wwPDB X-ray Structure Validation Summary Report (i)

Nov 25, 2024 – 07:27 PM EST

PDB ID	:	5IVK
Title	:	The alpha-esterase-7 carboxylesterase, E3, from the blowfly Lucilia cuprina: phosphorylated-enzyme ensemble refinement
Authors	:	Correy, G.J.; Jackson, C.J.
Deposited on	:	2016-03-21
Resolution	:	1.53 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 (i) 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 (i)) were used in the production of this report:

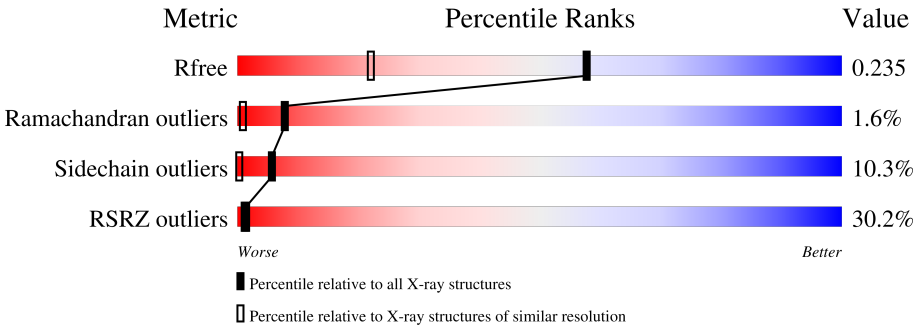
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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}	164625	3511 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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 <=5%

Mol	Chain	Length	Quality of chain
1	1-A	577	30% 87% 10%
1	10-A	577	88% 9%
1	11-A	577	89% 8%
1	12-A	577	90% 7%
1	13-A	577	87% 10%
1	14-A	577	89% 8%
1	15-A	577	86% 11%

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Mol	Chain	Length	Quality of chain
1	16-A	577	88% 9%
1	17-A	577	86% 10%
1	18-A	577	87% 9%
1	19-A	577	86% 11%
1	2-A	577	88% 9%
1	20-A	577	86% 11%
1	21-A	577	85% 12%
1	22-A	577	87% 10%
1	23-A	577	87% 10%
1	24-A	577	86% 11%
1	25-A	577	85% 12%
1	26-A	577	86% 11%
1	27-A	577	88% 9%
1	28-A	577	87% 10%
1	29-A	577	87% 10%
1	3-A	577	89% 8%
1	30-A	577	89% 8%
1	31-A	577	87% 10%
1	32-A	577	86% 10%
1	33-A	577	87% 10%
1	34-A	577	86% 10%
1	35-A	577	88% 9%
1	36-A	577	88% 9%
1	37-A	577	89% 7%
1	38-A	577	88% 8%

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Mol	Chain	Length	Quality of chain
1	39-A	577	86% 10%
1	4-A	577	87% 10%
1	40-A	577	86% 11%
1	41-A	577	87% 9%
1	42-A	577	87% 10%
1	43-A	577	86% 11%
1	5-A	577	86% 11%
1	6-A	577	89% 9%
1	7-A	577	89% 8%
1	8-A	577	89% 8%
1	9-A	577	88% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 405539 atoms, of which 192984 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
			9035	2911	4478	766	846	34			
1	2-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	3-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	4-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	5-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	6-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	7-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	8-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	9-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	10-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	11-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	12-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	13-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	14-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	15-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	16-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	18-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	19-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	20-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	21-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	22-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	23-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	24-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	25-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	26-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	27-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	28-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	29-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	30-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	31-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	32-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	33-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	34-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	35-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	36-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	37-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			

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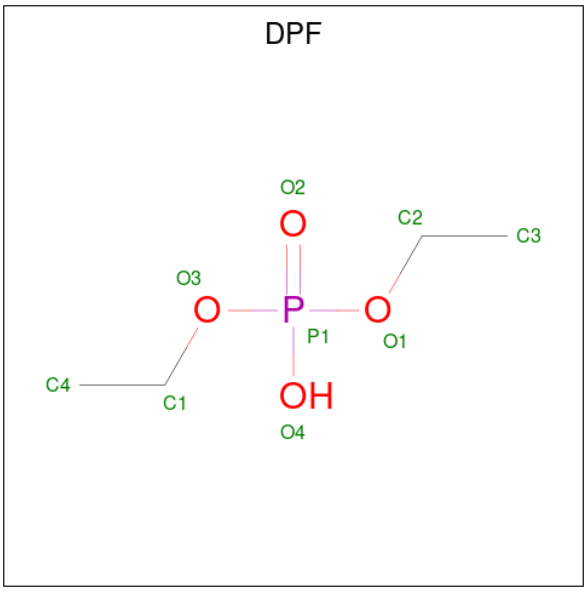
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	39-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	40-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	41-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	42-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			
1	43-A	566	Total	C	H	N	O	S	0	0	0
			9035	2911	4478	766	846	34			

There are 13 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	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 DIETHYL HYDROGEN PHOSPHATE (three-letter code: DPF) (formula: $C_4H_{11}O_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	2-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	3-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	4-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	5-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	6-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	7-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	8-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	9-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	10-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	11-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	12-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	13-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	14-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	16-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	17-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	18-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	19-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	20-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	21-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	22-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	23-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	24-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	25-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	26-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	27-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	28-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	29-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	30-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	31-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	32-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	33-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	34-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	35-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	36-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	37-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	38-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	39-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	40-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	41-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	42-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		
2	43-A	1	Total	C	H	O	P	0	0
			18	4	10	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	399	Total	O	0	0
			399	399		
3	2-A	380	Total	O	0	0
			380	380		
3	3-A	356	Total	O	0	0
			356	356		
3	4-A	389	Total	O	0	0
			389	389		
3	5-A	386	Total	O	0	0
			386	386		
3	6-A	379	Total	O	0	0
			379	379		
3	7-A	375	Total	O	0	0
			375	375		
3	8-A	365	Total	O	0	0
			365	365		
3	9-A	373	Total	O	0	0
			373	373		
3	10-A	365	Total	O	0	0
			365	365		
3	11-A	360	Total	O	0	0
			360	360		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	12-A	396	Total O 396 396	0	0
3	13-A	406	Total O 406 406	0	0
3	14-A	378	Total O 378 378	0	0
3	15-A	374	Total O 374 374	0	0
3	16-A	386	Total O 386 386	0	0
3	17-A	357	Total O 357 357	0	0
3	18-A	353	Total O 353 353	0	0
3	19-A	363	Total O 363 363	0	0
3	20-A	399	Total O 399 399	0	0
3	21-A	389	Total O 389 389	0	0
3	22-A	380	Total O 380 380	0	0
3	23-A	376	Total O 376 376	0	0
3	24-A	381	Total O 381 381	0	0
3	25-A	359	Total O 359 359	0	0
3	26-A	362	Total O 362 362	0	0
3	27-A	379	Total O 379 379	0	0
3	28-A	389	Total O 389 389	0	0
3	29-A	377	Total O 377 377	0	0
3	30-A	363	Total O 363 363	0	0
3	31-A	365	Total O 365 365	0	0
3	32-A	393	Total O 393 393	0	0

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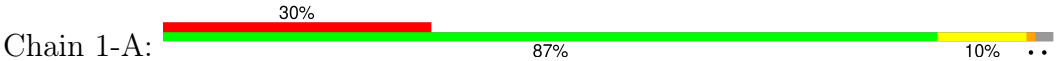
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	33-A	378	Total O 378 378	0	0
3	34-A	384	Total O 384 384	0	0
3	35-A	383	Total O 383 383	0	0
3	36-A	390	Total O 390 390	0	0
3	37-A	358	Total O 358 358	0	0
3	38-A	377	Total O 377 377	0	0
3	39-A	393	Total O 393 393	0	0
3	40-A	388	Total O 388 388	0	0
3	41-A	390	Total O 390 390	0	0
3	42-A	390	Total O 390 390	0	0
3	43-A	377	Total O 377 377	0	0

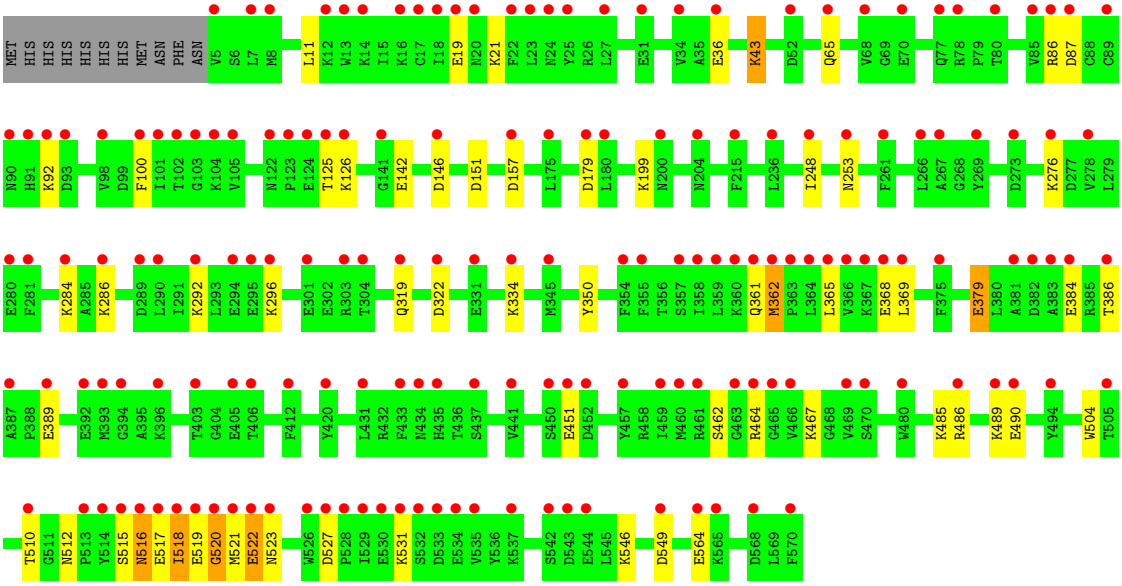
3 Residue-property plots (i)

