13-A	500/511 (98%)	445 (89%)	55 (11%)	6	1
1	14-A	500/511 (98%)	447 (89%)	53 (11%)	6	1
1	15-A	500/511 (98%)	444 (89%)	56 (11%)	6	1
1	16-A	500/511 (98%)	443 (89%)	57 (11%)	5	1
1	17-A	500/511 (98%)	439 (88%)	61 (12%)	5	1
1	18-A	500/511 (98%)	436 (87%)	64 (13%)	4	1
1	19-A	500/511 (98%)	442 (88%)	58 (12%)	5	1
1	20-A	500/511 (98%)	438 (88%)	62 (12%)	4	1
1	21-A	500/511 (98%)	443 (89%)	57 (11%)	5	1
1	22-A	500/511 (98%)	435 (87%)	65 (13%)	4	1
1	23-A	500/511 (98%)	434 (87%)	66 (13%)	4	1
1	24-A	500/511 (98%)	429 (86%)	71 (14%)	3	0
1	25-A	500/511 (98%)	440 (88%)	60 (12%)	5	1
1	26-A	500/511 (98%)	447 (89%)	53 (11%)	6	1
1	27-A	500/511 (98%)	436 (87%)	64 (13%)	4	1
1	28-A	500/511 (98%)	449 (90%)	51 (10%)	7	1
1	29-A	500/511 (98%)	438 (88%)	62 (12%)	4	1
1	30-A	500/511 (98%)	446 (89%)	54 (11%)	6	1
1	31-A	500/511 (98%)	448 (90%)	52 (10%)	7	1
1	32-A	500/511 (98%)	438 (88%)	62 (12%)	4	1
1	33-A	500/511 (98%)	453 (91%)	47 (9%)	8	1
1	34-A	500/511 (98%)	440 (88%)	60 (12%)	5	1
1	35-A	500/511 (98%)	446 (89%)	54 (11%)	6	1
1	36-A	500/511 (98%)	435 (87%)	65 (13%)	4	1
1	37-A	500/511 (98%)	436 (87%)	64 (13%)	4	1
1	38-A	500/511 (98%)	434 (87%)	66 (13%)	4	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	39-A	500/511 (98%)	429 (86%)	71 (14%)	3	0
1	40-A	500/511 (98%)	441 (88%)	59 (12%)	5	1
1	41-A	500/511 (98%)	444 (89%)	56 (11%)	6	1
1	42-A	500/511 (98%)	443 (89%)	57 (11%)	5	1
1	43-A	500/511 (98%)	435 (87%)	65 (13%)	4	1
1	44-A	500/511 (98%)	436 (87%)	64 (13%)	4	1
All	All	22000/22484 (98%)	19407 (88%)	2593 (12%)	5	1

5 of 2593 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	21-A	236	LEU
1	25-A	405	GLU
1	41-A	486	ARG
1	22-A	8	MET
1	23-A	439	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 490 such sidechains are listed below:

Mol	Chain	Res	Type
1	21-A	258	HIS
1	26-A	91	HIS
1	41-A	176	ASN
1	22-A	120	ASN
1	23-A	418	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	2-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	3-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	4-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	5-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	6-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	7-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	8-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	9-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	10-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	11-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	12-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	13-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	14-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	15-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	16-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	17-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	18-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	19-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	20-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	21-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	22-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	23-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)
1	24-A	566/577 (98%)	0.40	39 (6%)	16 19	27, 30, 35, 39	566 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	25-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	26-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	27-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	28-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	29-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	30-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	31-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	32-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	33-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	34-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	35-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	36-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	37-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	38-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	39-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	40-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	41-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	42-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	43-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
1	44-A	566/577 (98%)	0.40	39 (6%) 16 19	27, 30, 35, 39	566 (100%)
All	All	24904/25388 (98%)	0.40	1716 (6%) 20 19	27, 30, 35, 39	24904 (100%)

The worst 5 of 1716 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	464	ARG	20.3
1	2-A	464	ARG	20.3
1	3-A	464	ARG	20.3
1	4-A	464	ARG	20.3
1	5-A	464	ARG	20.3

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.