



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2022 – 10:52 AM EDT

PDB ID : 7MHM
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 240 K
Authors : Ebrahim, A.; Riley, B.T.; Kumaran, D.; Andi, B.; Fuchs, M.R.; McSweeney, S.; Keedy, D.A.
Deposited on : 2021-04-15
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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

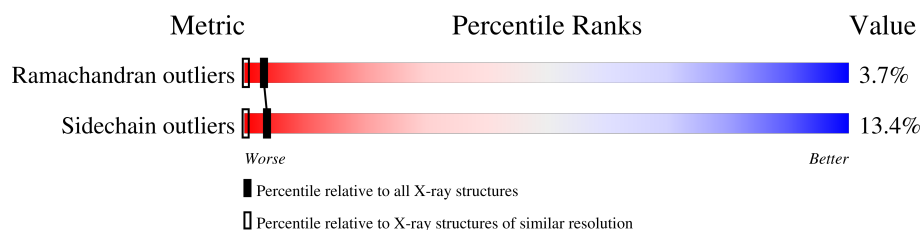
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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))
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	306	85% 12% .
1	10-A	306	85% 14% .
1	11-A	306	83% 14% .
1	12-A	306	85% 13% .
1	13-A	306	84% 14% .
1	14-A	306	85% 13% .
1	15-A	306	84% 12% . .
1	16-A	306	85% 12% .
1	17-A	306	86% 11% .










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Mol	Chain	Length	Quality of chain
1	18-A	306	 85% 14% .
1	19-A	306	 85% 12% .
1	2-A	306	 81% 15% ..
1	20-A	306	 86% 12% .
1	21-A	306	 87% 12% .
1	22-A	306	 92% 7% .
1	23-A	306	 83% 14% ..
1	24-A	306	 83% 13% ..
1	25-A	306	 84% 12% ..
1	26-A	306	 85% 13% .
1	27-A	306	 84% 12% ..
1	28-A	306	 85% 13% ..
1	29-A	306	 79% 18% .
1	3-A	306	 85% 11% ..
1	30-A	306	 86% 11% .
1	31-A	306	 83% 15% .
1	32-A	306	 83% 15% .
1	33-A	306	 83% 13% ..
1	34-A	306	 83% 13% .
1	35-A	306	 81% 14% ..
1	36-A	306	 87% 9% .
1	37-A	306	 83% 14% ..
1	38-A	306	 79% 17% ..
1	39-A	306	 82% 14% ..
1	4-A	306	 82% 14% ..

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Mol	Chain	Length	Quality of chain
1	40-A	306	 86% 12% .
1	41-A	306	 83% 14% .
1	42-A	306	 82% 14% . .
1	43-A	306	 79% 17% .
1	5-A	306	 84% 13% .
1	6-A	306	 85% 12% . .
1	7-A	306	 82% 16% .
1	8-A	306	 85% 12% .
1	9-A	306	 81% 15% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 210185 atoms, of which 101308 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 3C-like proteinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	2-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	3-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	4-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	5-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	6-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	7-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	8-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	9-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	10-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	11-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	12-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	13-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	14-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	15-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	16-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			

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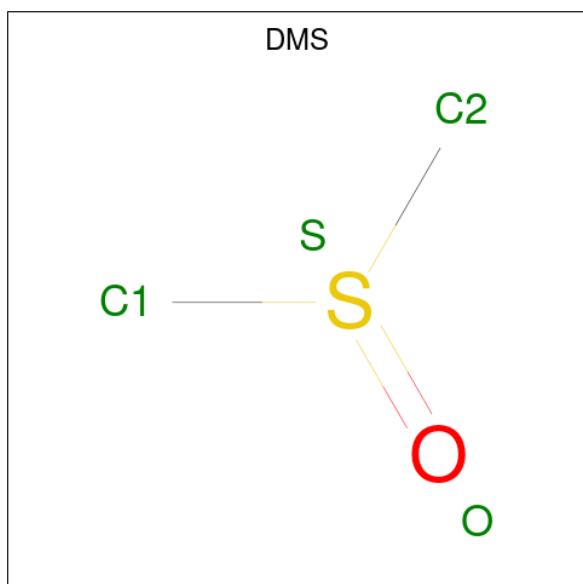
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	18-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	19-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	20-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	21-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	22-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	23-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	24-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	25-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	26-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	27-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	28-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	29-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	30-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	31-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	32-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	33-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	34-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	35-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	36-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	37-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	39-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	40-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	41-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	42-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	43-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	21-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	22-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	23-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	24-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	25-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	26-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	27-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	28-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	29-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	1	Total	Zn	0	0
			1	1		
3	2-A	1	Total	Zn	0	0
			1	1		
3	3-A	1	Total	Zn	0	0
			1	1		
3	4-A	1	Total	Zn	0	0
			1	1		
3	5-A	1	Total	Zn	0	0
			1	1		
3	6-A	1	Total	Zn	0	0
			1	1		
3	7-A	1	Total	Zn	0	0
			1	1		
3	8-A	1	Total	Zn	0	0
			1	1		
3	9-A	1	Total	Zn	0	0
			1	1		
3	10-A	1	Total	Zn	0	0
			1	1		
3	11-A	1	Total	Zn	0	0
			1	1		
3	12-A	1	Total	Zn	0	0
			1	1		
3	13-A	1	Total	Zn	0	0
			1	1		
3	14-A	1	Total	Zn	0	0
			1	1		
3	15-A	1	Total	Zn	0	0
			1	1		
3	16-A	1	Total	Zn	0	0
			1	1		
3	17-A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	18-A	1	Total 1	Zn 1	0	0
3	19-A	1	Total 1	Zn 1	0	0
3	20-A	1	Total 1	Zn 1	0	0
3	21-A	1	Total 1	Zn 1	0	0
3	22-A	1	Total 1	Zn 1	0	0
3	23-A	1	Total 1	Zn 1	0	0
3	24-A	1	Total 1	Zn 1	0	0
3	25-A	1	Total 1	Zn 1	0	0
3	26-A	1	Total 1	Zn 1	0	0
3	27-A	1	Total 1	Zn 1	0	0
3	28-A	1	Total 1	Zn 1	0	0
3	29-A	1	Total 1	Zn 1	0	0
3	30-A	1	Total 1	Zn 1	0	0
3	31-A	1	Total 1	Zn 1	0	0
3	32-A	1	Total 1	Zn 1	0	0
3	33-A	1	Total 1	Zn 1	0	0
3	34-A	1	Total 1	Zn 1	0	0
3	35-A	1	Total 1	Zn 1	0	0
3	36-A	1	Total 1	Zn 1	0	0
3	37-A	1	Total 1	Zn 1	0	0
3	38-A	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	39-A	1	Total 1	Zn 1	0	0
3	40-A	1	Total 1	Zn 1	0	0
3	41-A	1	Total 1	Zn 1	0	0
3	42-A	1	Total 1	Zn 1	0	0
3	43-A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	148	Total 148	O 148	0	0
4	2-A	135	Total 135	O 135	0	0
4	3-A	134	Total 134	O 134	0	0
4	4-A	142	Total 142	O 142	0	0
4	5-A	140	Total 140	O 140	0	0
4	6-A	145	Total 145	O 145	0	0
4	7-A	133	Total 133	O 133	0	0
4	8-A	131	Total 131	O 131	0	0
4	9-A	147	Total 147	O 147	0	0
4	10-A	146	Total 146	O 146	0	0
4	11-A	137	Total 137	O 137	0	0
4	12-A	141	Total 141	O 141	0	0
4	13-A	130	Total 130	O 130	0	0
4	14-A	135	Total 135	O 135	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	15-A	136	Total 136	O 136	0	0
4	16-A	121	Total 121	O 121	0	0
4	17-A	152	Total 152	O 152	0	0
4	18-A	122	Total 122	O 122	0	0
4	19-A	141	Total 141	O 141	0	0
4	20-A	131	Total 131	O 131	0	0
4	21-A	142	Total 142	O 142	0	0
4	22-A	139	Total 139	O 139	0	0
4	23-A	134	Total 134	O 134	0	0
4	24-A	138	Total 138	O 138	0	0
4	25-A	145	Total 145	O 145	0	0
4	26-A	125	Total 125	O 125	0	0
4	27-A	144	Total 144	O 144	0	0
4	28-A	135	Total 135	O 135	0	0
4	29-A	144	Total 144	O 144	0	0
4	30-A	146	Total 146	O 146	0	0
4	31-A	136	Total 136	O 136	0	0
4	32-A	122	Total 122	O 122	0	0
4	33-A	134	Total 134	O 134	0	0
4	34-A	123	Total 123	O 123	0	0
4	35-A	130	Total 130	O 130	0	0