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. 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. 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: Carboxylic ester hydrolase

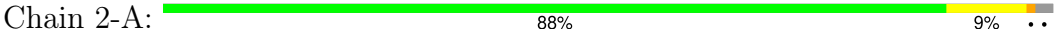
Chain 1-A:

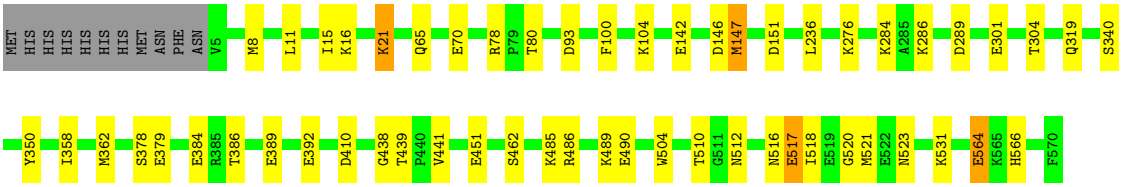




• Molecule 1: Carboxylic ester hydrolase

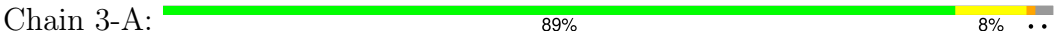
Chain 2-A:

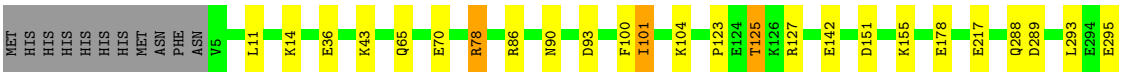


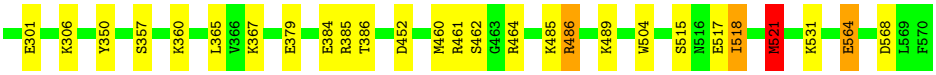


• Molecule 1: Carboxylic ester hydrolase

Chain 3-A:

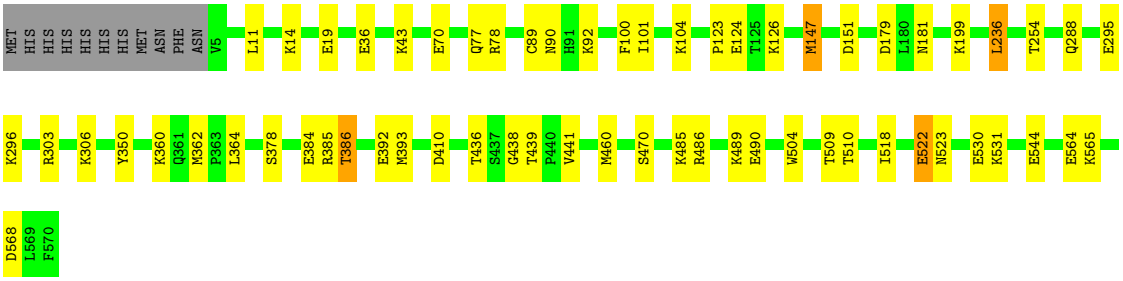






• Molecule 1: Carboxylic ester hydrolase

Chain 4-A:

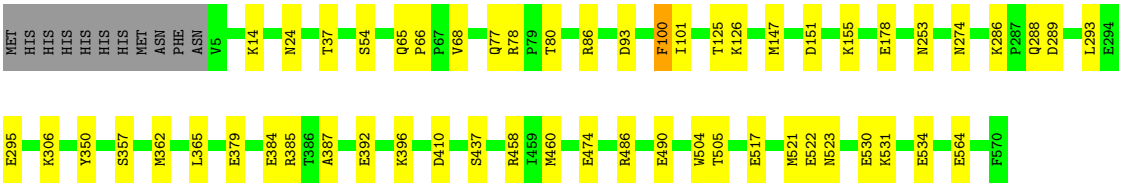


• Molecule 1: Carboxylic ester hydrolase

Chain 5-A:

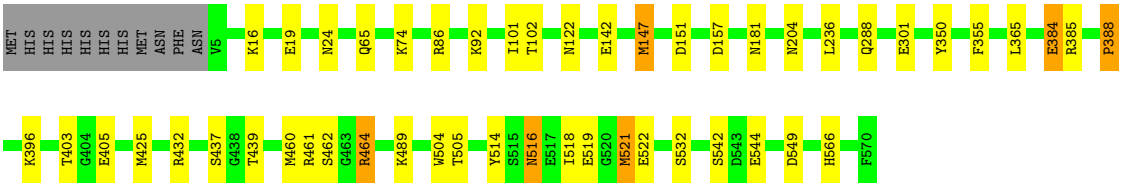
• Molecule 1: Carboxylic ester hydrolase

Chain 6-A:



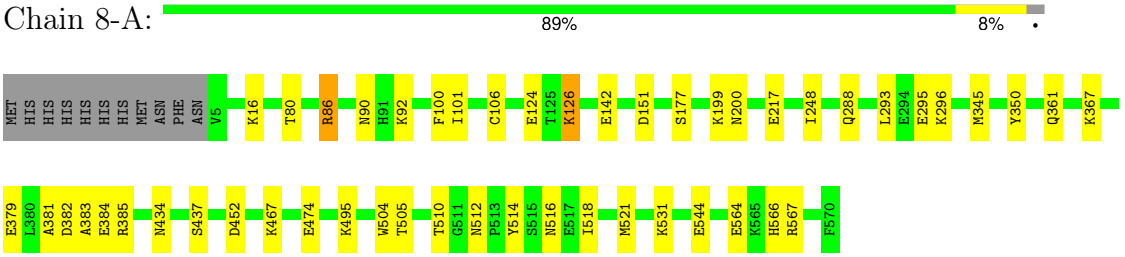
• Molecule 1: Carboxylic ester hydrolase

Chain 7-A:



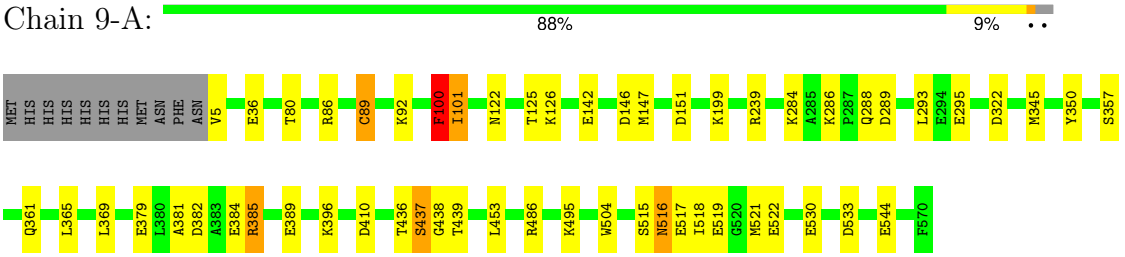
• Molecule 1: Carboxylic ester hydrolase

Chain 8-A:



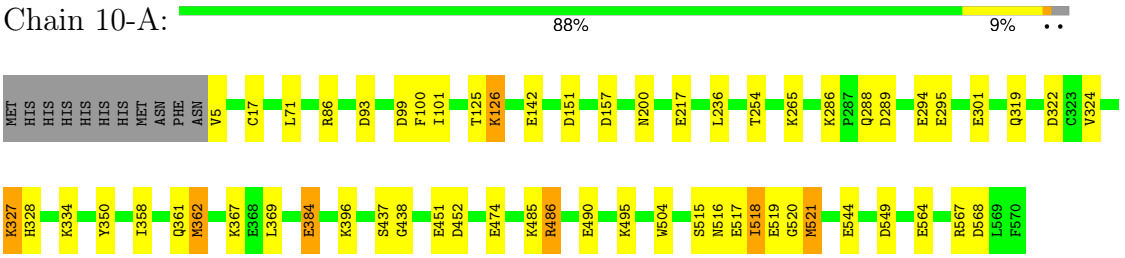
• Molecule 1: Carboxylic ester hydrolase

Chain 9-A:



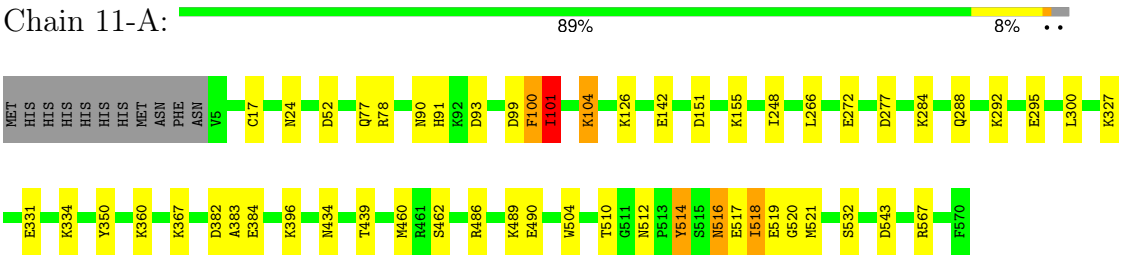
• Molecule 1: Carboxylic ester hydrolase

Chain 10-A:



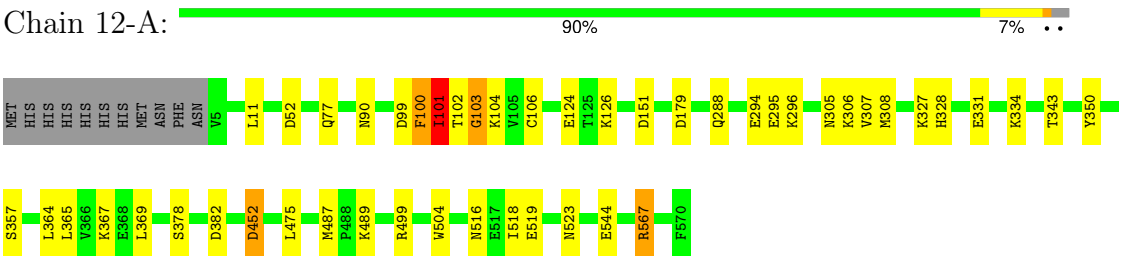
• Molecule 1: Carboxylic ester hydrolase

Chain 11-A:



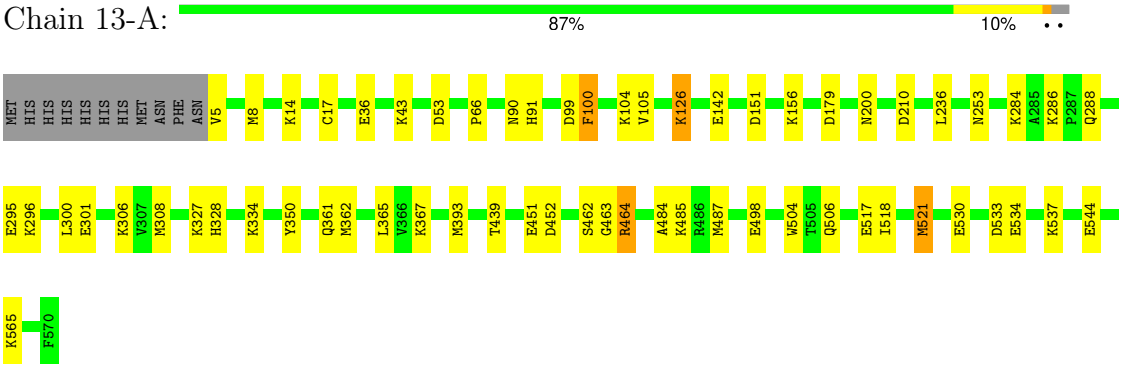
• Molecule 1: Carboxylic ester hydrolase

Chain 12-A:



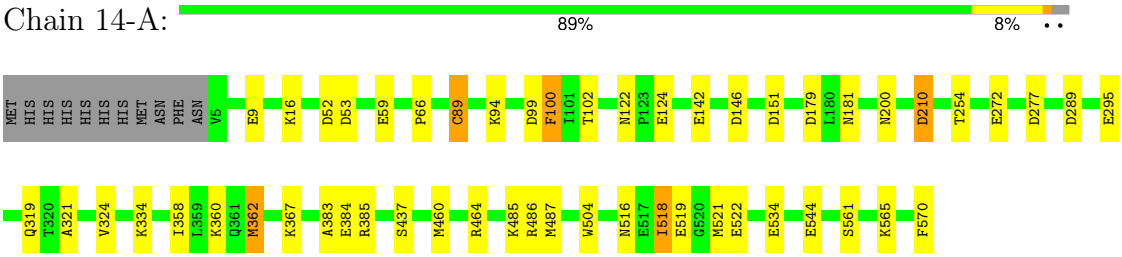
• Molecule 1: Carboxylic ester hydrolase

Chain 13-A:



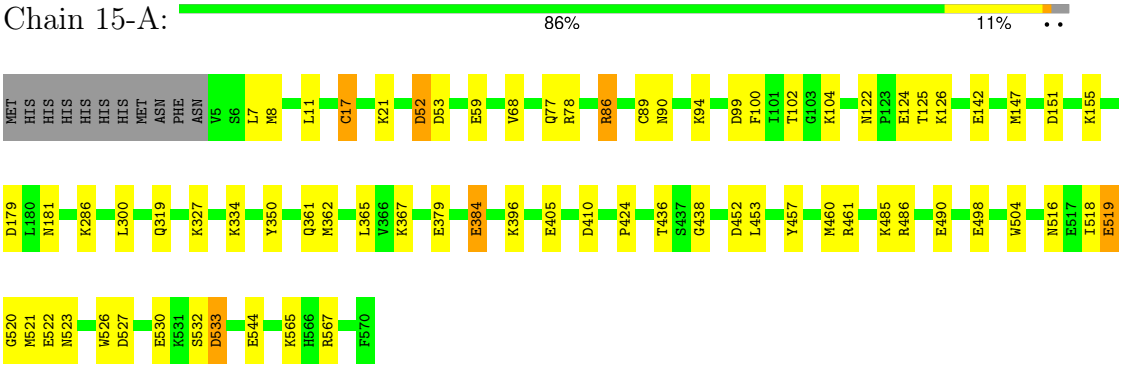
• Molecule 1: Carboxylic ester hydrolase

Chain 14-A:



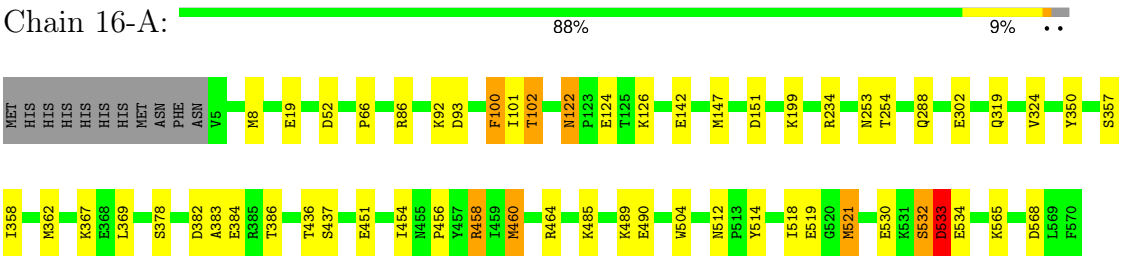
• Molecule 1: Carboxylic ester hydrolase

Chain 15-A:



• Molecule 1: Carboxylic ester hydrolase

Chain 16-A:

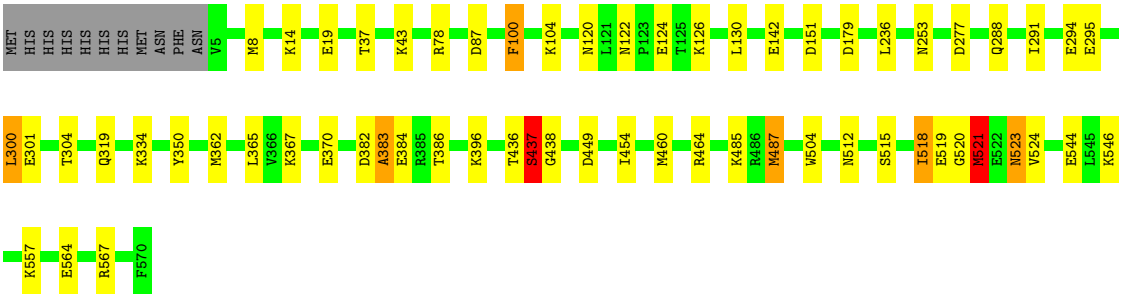


• Molecule 1: Carboxylic ester hydrolase

Chain 17-A:

• Molecule 1: Carboxylic ester hydrolase

Chain 18-A:



• Molecule 1: Carboxylic ester hydrolase

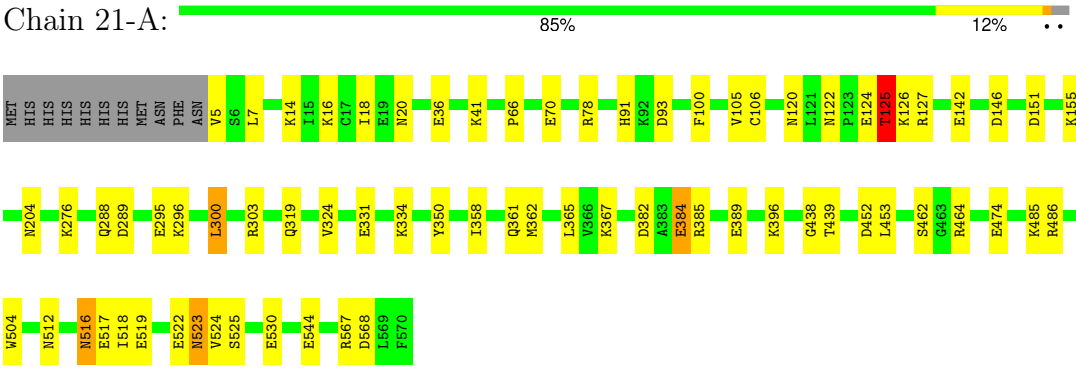
Chain 19-A:

• Molecule 1: Carboxylic ester hydrolase

Chain 20-A:

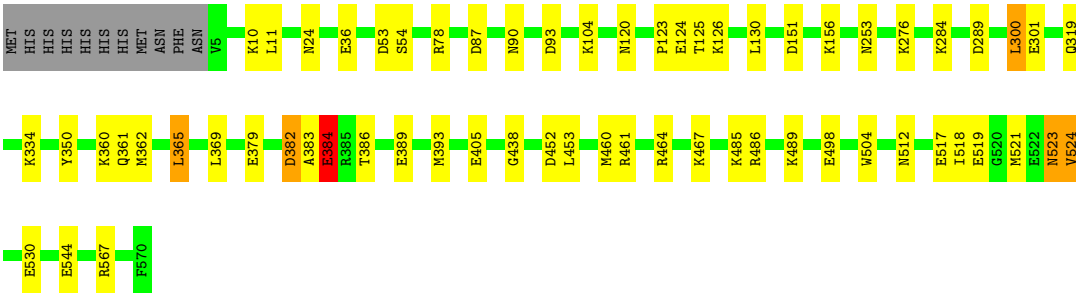
• Molecule 1: Carboxylic ester hydrolase

Chain 21-A:



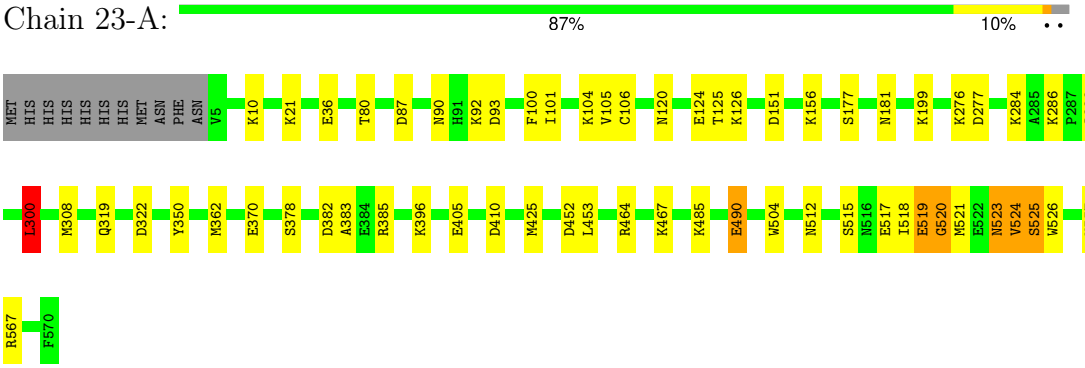
• Molecule 1: Carboxylic ester hydrolase

Chain 22-A:



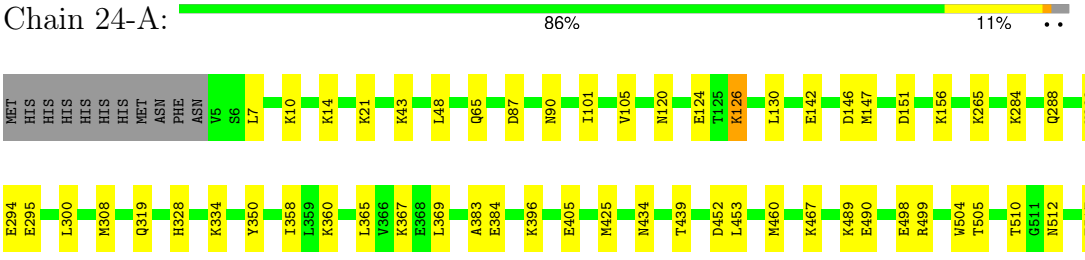
• Molecule 1: Carboxylic ester hydrolase

Chain 23-A:



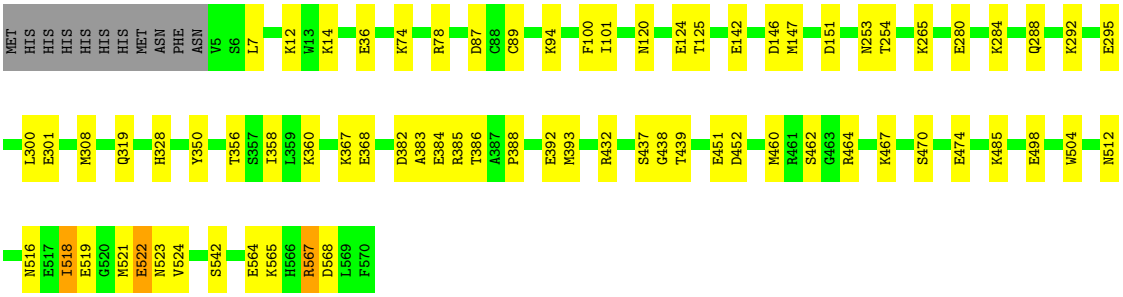
• Molecule 1: Carboxylic ester hydrolase

Chain 24-A:



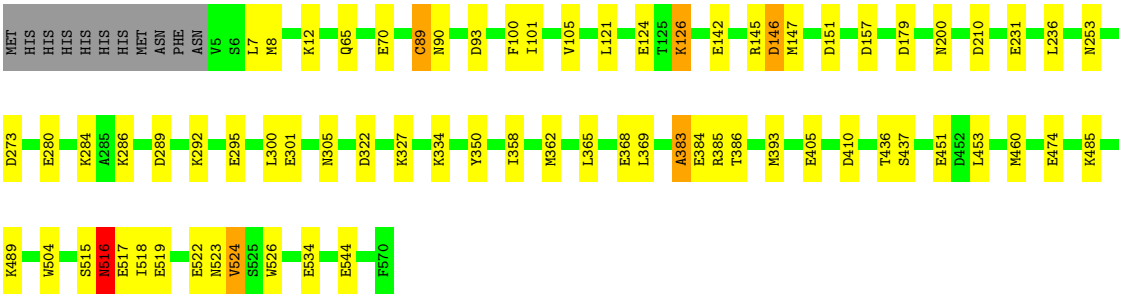
• Molecule 1: Carboxylic ester hydrolase

Chain 25-A:



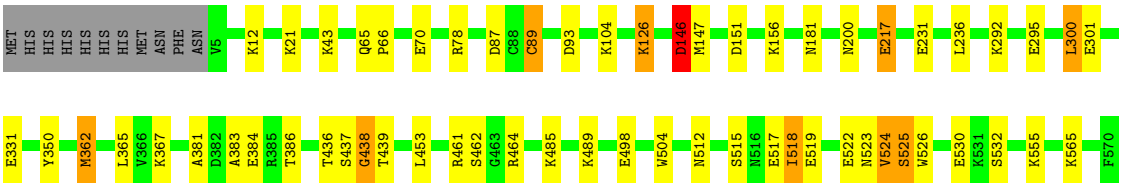
• Molecule 1: Carboxylic ester hydrolase

Chain 26-A:



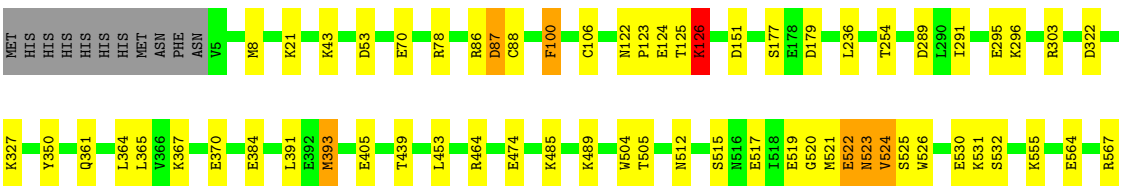
• Molecule 1: Carboxylic ester hydrolase

Chain 27-A:



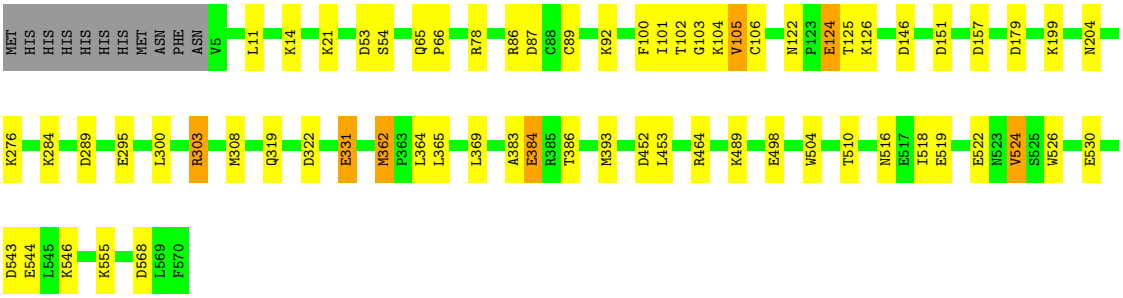
• Molecule 1: Carboxylic ester hydrolase

Chain 28-A:



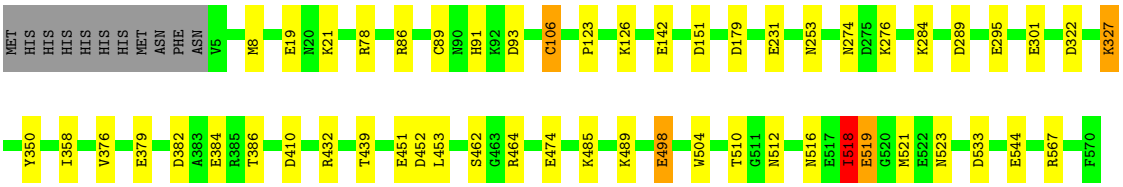
• Molecule 1: Carboxylic ester hydrolase

Chain 29-A:



• Molecule 1: Carboxylic ester hydrolase

Chain 30-A:

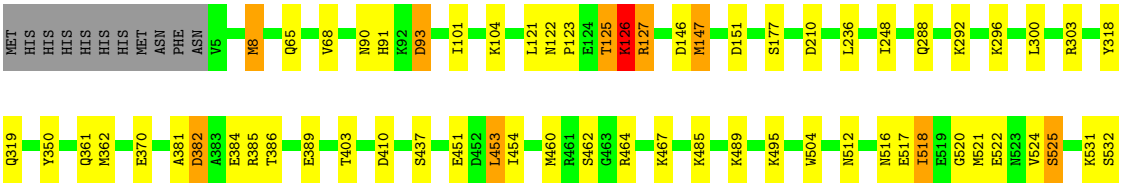


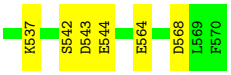
• Molecule 1: Carboxylic ester hydrolase

Chain 31-A:

• Molecule 1: Carboxylic ester hydrolase

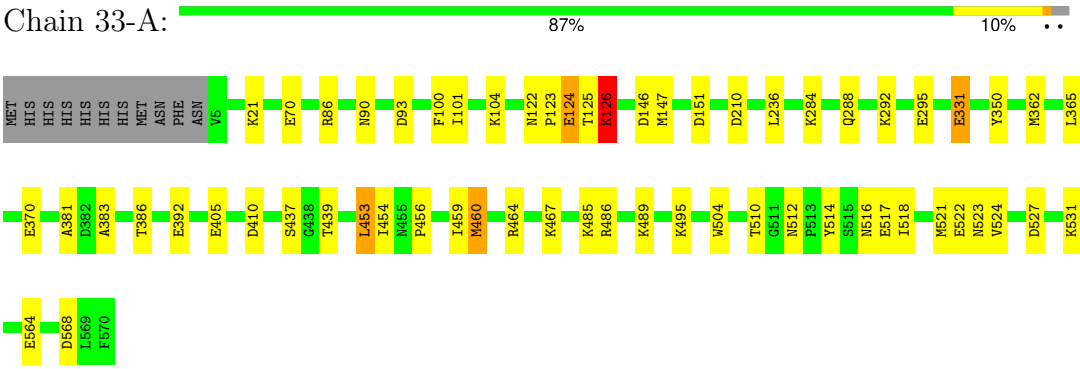
Chain 32-A:





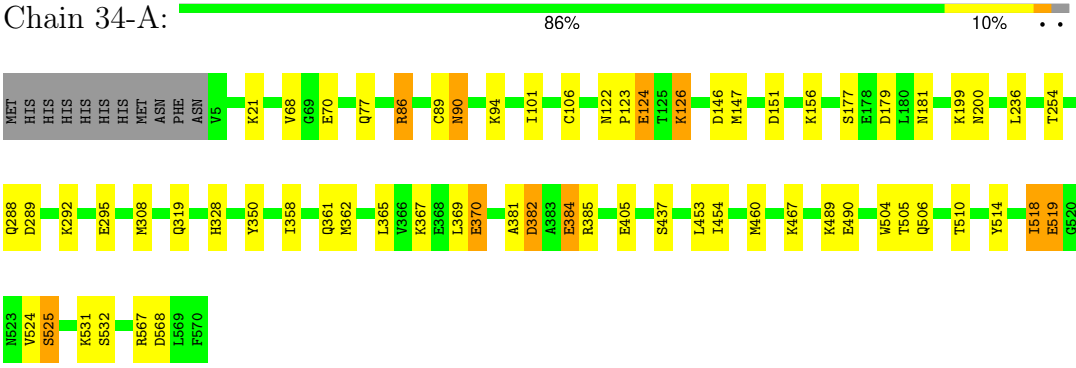
• Molecule 1: Carboxylic ester hydrolase

Chain 33-A:



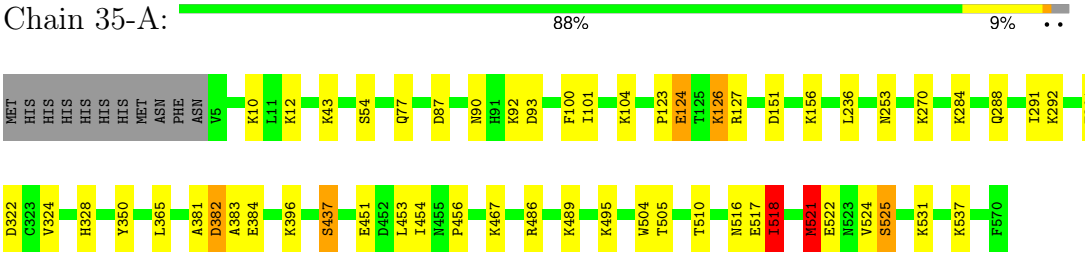
• Molecule 1: Carboxylic ester hydrolase

Chain 34-A:



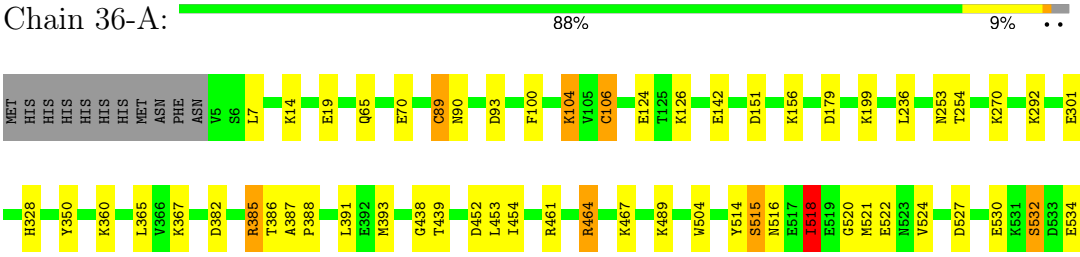
• Molecule 1: Carboxylic ester hydrolase

Chain 35-A:



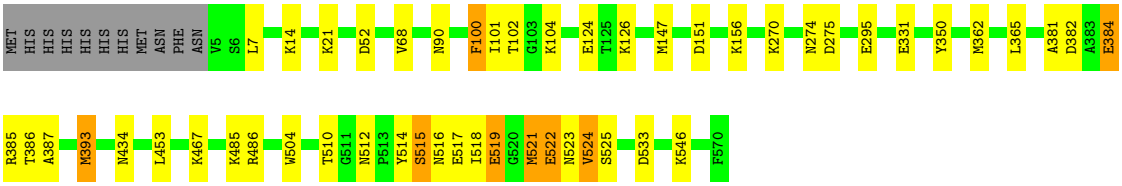
• Molecule 1: Carboxylic ester hydrolase

Chain 36-A:



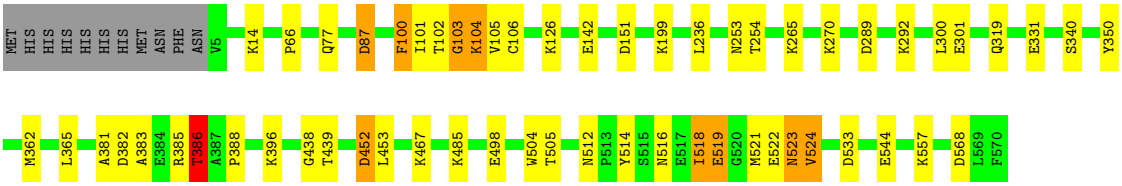
• Molecule 1: Carboxylic ester hydrolase

Chain 37-A:



• Molecule 1: Carboxylic ester hydrolase

Chain 38-A:



• Molecule 1: Carboxylic ester hydrolase

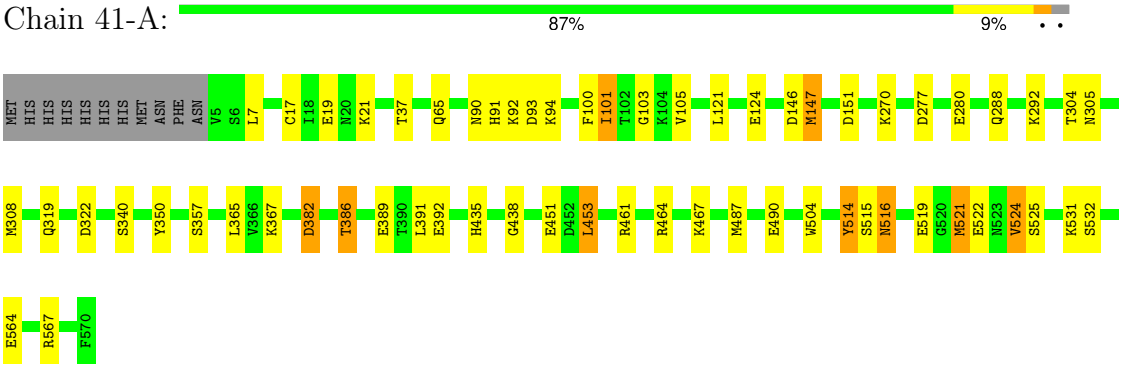
Chain 39-A:

• Molecule 1: Carboxylic ester hydrolase

Chain 40-A:

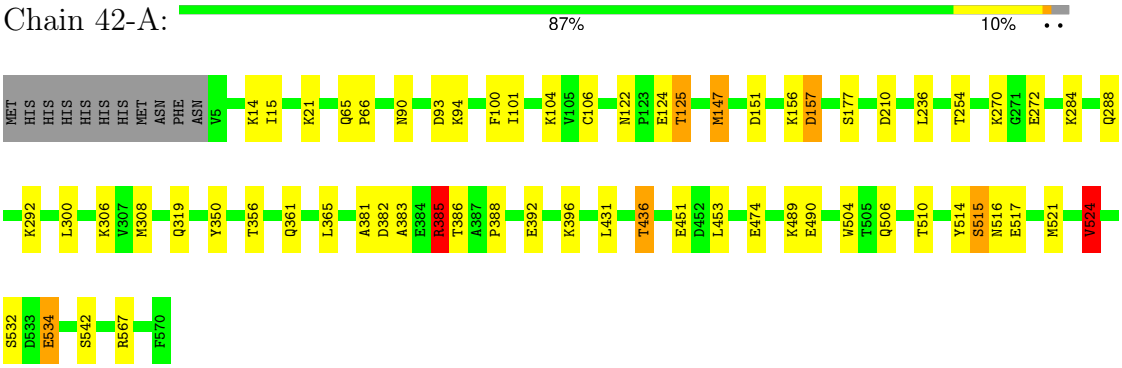
• Molecule 1: Carboxylic ester hydrolase

Chain 41-A:



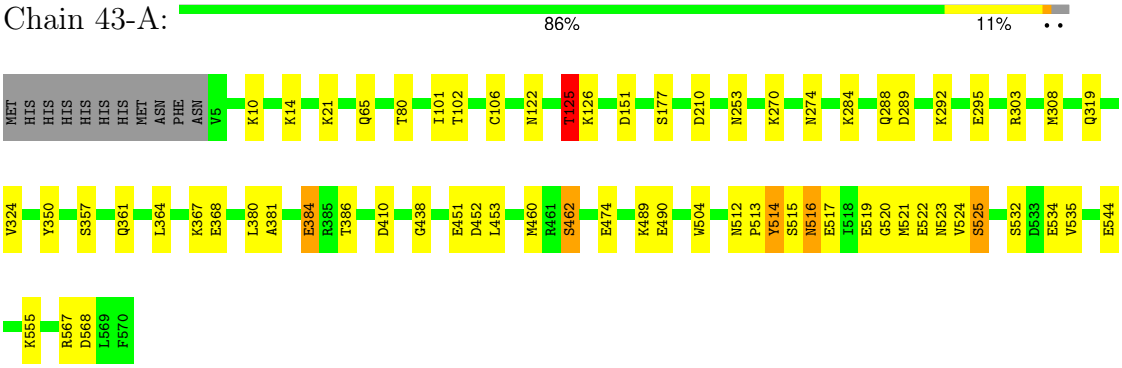
• Molecule 1: Carboxylic ester hydrolase