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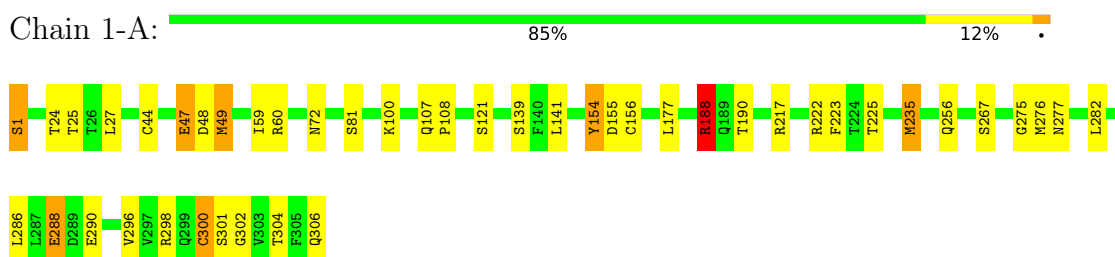
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	36-A	139	Total 139	O 139	0	0
4	37-A	140	Total 140	O 140	0	0
4	38-A	120	Total 120	O 120	0	0
4	39-A	145	Total 145	O 145	0	0
4	40-A	121	Total 121	O 121	0	0
4	41-A	127	Total 127	O 127	0	0
4	42-A	133	Total 133	O 133	0	0
4	43-A	140	Total 140	O 140	0	0

3 Residue-property plots [i](#)

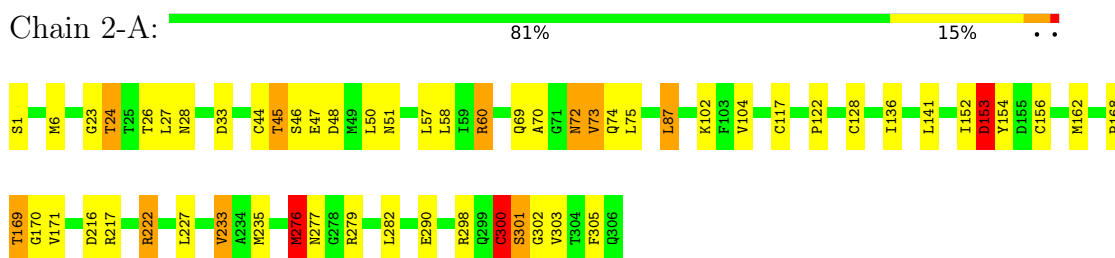
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

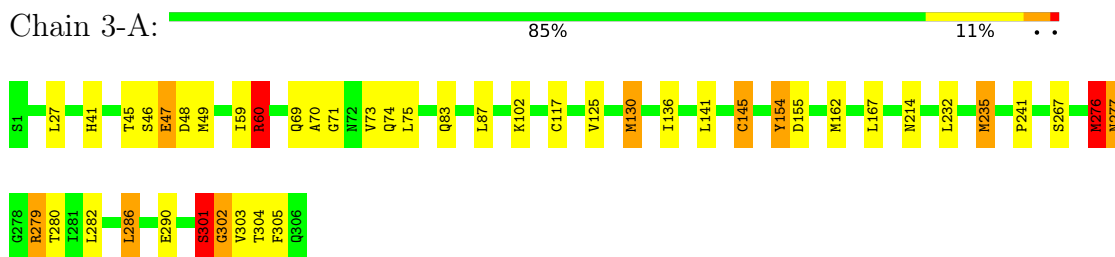
- Molecule 1: 3C-like proteinase



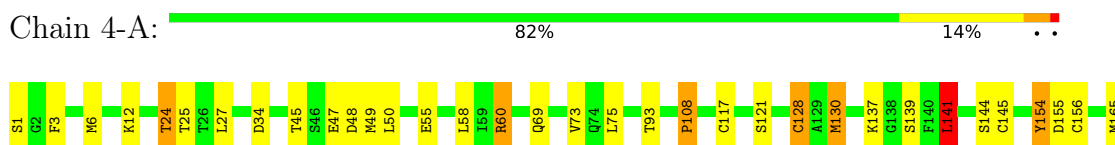
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



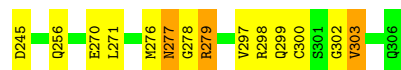
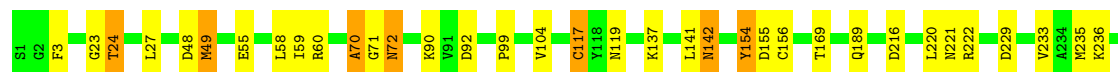
- Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase

Chain 5-A: 84% 13% .



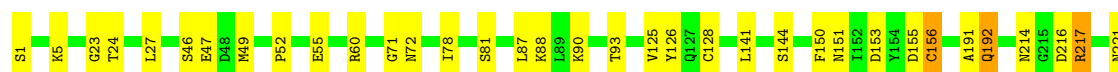
- Molecule 1: 3C-like proteinase

Chain 6-A: 85% 12% . .



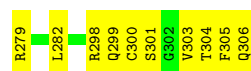
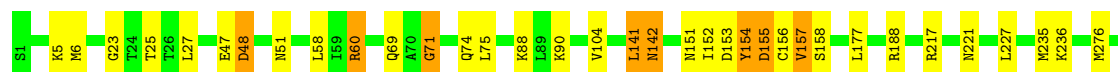
- Molecule 1: 3C-like proteinase

Chain 7-A: 82% 16% .



- Molecule 1: 3C-like proteinase

Chain 8-A: 85% 12% .



- Molecule 1: 3C-like proteinase

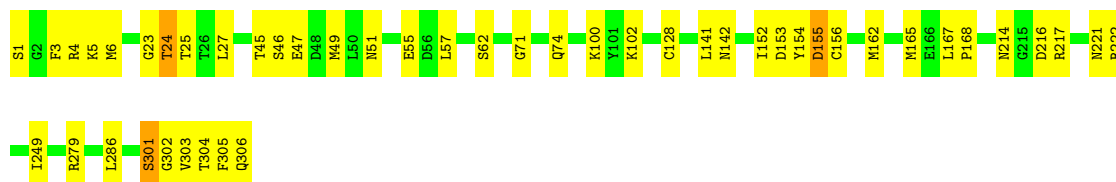
Chain 9-A: 81% 15% .