Chain 42-A:



• Molecule 1: Carboxylic ester hydrolase

Chain 43-A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	51.82Å 101.25Å 225.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.01 – 1.53 42.01 – 1.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.01-1.53) 95.8 (42.01-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.181 , 0.220 0.193 , 0.235	Depositor DCC
R_{free} test set	4499 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.01 , 23.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	405539	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2/4672 (0.0%)	0.78	5/6320 (0.1%)
1	2-A	0.57	0/4672	0.73	2/6320 (0.0%)
1	3-A	0.62	0/4672	0.76	7/6320 (0.1%)
1	4-A	0.65	2/4672 (0.0%)	0.78	7/6320 (0.1%)
1	5-A	0.62	2/4672 (0.0%)	0.74	0/6320
1	6-A	0.58	2/4672 (0.0%)	0.74	3/6320 (0.0%)
1	7-A	0.60	0/4672	0.75	4/6320 (0.1%)
1	8-A	0.59	1/4672 (0.0%)	0.73	2/6320 (0.0%)
1	9-A	0.62	3/4672 (0.1%)	0.76	5/6320 (0.1%)
1	10-A	0.62	3/4672 (0.1%)	0.78	3/6320 (0.0%)
1	11-A	0.59	3/4672 (0.1%)	0.75	3/6320 (0.0%)
1	12-A	0.61	3/4672 (0.1%)	0.79	7/6320 (0.1%)
1	13-A	0.65	6/4672 (0.1%)	0.79	4/6320 (0.1%)
1	14-A	0.61	2/4672 (0.0%)	0.77	6/6320 (0.1%)
1	15-A	0.62	3/4672 (0.1%)	0.80	7/6320 (0.1%)
1	16-A	0.62	1/4672 (0.0%)	0.79	3/6320 (0.0%)
1	17-A	0.63	2/4672 (0.0%)	0.78	7/6320 (0.1%)
1	18-A	0.61	0/4672	0.78	8/6320 (0.1%)
1	19-A	0.60	0/4672	0.79	8/6320 (0.1%)
1	20-A	0.64	1/4672 (0.0%)	0.80	8/6320 (0.1%)
1	21-A	0.61	2/4672 (0.0%)	0.77	5/6320 (0.1%)
1	22-A	0.60	2/4672 (0.0%)	0.78	5/6320 (0.1%)
1	23-A	0.65	1/4672 (0.0%)	0.79	9/6320 (0.1%)
1	24-A	0.61	3/4672 (0.1%)	0.78	3/6320 (0.0%)
1	25-A	0.59	1/4672 (0.0%)	0.77	2/6320 (0.0%)
1	26-A	0.61	2/4672 (0.0%)	0.78	3/6320 (0.0%)
1	27-A	0.63	4/4672 (0.1%)	0.78	4/6320 (0.1%)
1	28-A	0.63	1/4672 (0.0%)	0.77	3/6320 (0.0%)
1	29-A	0.62	3/4672 (0.1%)	0.77	6/6320 (0.1%)
1	30-A	0.64	5/4672 (0.1%)	0.77	5/6320 (0.1%)
1	31-A	0.63	5/4672 (0.1%)	0.77	1/6320 (0.0%)
1	32-A	0.69	4/4672 (0.1%)	0.81	10/6320 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	33-A	0.60	4/4672 (0.1%)	0.77	7/6320 (0.1%)
1	34-A	0.64	4/4672 (0.1%)	0.78	4/6320 (0.1%)
1	35-A	0.61	1/4672 (0.0%)	0.75	0/6320
1	36-A	0.59	1/4672 (0.0%)	0.78	3/6320 (0.0%)
1	37-A	0.58	0/4672	0.77	1/6320 (0.0%)
1	38-A	0.60	2/4672 (0.0%)	0.77	3/6320 (0.0%)
1	39-A	0.61	2/4672 (0.0%)	0.76	5/6320 (0.1%)
1	40-A	0.61	4/4672 (0.1%)	0.77	0/6320
1	41-A	0.60	3/4672 (0.1%)	0.77	7/6320 (0.1%)
1	42-A	0.63	4/4672 (0.1%)	0.79	5/6320 (0.1%)
1	43-A	0.62	4/4672 (0.1%)	0.77	2/6320 (0.0%)
All	All	0.62	98/200896 (0.0%)	0.77	192/271760 (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	3
1	3-A	0	3
1	4-A	0	2
1	5-A	0	1
1	7-A	0	1
1	8-A	0	1
1	9-A	0	3
1	10-A	0	5
1	11-A	0	3
1	12-A	0	4
1	13-A	0	3
1	14-A	0	1
1	15-A	0	5
1	16-A	0	4
1	17-A	0	5
1	18-A	0	5
1	19-A	0	3
1	20-A	0	4
1	21-A	0	7
1	22-A	0	5
1	23-A	0	6
1	24-A	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	25-A	0	1
1	26-A	0	4
1	27-A	0	5
1	28-A	0	2
1	29-A	0	2
1	30-A	0	2
1	31-A	0	1
1	32-A	0	3
1	33-A	0	2
1	34-A	0	5
1	35-A	0	6
1	36-A	0	3
1	37-A	0	4
1	38-A	0	5
1	39-A	0	3
1	40-A	0	6
1	41-A	0	2
1	42-A	0	4
1	43-A	0	5
All	All	0	143

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	32-A	125	THR	C-N	21.17	1.82	1.34
1	9-A	89	CYS	CB-SG	11.56	2.01	1.82
1	23-A	106	CYS	CB-SG	11.46	2.01	1.82
1	13-A	126	LYS	C-N	11.18	1.59	1.34
1	34-A	126	LYS	C-N	10.49	1.58	1.34

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	22-A	130	LEU	CA-CB-CG	13.13	145.50	115.30
1	15-A	17	CYS	CA-CB-SG	12.26	136.07	114.00
1	42-A	157	ASP	CB-CG-OD2	-9.89	109.40	118.30
1	17-A	147	MET	CG-SD-CE	-9.52	84.96	100.20
1	1-A	179	ASP	CB-CG-OD2	-8.96	110.23	118.30

There are no chirality outliers.