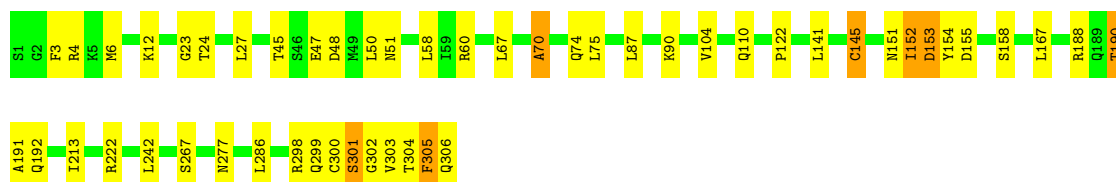
- Molecule 1: 3C-like proteinase

Chain 10-A: 85% 14% .



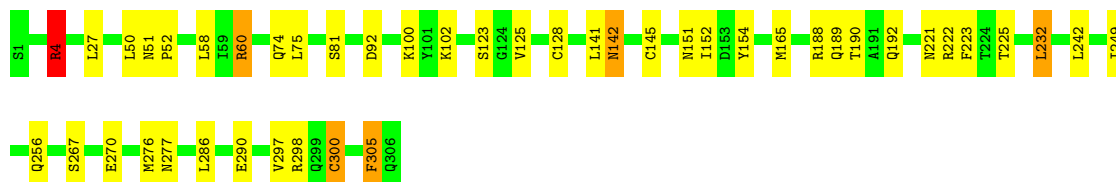
- Molecule 1: 3C-like proteinase

Chain 11-A: 83% 14% .



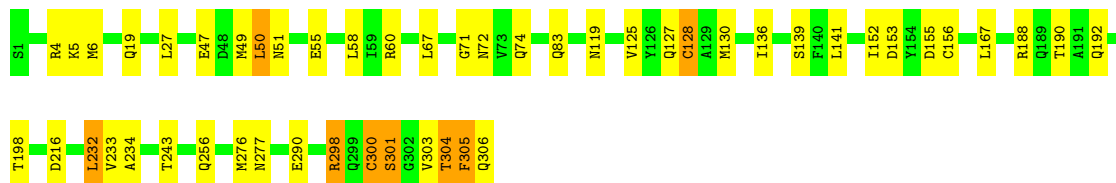
- Molecule 1: 3C-like proteinase

Chain 12-A: 85% 13% .



- Molecule 1: 3C-like proteinase

Chain 13-A: 84% 14% .



- Molecule 1: 3C-like proteinase

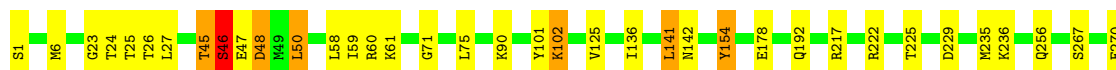
Chain 14-A: 85% 13% .





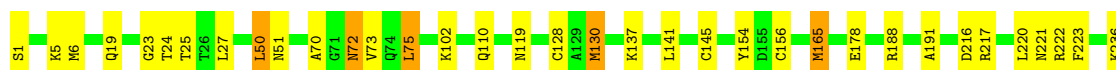
- Molecule 1: 3C-like proteinase

Chain 15-A: 84% 12% . .



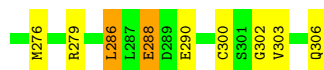
- Molecule 1: 3C-like proteinase

Chain 16-A: 85% 12% .



- Molecule 1: 3C-like proteinase

Chain 17-A: 86% 11% .



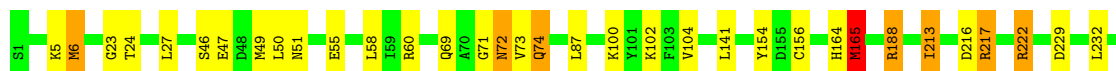
- Molecule 1: 3C-like proteinase

Chain 18-A: 85% 14% .



- Molecule 1: 3C-like proteinase

Chain 19-A: 85% 12% .





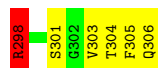
- Molecule 1: 3C-like proteinase

Chain 20-A: 86% 12% .



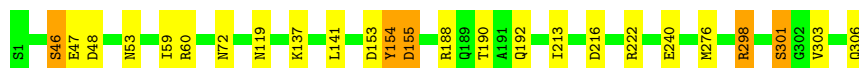
- Molecule 1: 3C-like proteinase

Chain 21-A: 87% 12% .



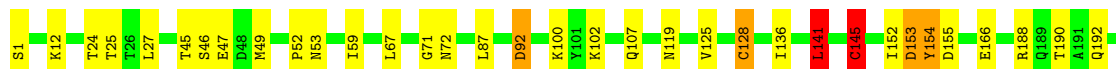
- Molecule 1: 3C-like proteinase

Chain 22-A: 92% 7% .



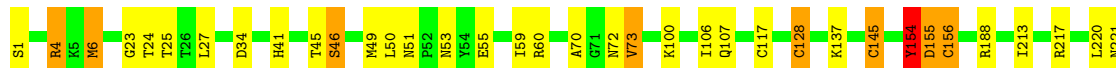
- Molecule 1: 3C-like proteinase

Chain 23-A: 83% 14% ..


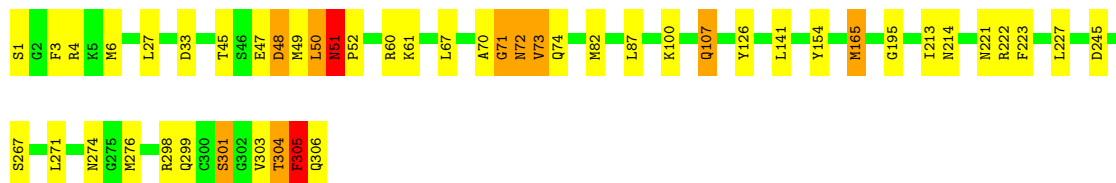


- Molecule 1: 3C-like proteinase


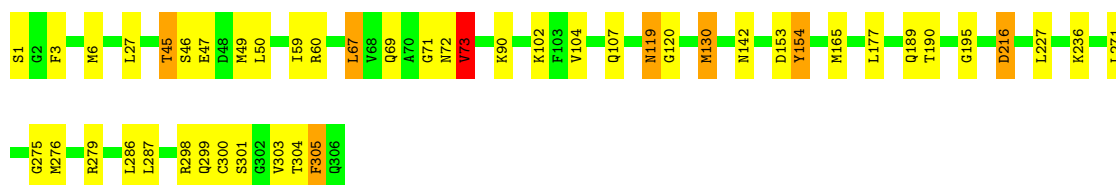
Chain 24-A: 83% 13% ..




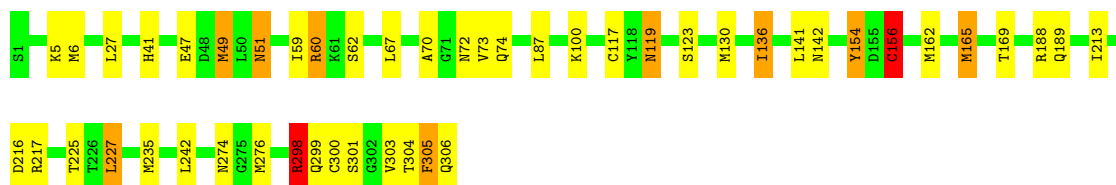
• Molecule 1: 3C-like proteinase

Chain 25-A:  84% 12% ..


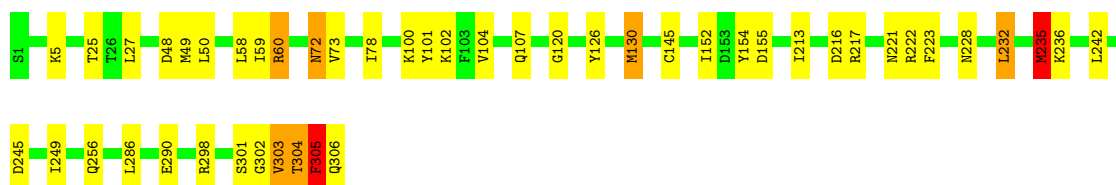
• Molecule 1: 3C-like proteinase

Chain 26-A:  85% 13% .


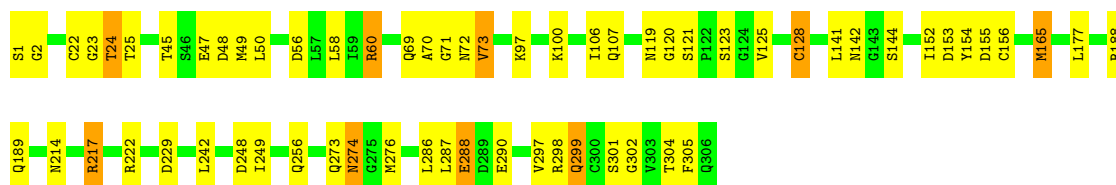
• Molecule 1: 3C-like proteinase

Chain 27-A:  84% 12% ..

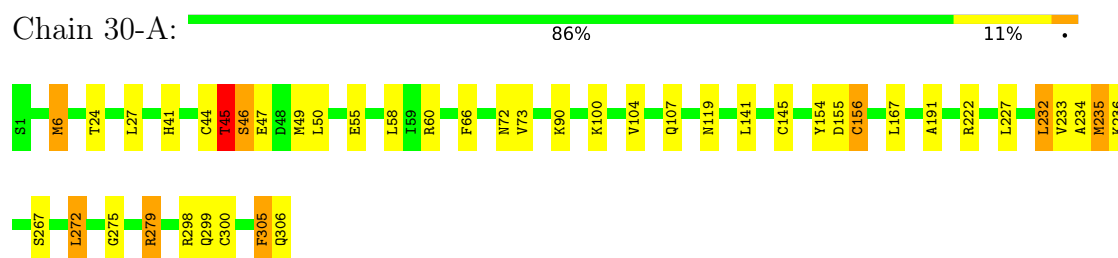
• Molecule 1: 3C-like proteinase

Chain 28-A:  85% 13% ..

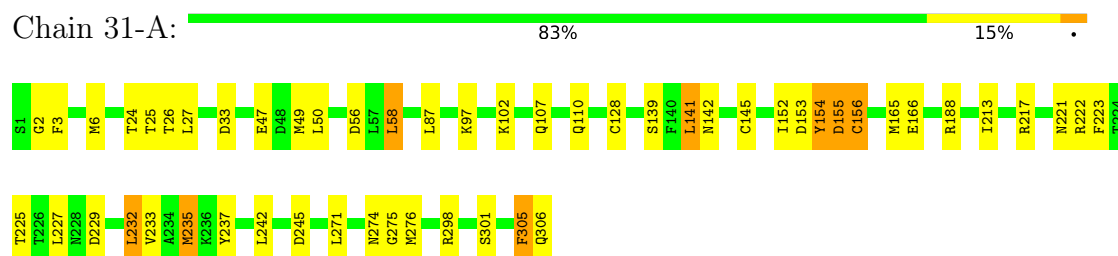
• Molecule 1: 3C-like proteinase

Chain 29-A:  79% 18% .