5 of 143 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	518	ILE	Peptide
1	1-A	520	GLY	Peptide
1	1-A	522	GLU	Peptide
1	2-A	517	GLU	Peptide
1	2-A	518	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	4557	4478	4476	0	0
1	2-A	4557	4478	4476	0	0
1	3-A	4557	4478	4476	0	0
1	4-A	4557	4478	4476	0	0
1	5-A	4557	4478	4476	0	0
1	6-A	4557	4478	4476	0	0
1	7-A	4557	4478	4476	0	0
1	8-A	4557	4478	4476	0	0
1	9-A	4557	4478	4476	0	0
1	10-A	4557	4478	4476	0	0
1	11-A	4557	4478	4476	0	0
1	12-A	4557	4478	4476	0	0
1	13-A	4557	4478	4476	0	0
1	14-A	4557	4478	4476	0	0
1	15-A	4557	4478	4476	0	0
1	16-A	4557	4478	4476	0	0
1	17-A	4557	4478	4476	0	0
1	18-A	4557	4478	4476	0	0
1	19-A	4557	4478	4475	0	0
1	20-A	4557	4478	4476	0	0
1	21-A	4557	4478	4476	0	0
1	22-A	4557	4478	4476	0	0
1	23-A	4557	4478	4476	0	0
1	24-A	4557	4478	4476	0	0
1	25-A	4557	4478	4476	0	0
1	26-A	4557	4478	4476	0	0
1	27-A	4557	4478	4476	0	0
1	28-A	4557	4478	4476	0	0
1	29-A	4557	4478	4476	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	30-A	4557	4478	4476	0	0
1	31-A	4557	4478	4476	0	0
1	32-A	4557	4478	4475	0	0
1	33-A	4557	4478	4476	0	0
1	34-A	4557	4478	4476	0	0
1	35-A	4557	4478	4476	0	0
1	36-A	4557	4478	4476	0	0
1	37-A	4557	4478	4476	0	0
1	38-A	4557	4478	4476	0	0
1	39-A	4557	4478	4476	0	0
1	40-A	4557	4478	4476	0	0
1	41-A	4557	4478	4476	0	0
1	42-A	4557	4478	4476	0	0
1	43-A	4557	4478	4476	0	0
2	1-A	8	10	10	0	0
2	2-A	8	10	10	0	0
2	3-A	8	10	10	0	0
2	4-A	8	10	10	0	0
2	5-A	8	10	10	0	0
2	6-A	8	10	10	0	0
2	7-A	8	10	10	0	0
2	8-A	8	10	10	0	0
2	9-A	8	10	10	0	0
2	10-A	8	10	10	0	0
2	11-A	8	10	10	0	0
2	12-A	8	10	10	0	0
2	13-A	8	10	10	0	0
2	14-A	8	10	10	0	0
2	15-A	8	10	10	0	0
2	16-A	8	10	10	0	0
2	17-A	8	10	10	0	0
2	18-A	8	10	10	0	0
2	19-A	8	10	10	0	0
2	20-A	8	10	10	0	0
2	21-A	8	10	10	0	0
2	22-A	8	10	10	0	0
2	23-A	8	10	10	0	0
2	24-A	8	10	10	0	0
2	25-A	8	10	10	0	0
2	26-A	8	10	10	0	0
2	27-A	8	10	10	0	0
2	28-A	8	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	29-A	8	10	10	0	0
2	30-A	8	10	10	0	0
2	31-A	8	10	10	0	0
2	32-A	8	10	10	0	0
2	33-A	8	10	10	0	0
2	34-A	8	10	10	0	0
2	35-A	8	10	10	0	0
2	36-A	8	10	10	0	0
2	37-A	8	10	10	0	0
2	38-A	8	10	10	0	0
2	39-A	8	10	10	0	0
2	40-A	8	10	10	0	0
2	41-A	8	10	10	0	0
2	42-A	8	10	10	0	0
2	43-A	8	10	10	0	0
3	1-A	399	0	0	0	0
3	2-A	380	0	0	0	0
3	3-A	356	0	0	0	0
3	4-A	389	0	0	0	0
3	5-A	386	0	0	0	0
3	6-A	379	0	0	0	0
3	7-A	375	0	0	0	0
3	8-A	365	0	0	0	0
3	9-A	373	0	0	0	0
3	10-A	365	0	0	0	0
3	11-A	360	0	0	0	0
3	12-A	396	0	0	0	0
3	13-A	406	0	0	0	0
3	14-A	378	0	0	0	0
3	15-A	374	0	0	0	0
3	16-A	386	0	0	0	0
3	17-A	357	0	0	0	0
3	18-A	353	0	0	0	0
3	19-A	363	0	0	0	0
3	20-A	399	0	0	0	0
3	21-A	389	0	0	0	0
3	22-A	380	0	0	0	0
3	23-A	376	0	0	0	0
3	24-A	381	0	0	0	0
3	25-A	359	0	0	0	0
3	26-A	362	0	0	0	0
3	27-A	379	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	28-A	389	0	0	0	0
3	29-A	377	0	0	0	0
3	30-A	363	0	0	0	0
3	31-A	365	0	0	0	0
3	32-A	393	0	0	0	0
3	33-A	378	0	0	0	0
3	34-A	384	0	0	0	0
3	35-A	383	0	0	0	0
3	36-A	390	0	0	0	0
3	37-A	358	0	0	0	0
3	38-A	377	0	0	0	0
3	39-A	393	0	0	0	0
3	40-A	388	0	0	0	0
3	41-A	390	0	0	0	0
3	42-A	390	0	0	0	0
3	43-A	377	0	0	0	0
All	All	212555	192984	192896	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%)	531 (94%)	27 (5%)	6 (1%)	12 2
1	2-A	564/577 (98%)	524 (93%)	34 (6%)	6 (1%)	12 2
1	3-A	564/577 (98%)	528 (94%)	29 (5%)	7 (1%)	11 1
1	4-A	564/577 (98%)	533 (94%)	27 (5%)	4 (1%)	19 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	564/577 (98%)	529 (94%)	28 (5%)	7 (1%)	11	1
1	6-A	564/577 (98%)	528 (94%)	30 (5%)	6 (1%)	12	2
1	7-A	564/577 (98%)	527 (93%)	31 (6%)	6 (1%)	12	2
1	8-A	564/577 (98%)	528 (94%)	28 (5%)	8 (1%)	9	1
1	9-A	564/577 (98%)	531 (94%)	26 (5%)	7 (1%)	11	1
1	10-A	564/577 (98%)	538 (95%)	20 (4%)	6 (1%)	12	2
1	11-A	564/577 (98%)	528 (94%)	30 (5%)	6 (1%)	12	2
1	12-A	564/577 (98%)	528 (94%)	28 (5%)	8 (1%)	9	1
1	13-A	564/577 (98%)	532 (94%)	27 (5%)	5 (1%)	14	3
1	14-A	564/577 (98%)	531 (94%)	25 (4%)	8 (1%)	9	1
1	15-A	564/577 (98%)	523 (93%)	32 (6%)	9 (2%)	8	1
1	16-A	564/577 (98%)	531 (94%)	24 (4%)	9 (2%)	8	1
1	17-A	564/577 (98%)	532 (94%)	23 (4%)	9 (2%)	8	1
1	18-A	564/577 (98%)	529 (94%)	26 (5%)	9 (2%)	8	1
1	19-A	564/577 (98%)	530 (94%)	29 (5%)	5 (1%)	14	3
1	20-A	564/577 (98%)	525 (93%)	30 (5%)	9 (2%)	8	1
1	21-A	564/577 (98%)	523 (93%)	34 (6%)	7 (1%)	11	1
1	22-A	564/577 (98%)	525 (93%)	29 (5%)	10 (2%)	7	1
1	23-A	564/577 (98%)	521 (92%)	31 (6%)	12 (2%)	5	0
1	24-A	564/577 (98%)	530 (94%)	30 (5%)	4 (1%)	19	4
1	25-A	564/577 (98%)	524 (93%)	32 (6%)	8 (1%)	9	1
1	26-A	564/577 (98%)	527 (93%)	28 (5%)	9 (2%)	8	1
1	27-A	564/577 (98%)	519 (92%)	34 (6%)	11 (2%)	6	0
1	28-A	564/577 (98%)	527 (93%)	25 (4%)	12 (2%)	5	0
1	29-A	564/577 (98%)	530 (94%)	24 (4%)	10 (2%)	7	1
1	30-A	564/577 (98%)	531 (94%)	29 (5%)	4 (1%)	19	4
1	31-A	564/577 (98%)	530 (94%)	22 (4%)	12 (2%)	5	0
1	32-A	564/577 (98%)	534 (95%)	17 (3%)	13 (2%)	5	0
1	33-A	564/577 (98%)	520 (92%)	36 (6%)	8 (1%)	9	1
1	34-A	564/577 (98%)	518 (92%)	34 (6%)	12 (2%)	5	0
1	35-A	564/577 (98%)	517 (92%)	39 (7%)	8 (1%)	9	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	36-A	564/577 (98%)	524 (93%)	27 (5%)	13 (2%)	5 0
1	37-A	564/577 (98%)	519 (92%)	31 (6%)	14 (2%)	4 0
1	38-A	564/577 (98%)	522 (93%)	30 (5%)	12 (2%)	5 0
1	39-A	564/577 (98%)	523 (93%)	28 (5%)	13 (2%)	5 0
1	40-A	564/577 (98%)	530 (94%)	22 (4%)	12 (2%)	5 0
1	41-A	564/577 (98%)	524 (93%)	27 (5%)	13 (2%)	5 0
1	42-A	564/577 (98%)	525 (93%)	28 (5%)	11 (2%)	6 0
1	43-A	564/577 (98%)	526 (93%)	23 (4%)	15 (3%)	4 0
All	All	24252/24811 (98%)	22655 (93%)	1214 (5%)	383 (2%)	8 1

5 of 383 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	515	SER
1	1-A	522	GLU
1	2-A	564	GLU
1	3-A	123	PRO
1	3-A	518	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1-A	500/512 (98%)	445 (89%)	55 (11%)	5 0
1	2-A	500/512 (98%)	451 (90%)	49 (10%)	6 0
1	3-A	500/512 (98%)	456 (91%)	44 (9%)	8 0
1	4-A	500/512 (98%)	446 (89%)	54 (11%)	5 0
1	5-A	500/512 (98%)	439 (88%)	61 (12%)	4 0
1	6-A	500/512 (98%)	455 (91%)	45 (9%)	8 0
1	7-A	500/512 (98%)	455 (91%)	45 (9%)	8 0
1	8-A	500/512 (98%)	460 (92%)	40 (8%)	10 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	9-A	500/512 (98%)	453 (91%)	47 (9%)	7 0
1	10-A	500/512 (98%)	449 (90%)	51 (10%)	6 0
1	11-A	500/512 (98%)	452 (90%)	48 (10%)	7 0
1	12-A	500/512 (98%)	466 (93%)	34 (7%)	13 1
1	13-A	500/512 (98%)	452 (90%)	48 (10%)	7 0
1	14-A	500/512 (98%)	459 (92%)	41 (8%)	9 0
1	15-A	500/512 (98%)	444 (89%)	56 (11%)	5 0
1	16-A	500/512 (98%)	450 (90%)	50 (10%)	6 0
1	17-A	500/512 (98%)	446 (89%)	54 (11%)	5 0
1	18-A	500/512 (98%)	448 (90%)	52 (10%)	5 0
1	19-A	500/512 (98%)	441 (88%)	59 (12%)	4 0
1	20-A	500/512 (98%)	439 (88%)	61 (12%)	4 0
1	21-A	500/512 (98%)	440 (88%)	60 (12%)	4 0
1	22-A	500/512 (98%)	446 (89%)	54 (11%)	5 0
1	23-A	500/512 (98%)	454 (91%)	46 (9%)	7 0
1	24-A	500/512 (98%)	439 (88%)	61 (12%)	4 0
1	25-A	500/512 (98%)	436 (87%)	64 (13%)	3 0
1	26-A	500/512 (98%)	439 (88%)	61 (12%)	4 0
1	27-A	500/512 (98%)	452 (90%)	48 (10%)	7 0
1	28-A	500/512 (98%)	446 (89%)	54 (11%)	5 0
1	29-A	500/512 (98%)	447 (89%)	53 (11%)	5 0
1	30-A	500/512 (98%)	454 (91%)	46 (9%)	7 0
1	31-A	500/512 (98%)	448 (90%)	52 (10%)	5 0
1	32-A	500/512 (98%)	448 (90%)	52 (10%)	5 0
1	33-A	500/512 (98%)	449 (90%)	51 (10%)	6 0
1	34-A	500/512 (98%)	445 (89%)	55 (11%)	5 0
1	35-A	500/512 (98%)	449 (90%)	51 (10%)	6 0
1	36-A	500/512 (98%)	449 (90%)	51 (10%)	6 0
1	37-A	500/512 (98%)	460 (92%)	40 (8%)	10 0
1	38-A	500/512 (98%)	452 (90%)	48 (10%)	7 0
1	39-A	500/512 (98%)	442 (88%)	58 (12%)	4 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	40-A	500/512 (98%)	441 (88%)	59 (12%)	4 0
1	41-A	500/512 (98%)	451 (90%)	49 (10%)	6 0
1	42-A	500/512 (98%)	447 (89%)	53 (11%)	5 0
1	43-A	500/512 (98%)	450 (90%)	50 (10%)	6 0
All	All	21500/22016 (98%)	19290 (90%)	2210 (10%)	6 0

5 of 2210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	36-A	544	GLU
1	38-A	265	LYS
1	36-A	534	GLU
1	41-A	308	MET
1	17-A	100	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 364 such sidechains are listed below:

Mol	Chain	Res	Type
1	28-A	181	ASN
1	35-A	77	GLN
1	29-A	20	ASN
1	31-A	523	ASN
1	36-A	328	HIS

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)

43 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	DPF	38-A	601	1	4,7,8	0.93	0	2,7,10	0.68	0
2	DPF	25-A	601	1	4,7,8	0.91	0	2,7,10	0.66	0
2	DPF	5-A	601	1	4,7,8	0.79	0	2,7,10	0.19	0
2	DPF	9-A	601	1	4,7,8	1.10	0	2,7,10	0.35	0
2	DPF	31-A	601	1	4,7,8	0.74	0	2,7,10	0.09	0
2	DPF	26-A	601	1	4,7,8	0.74	0	2,7,10	0.58	0
2	DPF	21-A	601	1	4,7,8	0.99	0	2,7,10	0.13	0
2	DPF	34-A	601	1	4,7,8	0.93	0	2,7,10	0.44	0
2	DPF	3-A	601	1	4,7,8	1.04	0	2,7,10	0.30	0
2	DPF	11-A	601	1	4,7,8	1.09	0	2,7,10	0.64	0
2	DPF	6-A	601	1	4,7,8	1.10	0	2,7,10	0.97	0
2	DPF	2-A	601	1	4,7,8	1.12	0	2,7,10	0.72	0
2	DPF	15-A	601	1	4,7,8	1.44	1 (25%)	2,7,10	0.97	0
2	DPF	18-A	601	1	4,7,8	1.00	0	2,7,10	0.90	0
2	DPF	22-A	601	1	4,7,8	1.19	1 (25%)	2,7,10	0.64	0
2	DPF	24-A	601	1	4,7,8	0.97	0	2,7,10	0.39	0
2	DPF	19-A	601	1	4,7,8	0.89	0	2,7,10	0.79	0
2	DPF	20-A	601	1	4,7,8	1.02	0	2,7,10	0.30	0
2	DPF	43-A	601	1	4,7,8	0.98	0	2,7,10	0.60	0
2	DPF	41-A	601	1	4,7,8	0.79	0	2,7,10	0.26	0
2	DPF	42-A	601	1	4,7,8	0.78	0	2,7,10	0.38	0
2	DPF	39-A	601	1	4,7,8	0.89	0	2,7,10	0.34	0
2	DPF	4-A	601	1	4,7,8	0.86	0	2,7,10	1.12	0
2	DPF	28-A	601	1	4,7,8	0.90	0	2,7,10	0.09	0
2	DPF	36-A	601	1	4,7,8	0.82	0	2,7,10	0.19	0
2	DPF	40-A	601	1	4,7,8	1.00	0	2,7,10	0.28	0
2	DPF	12-A	601	1	4,7,8	1.01	0	2,7,10	0.74	0
2	DPF	17-A	601	1	4,7,8	0.98	0	2,7,10	0.06	0
2	DPF	37-A	601	1	4,7,8	0.88	0	2,7,10	0.68	0
2	DPF	35-A	601	1	4,7,8	1.03	0	2,7,10	0.57	0
2	DPF	1-A	601	1	4,7,8	1.24	1 (25%)	2,7,10	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DPF	32-A	601	1	4,7,8	0.56	0	2,7,10	0.38	0
2	DPF	33-A	601	1	4,7,8	1.08	0	2,7,10	1.09	0
2	DPF	23-A	601	1	4,7,8	0.92	0	2,7,10	0.38	0
2	DPF	29-A	601	1	4,7,8	0.98	0	2,7,10	0.52	0
2	DPF	8-A	601	1	4,7,8	0.94	0	2,7,10	0.37	0
2	DPF	13-A	601	1	4,7,8	1.15	0	2,7,10	0.43	0
2	DPF	27-A	601	1	4,7,8	0.99	0	2,7,10	0.59	0
2	DPF	14-A	601	1	4,7,8	0.97	0	2,7,10	0.23	0
2	DPF	30-A	601	1	4,7,8	1.06	0	2,7,10	0.58	0
2	DPF	7-A	601	1	4,7,8	1.00	0	2,7,10	0.53	0
2	DPF	16-A	601	1	4,7,8	0.98	0	2,7,10	0.64	0
2	DPF	10-A	601	1	4,7,8	0.87	0	2,7,10	0.70	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
2	DPF	38-A	601	1	-	0/2/6/8	-
2	DPF	25-A	601	1	-	1/2/6/8	-
2	DPF	5-A	601	1	-	0/2/6/8	-
2	DPF	9-A	601	1	-	1/2/6/8	-
2	DPF	31-A	601	1	-	0/2/6/8	-
2	DPF	26-A	601	1	-	1/2/6/8	-
2	DPF	21-A	601	1	-	0/2/6/8	-
2	DPF	34-A	601	1	-	1/2/6/8	-
2	DPF	3-A	601	1	-	0/2/6/8	-
2	DPF	11-A	601	1	-	2/2/6/8	-
2	DPF	6-A	601	1	-	1/2/6/8	-
2	DPF	2-A	601	1	-	0/2/6/8	-
2	DPF	15-A	601	1	-	1/2/6/8	-
2	DPF	18-A	601	1	-	0/2/6/8	-
2	DPF	22-A	601	1	-	1/2/6/8	-
2	DPF	24-A	601	1	-	0/2/6/8	-
2	DPF	19-A	601	1	-	0/2/6/8	-
2	DPF	20-A	601	1	-	0/2/6/8	-
2	DPF	43-A	601	1	-	0/2/6/8	-
2	DPF	41-A	601	1	-	0/2/6/8	-
2	DPF	42-A	601	1	-	0/2/6/8	-
2	DPF	39-A	601	1	-	1/2/6/8	-
2	DPF	4-A	601	1	-	0/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPF	28-A	601	1	-	1/2/6/8	-
2	DPF	36-A	601	1	-	0/2/6/8	-
2	DPF	40-A	601	1	-	0/2/6/8	-
2	DPF	12-A	601	1	-	1/2/6/8	-
2	DPF	17-A	601	1	-	0/2/6/8	-
2	DPF	37-A	601	1	-	0/2/6/8	-
2	DPF	35-A	601	1	-	0/2/6/8	-
2	DPF	1-A	601	1	-	2/2/6/8	-
2	DPF	32-A	601	1	-	0/2/6/8	-
2	DPF	33-A	601	1	-	1/2/6/8	-
2	DPF	23-A	601	1	-	0/2/6/8	-
2	DPF	29-A	601	1	-	0/2/6/8	-
2	DPF	8-A	601	1	-	0/2/6/8	-
2	DPF	13-A	601	1	-	2/2/6/8	-
2	DPF	27-A	601	1	-	0/2/6/8	-
2	DPF	14-A	601	1	-	1/2/6/8	-
2	DPF	30-A	601	1	-	1/2/6/8	-
2	DPF	7-A	601	1	-	0/2/6/8	-
2	DPF	16-A	601	1	-	0/2/6/8	-
2	DPF	10-A	601	1	-	0/2/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	601	DPF	O1-C2	-2.23	1.37	1.44
2	1-A	601	DPF	O1-C2	-2.05	1.38	1.44
2	22-A	601	DPF	O1-C2	-2.02	1.38	1.44

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	601	DPF	C4-C1-O3-P1
2	1-A	601	DPF	C3-C2-O1-P1
2	6-A	601	DPF	C4-C1-O3-P1
2	9-A	601	DPF	C4-C1-O3-P1
2	11-A	601	DPF	C4-C1-O3-P1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	32-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
32	A	125:THR	C	126:LYS	N	1.82

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.2977, which does not match the depositor's R factor of 0.181. Please interpret the results in this section carefully.

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, 95^{th} 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%)	1.63	171 (30%) 1 1	0, 0, 0, 0	566 (100%)
1	2-A	0/577	-	-	-	-
1	3-A	0/577	-	-	-	-
1	4-A	0/577	-	-	-	-
1	5-A	0/577	-	-	-	-
1	6-A	0/577	-	-	-	-
1	7-A	0/577	-	-	-	-
1	8-A	0/577	-	-	-	-
1	9-A	0/577	-	-	-	-
1	10-A	0/577	-	-	-	-
1	11-A	0/577	-	-	-	-
1	12-A	0/577	-	-	-	-
1	13-A	0/577	-	-	-	-
1	14-A	0/577	-	-	-	-
1	15-A	0/577	-	-	-	-
1	16-A	0/577	-	-	-	-
1	17-A	0/577	-	-	-	-
1	18-A	0/577	-	-	-	-
1	19-A	0/577	-	-	-	-
1	20-A	0/577	-	-	-	-
1	21-A	0/577	-	-	-	-
1	22-A	0/577	-	-	-	-
1	23-A	0/577	-	-	-	-
1	24-A	0/577	-	-	-	-
1	25-A	0/577	-	-	-	-
1	26-A	0/577	-	-	-	-
1	27-A	0/577	-	-	-	-
1	28-A	0/577	-	-	-	-
1	29-A	0/577	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	30-A	0/577	-	-	-	-
1	31-A	0/577	-	-	-	-
1	32-A	0/577	-	-	-	-
1	33-A	0/577	-	-	-	-
1	34-A	0/577	-	-	-	-
1	35-A	0/577	-	-	-	-
1	36-A	0/577	-	-	-	-
1	37-A	0/577	-	-	-	-
1	38-A	0/577	-	-	-	-
1	39-A	0/577	-	-	-	-
1	40-A	0/577	-	-	-	-
1	41-A	0/577	-	-	-	-
1	42-A	0/577	-	-	-	-
1	43-A	0/577	-	-	-	-
All	All	566/24811 (2%)	1.63	171 (30%) 1 1	0, 0, 0, 0	566 (100%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	515	SER	8.0
1	1-A	514	TYR	7.7
1	1-A	100	PHE	7.5
1	1-A	519	GLU	7.1
1	1-A	518	ILE	6.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.