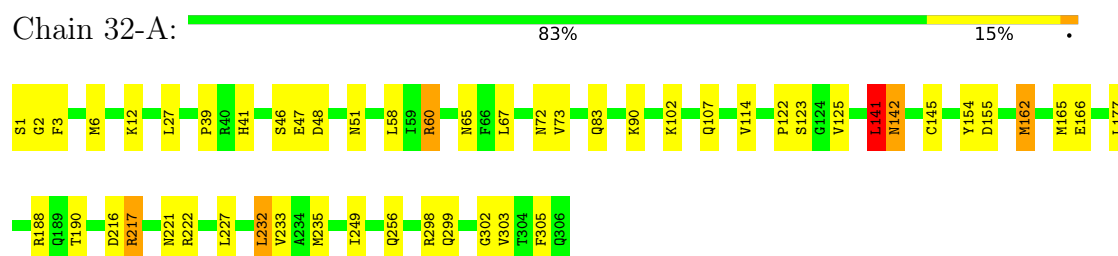
• Molecule 1: 3C-like proteinase



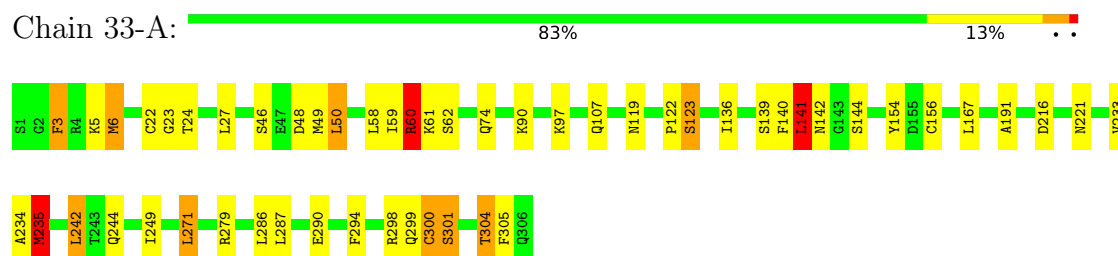
• Molecule 1: 3C-like proteinase



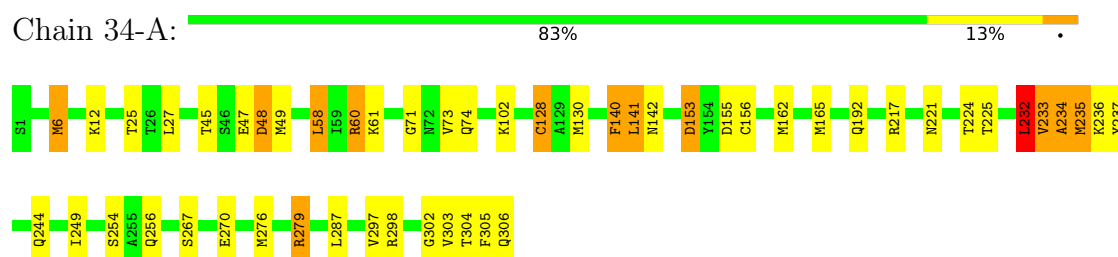
• Molecule 1: 3C-like proteinase



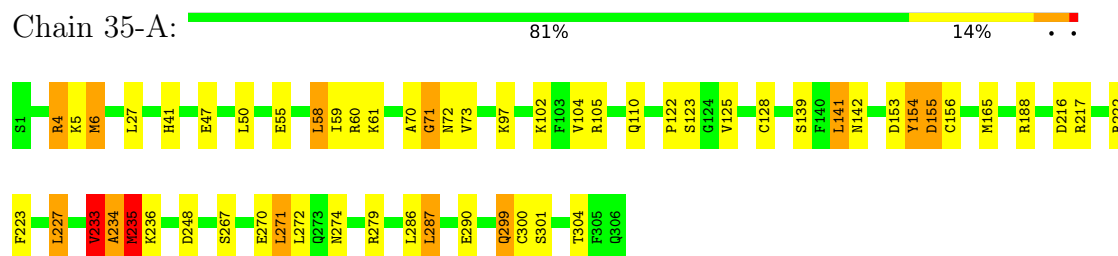
• Molecule 1: 3C-like proteinase



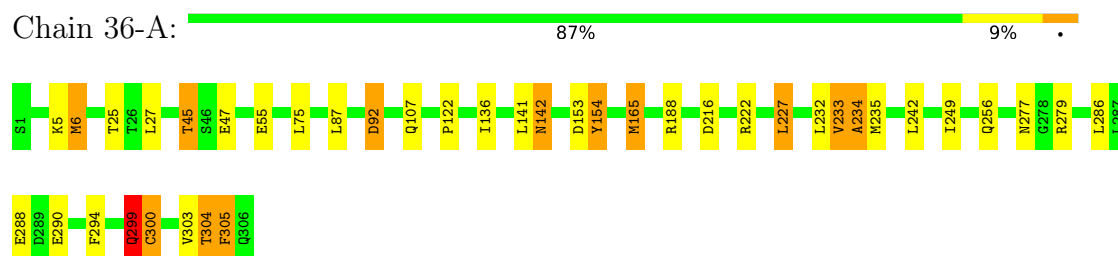
• Molecule 1: 3C-like proteinase



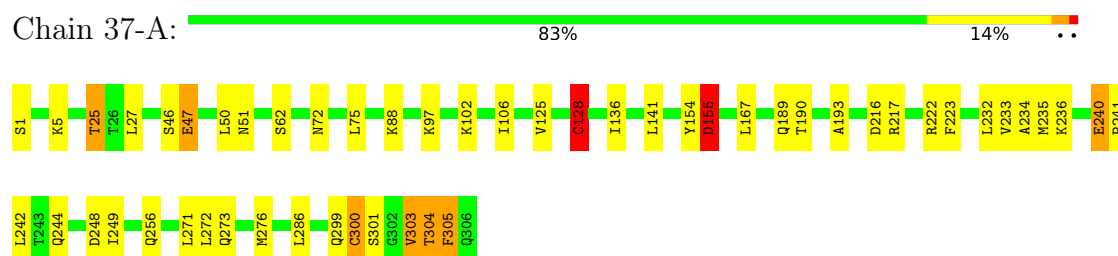
• Molecule 1: 3C-like proteinase



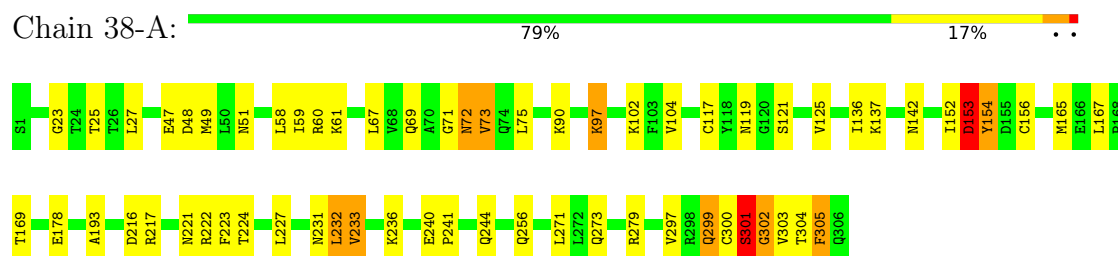
• Molecule 1: 3C-like proteinase



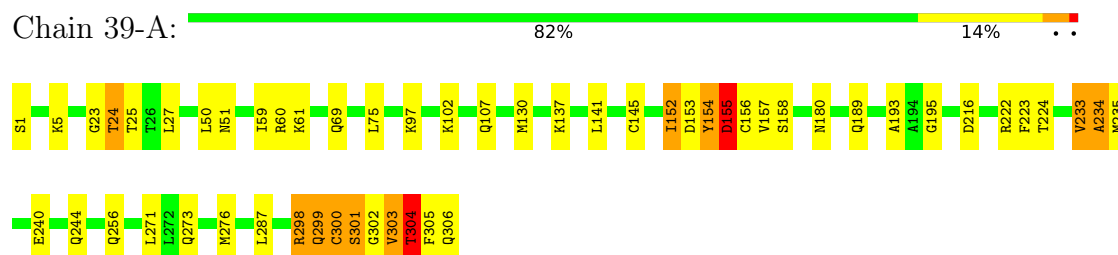
• Molecule 1: 3C-like proteinase



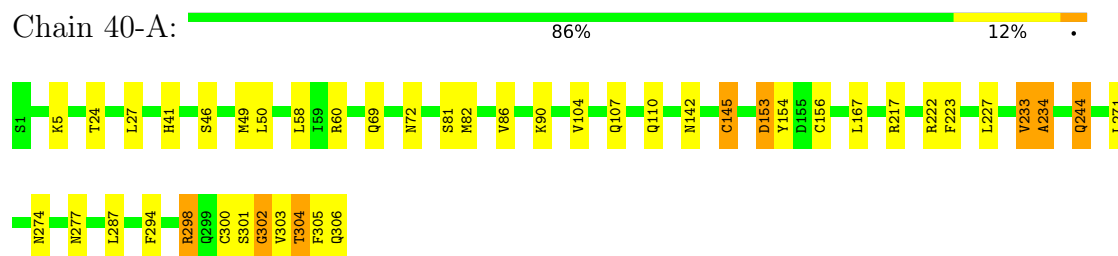
• Molecule 1: 3C-like proteinase



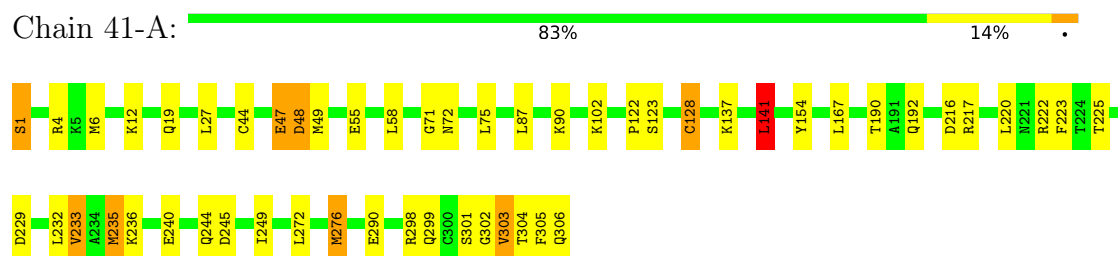
• Molecule 1: 3C-like proteinase



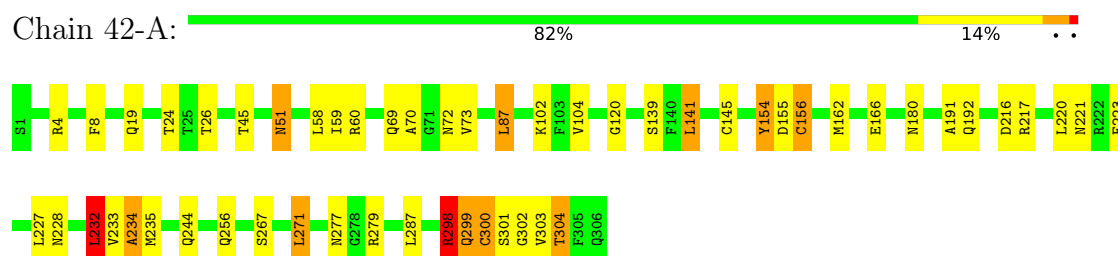
● Molecule 1: 3C-like proteinase



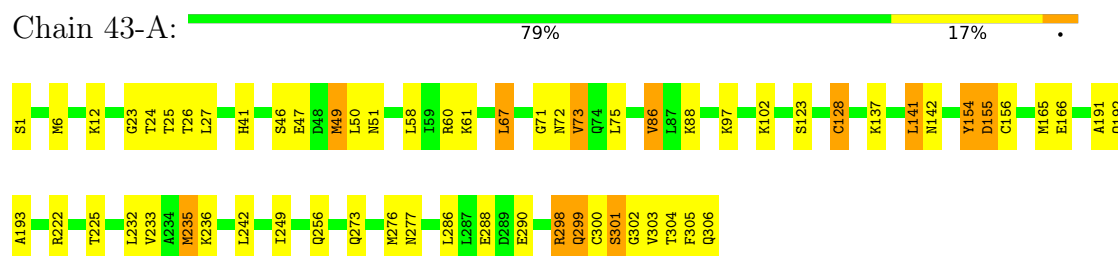
● Molecule 1: 3C-like proteinase



● Molecule 1: 3C-like proteinase



● Molecule 1: 3C-like proteinase



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.19Å 53.49Å 45.00Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	48.20 – 1.53	Depositor
% Data completeness (in resolution range)	99.9 (48.20-1.53)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 1.53Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.158 , 0.197	Depositor
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.260	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	210185	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% 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 ⓘ

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

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	0.78	4/2420 (0.2%)	0.89	2/3289 (0.1%)
1	2-A	0.81	2/2420 (0.1%)	0.96	7/3289 (0.2%)
1	3-A	0.77	4/2420 (0.2%)	0.91	3/3289 (0.1%)
1	4-A	0.80	3/2420 (0.1%)	0.97	7/3289 (0.2%)
1	5-A	0.74	1/2420 (0.0%)	0.92	3/3289 (0.1%)
1	6-A	0.79	3/2420 (0.1%)	0.95	8/3289 (0.2%)
1	7-A	0.77	3/2420 (0.1%)	0.86	3/3289 (0.1%)
1	8-A	0.73	0/2420	0.91	1/3289 (0.0%)
1	9-A	0.83	6/2420 (0.2%)	0.94	7/3289 (0.2%)
1	10-A	0.86	3/2420 (0.1%)	0.89	1/3289 (0.0%)
1	11-A	0.83	1/2420 (0.0%)	0.93	3/3289 (0.1%)
1	12-A	0.96	2/2420 (0.1%)	0.96	4/3289 (0.1%)
1	13-A	0.79	4/2420 (0.2%)	0.92	6/3289 (0.2%)
1	14-A	0.79	3/2420 (0.1%)	0.90	1/3289 (0.0%)
1	15-A	0.74	0/2420	0.88	4/3289 (0.1%)
1	16-A	0.79	6/2420 (0.2%)	0.93	3/3289 (0.1%)
1	17-A	1.06	9/2420 (0.4%)	0.93	4/3289 (0.1%)
1	18-A	0.76	3/2420 (0.1%)	0.91	4/3289 (0.1%)
1	19-A	0.80	6/2420 (0.2%)	0.91	5/3289 (0.2%)
1	20-A	0.78	1/2420 (0.0%)	0.89	2/3289 (0.1%)
1	21-A	0.70	1/2420 (0.0%)	0.87	6/3289 (0.2%)
1	22-A	0.74	0/2420	0.88	3/3289 (0.1%)
1	23-A	0.82	3/2420 (0.1%)	0.92	6/3289 (0.2%)
1	24-A	1.36	10/2420 (0.4%)	0.99	6/3289 (0.2%)
1	25-A	0.79	3/2420 (0.1%)	0.93	5/3289 (0.2%)
1	26-A	0.77	3/2420 (0.1%)	0.91	4/3289 (0.1%)
1	27-A	0.74	5/2420 (0.2%)	0.94	6/3289 (0.2%)
1	28-A	0.83	2/2420 (0.1%)	0.94	5/3289 (0.2%)
1	29-A	0.77	6/2420 (0.2%)	0.93	5/3289 (0.2%)
1	30-A	0.78	4/2420 (0.2%)	0.91	3/3289 (0.1%)
1	31-A	0.78	4/2420 (0.2%)	0.97	6/3289 (0.2%)
1	32-A	0.76	1/2420 (0.0%)	0.93	3/3289 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.78	2/2420 (0.1%)	0.94	6/3289 (0.2%)
1	34-A	0.75	3/2420 (0.1%)	0.95	7/3289 (0.2%)
1	35-A	0.82	4/2420 (0.2%)	0.99	11/3289 (0.3%)
1	36-A	0.80	5/2420 (0.2%)	0.98	7/3289 (0.2%)
1	37-A	0.74	3/2420 (0.1%)	0.93	3/3289 (0.1%)
1	38-A	0.76	1/2420 (0.0%)	0.94	3/3289 (0.1%)
1	39-A	0.84	4/2420 (0.2%)	0.91	3/3289 (0.1%)
1	40-A	0.82	5/2420 (0.2%)	0.85	0/3289
1	41-A	0.74	1/2420 (0.0%)	0.92	5/3289 (0.2%)
1	42-A	0.89	3/2420 (0.1%)	0.95	7/3289 (0.2%)
1	43-A	0.84	5/2420 (0.2%)	0.94	7/3289 (0.2%)
All	All	0.82	142/104060 (0.1%)	0.93	195/141427 (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	5
1	2-A	0	12
1	3-A	0	10
1	4-A	0	8
1	5-A	0	14
1	6-A	0	4
1	7-A	0	7
1	8-A	0	5
1	9-A	0	7
1	10-A	0	4
1	11-A	0	7
1	12-A	0	6
1	13-A	0	5
1	14-A	0	6
1	15-A	0	8
1	16-A	0	6
1	17-A	0	5
1	18-A	0	2
1	19-A	0	11
1	20-A	0	5
1	21-A	0	4
1	22-A	0	1
1	23-A	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	24-A	0	9
1	25-A	0	8
1	26-A	0	2
1	27-A	0	9
1	28-A	0	8
1	29-A	0	8
1	30-A	0	9
1	31-A	0	3
1	32-A	0	6
1	33-A	0	9
1	34-A	0	9
1	35-A	0	6
1	36-A	0	7
1	37-A	0	3
1	38-A	0	7
1	39-A	0	9
1	40-A	0	4
1	41-A	0	7
1	42-A	0	12
1	43-A	0	9
All	All	0	292

The worst 5 of 142 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	24-A	145	CYS	CB-SG	52.09	2.70	1.82
1	17-A	145	CYS	CB-SG	32.91	2.38	1.82
1	12-A	145	CYS	CB-SG	29.14	2.31	1.82
1	42-A	145	CYS	CB-SG	21.65	2.19	1.82
1	10-A	128	CYS	CB-SG	-20.32	1.47	1.82

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	24-A	145	CYS	CA-CB-SG	18.24	146.83	114.00
1	12-A	145	CYS	CA-CB-SG	14.00	139.19	114.00
1	31-A	145	CYS	CA-CB-SG	13.24	137.83	114.00
1	17-A	145	CYS	CA-CB-SG	13.01	137.43	114.00
1	36-A	227	LEU	CA-CB-CG	12.38	143.77	115.30

There are no chirality outliers.

5 of 292 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	1	SER	Peptide
1	1-A	188	ARG	Sidechain
1	1-A	25	THR	Peptide
1	1-A	300	CYS	Peptide
1	1-A	44	CYS	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	2367	2314	2313	0	0
1	2-A	2367	2314	2313	0	0
1	3-A	2367	2314	2313	0	0
1	4-A	2367	2314	2313	0	0
1	5-A	2367	2314	2313	0	0
1	6-A	2367	2314	2314	0	0
1	7-A	2367	2314	2313	0	0
1	8-A	2367	2314	2313	0	0
1	9-A	2367	2314	2313	0	0
1	10-A	2367	2314	2313	0	0
1	11-A	2367	2314	2314	0	0
1	12-A	2367	2314	2313	0	0
1	13-A	2367	2314	2313	0	0
1	14-A	2367	2314	2313	0	0
1	15-A	2367	2314	2313	0	0
1	16-A	2367	2314	2313	0	0
1	17-A	2367	2314	2314	0	0
1	18-A	2367	2314	2313	0	0
1	19-A	2367	2314	2313	0	0
1	20-A	2367	2314	2313	0	0
1	21-A	2367	2314	2313	0	0
1	22-A	2367	2314	2313	0	0
1	23-A	2367	2314	2313	0	0
1	24-A	2367	2314	2314	0	0
1	25-A	2367	2314	2313	0	0
1	26-A	2367	2314	2313	0	0
1	27-A	2367	2314	2313	0	0
1	28-A	2367	2314	2314	0	0
1	29-A	2367	2314	2313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	30-A	2367	2314	2313	0	0
1	31-A	2367	2314	2313	0	0
1	32-A	2367	2314	2313	0	0
1	33-A	2367	2314	2313	0	0
1	34-A	2367	2314	2313	0	0
1	35-A	2367	2314	2313	0	0
1	36-A	2367	2314	2313	0	0
1	37-A	2367	2314	2313	0	0
1	38-A	2367	2314	2313	0	0
1	39-A	2367	2314	2313	0	0
1	40-A	2367	2314	2313	0	0
1	41-A	2367	2314	2313	0	0
1	42-A	2367	2314	2314	0	0
1	43-A	2367	2314	2313	0	0
2	1-A	28	42	42	0	0
2	2-A	28	42	42	0	0
2	3-A	28	42	42	0	0
2	4-A	28	42	42	0	0
2	5-A	28	42	42	0	0
2	6-A	28	42	42	0	0
2	7-A	28	42	42	0	0
2	8-A	28	42	42	0	0
2	9-A	28	42	42	0	0
2	10-A	28	42	42	0	0
2	11-A	28	42	42	0	0
2	12-A	28	42	42	0	0
2	13-A	28	42	42	0	0
2	14-A	28	42	42	0	0
2	15-A	28	42	42	0	0
2	16-A	28	42	42	0	0
2	17-A	28	42	42	0	0
2	18-A	28	42	42	0	0
2	19-A	28	42	42	0	0
2	20-A	28	42	42	0	0
2	21-A	28	42	42	0	0
2	22-A	28	42	42	0	0
2	23-A	28	42	42	0	0
2	24-A	28	42	42	0	0
2	25-A	28	42	42	0	0
2	26-A	28	42	42	0	0
2	27-A	28	42	42	0	0
2	28-A	28	42	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	29-A	28	42	42	0	0
2	30-A	28	42	42	0	0
2	31-A	28	42	42	0	0
2	32-A	28	42	42	0	0
2	33-A	28	42	42	0	0
2	34-A	28	42	42	0	0
2	35-A	28	42	42	0	0
2	36-A	28	42	42	0	0
2	37-A	28	42	42	0	0
2	38-A	28	42	42	0	0
2	39-A	28	42	42	0	0
2	40-A	28	42	42	0	0
2	41-A	28	42	42	0	0
2	42-A	28	42	42	0	0
2	43-A	28	42	42	0	0
3	1-A	1	0	0	0	0
3	2-A	1	0	0	0	0
3	3-A	1	0	0	0	0
3	4-A	1	0	0	0	0
3	5-A	1	0	0	0	0
3	6-A	1	0	0	0	0
3	7-A	1	0	0	0	0
3	8-A	1	0	0	0	0
3	9-A	1	0	0	0	0
3	10-A	1	0	0	0	0
3	11-A	1	0	0	0	0
3	12-A	1	0	0	0	0
3	13-A	1	0	0	0	0
3	14-A	1	0	0	0	0
3	15-A	1	0	0	0	0
3	16-A	1	0	0	0	0
3	17-A	1	0	0	0	0
3	18-A	1	0	0	0	0
3	19-A	1	0	0	0	0
3	20-A	1	0	0	0	0
3	21-A	1	0	0	0	0
3	22-A	1	0	0	0	0
3	23-A	1	0	0	0	0
3	24-A	1	0	0	0	0
3	25-A	1	0	0	0	0
3	26-A	1	0	0	0	0
3	27-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	28-A	1	0	0	0	0
3	29-A	1	0	0	0	0
3	30-A	1	0	0	0	0
3	31-A	1	0	0	0	0
3	32-A	1	0	0	0	0
3	33-A	1	0	0	0	0
3	34-A	1	0	0	0	0
3	35-A	1	0	0	0	0
3	36-A	1	0	0	0	0
3	37-A	1	0	0	0	0
3	38-A	1	0	0	0	0
3	39-A	1	0	0	0	0
3	40-A	1	0	0	0	0
3	41-A	1	0	0	0	0
3	42-A	1	0	0	0	0
3	43-A	1	0	0	0	0
4	1-A	148	0	0	0	0
4	2-A	135	0	0	0	0
4	3-A	134	0	0	0	0
4	4-A	142	0	0	0	0
4	5-A	140	0	0	0	0
4	6-A	145	0	0	0	0
4	7-A	133	0	0	0	0
4	8-A	131	0	0	0	0
4	9-A	147	0	0	0	0
4	10-A	146	0	0	0	0
4	11-A	137	0	0	0	0
4	12-A	141	0	0	0	0
4	13-A	130	0	0	0	0
4	14-A	135	0	0	0	0
4	15-A	136	0	0	0	0
4	16-A	121	0	0	0	0
4	17-A	152	0	0	0	0
4	18-A	122	0	0	0	0
4	19-A	141	0	0	0	0
4	20-A	131	0	0	0	0
4	21-A	142	0	0	0	0
4	22-A	139	0	0	0	0
4	23-A	134	0	0	0	0
4	24-A	138	0	0	0	0
4	25-A	145	0	0	0	0
4	26-A	125	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	27-A	144	0	0	0	0
4	28-A	135	0	0	0	0
4	29-A	144	0	0	0	0
4	30-A	146	0	0	0	0
4	31-A	136	0	0	0	0
4	32-A	122	0	0	0	0
4	33-A	134	0	0	0	0
4	34-A	123	0	0	0	0
4	35-A	130	0	0	0	0
4	36-A	139	0	0	0	0
4	37-A	140	0	0	0	0
4	38-A	120	0	0	0	0
4	39-A	145	0	0	0	0
4	40-A	121	0	0	0	0
4	41-A	127	0	0	0	0
4	42-A	133	0	0	0	0
4	43-A	140	0	0	0	0
All	All	108877	101308	101271	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	304/306 (99%)	274 (90%)	21 (7%)	9 (3%)	4 0
1	2-A	304/306 (99%)	269 (88%)	15 (5%)	20 (7%)	1 0
1	3-A	304/306 (99%)	274 (90%)	20 (7%)	10 (3%)	4 0
1	4-A	304/306 (99%)	269 (88%)	20 (7%)	15 (5%)	2 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	304/306 (99%)	274 (90%)	21 (7%)	9 (3%)	4	0
1	6-A	304/306 (99%)	277 (91%)	12 (4%)	15 (5%)	2	0
1	7-A	304/306 (99%)	272 (90%)	21 (7%)	11 (4%)	3	0
1	8-A	304/306 (99%)	275 (90%)	15 (5%)	14 (5%)	2	0
1	9-A	304/306 (99%)	275 (90%)	17 (6%)	12 (4%)	3	0
1	10-A	304/306 (99%)	281 (92%)	13 (4%)	10 (3%)	4	0
1	11-A	304/306 (99%)	274 (90%)	19 (6%)	11 (4%)	3	0
1	12-A	304/306 (99%)	282 (93%)	17 (6%)	5 (2%)	9	1
1	13-A	304/306 (99%)	288 (95%)	13 (4%)	3 (1%)	15	3
1	14-A	304/306 (99%)	289 (95%)	9 (3%)	6 (2%)	7	1
1	15-A	304/306 (99%)	274 (90%)	16 (5%)	14 (5%)	2	0
1	16-A	304/306 (99%)	285 (94%)	10 (3%)	9 (3%)	4	0
1	17-A	304/306 (99%)	282 (93%)	16 (5%)	6 (2%)	7	1
1	18-A	304/306 (99%)	276 (91%)	19 (6%)	9 (3%)	4	0
1	19-A	304/306 (99%)	274 (90%)	19 (6%)	11 (4%)	3	0
1	20-A	304/306 (99%)	288 (95%)	8 (3%)	8 (3%)	5	0
1	21-A	304/306 (99%)	281 (92%)	12 (4%)	11 (4%)	3	0
1	22-A	304/306 (99%)	277 (91%)	20 (7%)	7 (2%)	6	0
1	23-A	304/306 (99%)	271 (89%)	23 (8%)	10 (3%)	4	0
1	24-A	304/306 (99%)	272 (90%)	19 (6%)	13 (4%)	2	0
1	25-A	304/306 (99%)	279 (92%)	15 (5%)	10 (3%)	4	0
1	26-A	304/306 (99%)	268 (88%)	19 (6%)	17 (6%)	2	0
1	27-A	304/306 (99%)	279 (92%)	14 (5%)	11 (4%)	3	0
1	28-A	304/306 (99%)	277 (91%)	17 (6%)	10 (3%)	4	0
1	29-A	304/306 (99%)	271 (89%)	21 (7%)	12 (4%)	3	0
1	30-A	304/306 (99%)	279 (92%)	16 (5%)	9 (3%)	4	0
1	31-A	304/306 (99%)	268 (88%)	27 (9%)	9 (3%)	4	0
1	32-A	304/306 (99%)	273 (90%)	19 (6%)	12 (4%)	3	0
1	33-A	304/306 (99%)	268 (88%)	16 (5%)	20 (7%)	1	0
1	34-A	304/306 (99%)	275 (90%)	17 (6%)	12 (4%)	3	0
1	35-A	304/306 (99%)	278 (91%)	14 (5%)	12 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	36-A	304/306 (99%)	277 (91%)	18 (6%)	9 (3%)	4	0
1	37-A	304/306 (99%)	272 (90%)	18 (6%)	14 (5%)	2	0
1	38-A	304/306 (99%)	268 (88%)	20 (7%)	16 (5%)	2	0
1	39-A	304/306 (99%)	270 (89%)	19 (6%)	15 (5%)	2	0
1	40-A	304/306 (99%)	287 (94%)	10 (3%)	7 (2%)	6	0
1	41-A	304/306 (99%)	273 (90%)	15 (5%)	16 (5%)	2	0
1	42-A	304/306 (99%)	275 (90%)	17 (6%)	12 (4%)	3	0
1	43-A	304/306 (99%)	270 (89%)	21 (7%)	13 (4%)	2	0
All	All	13072/13158 (99%)	11860 (91%)	728 (6%)	484 (4%)	3	0

5 of 484 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	24	THR
1	1-A	47	GLU
1	1-A	154	TYR
1	1-A	304	THR
1	2-A	24	THR

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	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	2-A	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	3-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	4-A	263/263 (100%)	225 (86%)	38 (14%)	3	0
1	5-A	263/263 (100%)	231 (88%)	32 (12%)	5	0
1	6-A	263/263 (100%)	232 (88%)	31 (12%)	5	0
1	7-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	8-A	263/263 (100%)	230 (88%)	33 (12%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	9-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	10-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	11-A	263/263 (100%)	225 (86%)	38 (14%)	3	0
1	12-A	263/263 (100%)	226 (86%)	37 (14%)	3	0
1	13-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	14-A	263/263 (100%)	225 (86%)	38 (14%)	3	0
1	15-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	16-A	263/263 (100%)	233 (89%)	30 (11%)	5	0
1	17-A	263/263 (100%)	231 (88%)	32 (12%)	5	0
1	18-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	19-A	263/263 (100%)	234 (89%)	29 (11%)	6	0
1	20-A	263/263 (100%)	231 (88%)	32 (12%)	5	0
1	21-A	263/263 (100%)	237 (90%)	26 (10%)	8	0
1	22-A	263/263 (100%)	244 (93%)	19 (7%)	14	1
1	23-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	24-A	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	25-A	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	26-A	263/263 (100%)	233 (89%)	30 (11%)	5	0
1	27-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	28-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	29-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	30-A	263/263 (100%)	234 (89%)	29 (11%)	6	0
1	31-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	32-A	263/263 (100%)	226 (86%)	37 (14%)	3	0
1	33-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	34-A	263/263 (100%)	226 (86%)	37 (14%)	3	0
1	35-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	36-A	263/263 (100%)	236 (90%)	27 (10%)	7	0
1	37-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	38-A	263/263 (100%)	214 (81%)	49 (19%)	1	0
1	39-A	263/263 (100%)	224 (85%)	39 (15%)	3	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	40-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	41-A	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	42-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	43-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
All	All	11309/11309 (100%)	9795 (87%)	1514 (13%)	4	0

5 of 1514 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	28-A	155	ASP
1	34-A	156	CYS
1	29-A	49	MET
1	28-A	130	MET
1	31-A	155	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 329 such sidechains are listed below:

Mol	Chain	Res	Type
1	31-A	228	ASN
1	39-A	69	GLN
1	33-A	28	ASN
1	35-A	214	ASN
1	40-A	119	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 344 ligands modelled in this entry, 43 are monoatomic - leaving 301 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DMS	1-A	404	-	3,3,3	0.61	0	3,3,3	0.95	0
2	DMS	1-A	403	-	3,3,3	0.73	0	3,3,3	1.16	0
2	DMS	1-A	401	-	3,3,3	0.64	0	3,3,3	1.35	1 (33%)
2	DMS	1-A	402	-	3,3,3	0.82	0	3,3,3	0.48	0
2	DMS	1-A	405	-	3,3,3	0.63	0	3,3,3	1.63	1 (33%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	405	DMS	O-S-C2	2.57	119.66	106.54
2	1-A	401	DMS	O-S-C2	2.28	118.19	106.54

There are no chirality outliers.

There are no torsion outliers.

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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.