



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2022 – 10:38 AM EDT

PDB ID : 7MHN
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 277 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 : 2.19 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **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

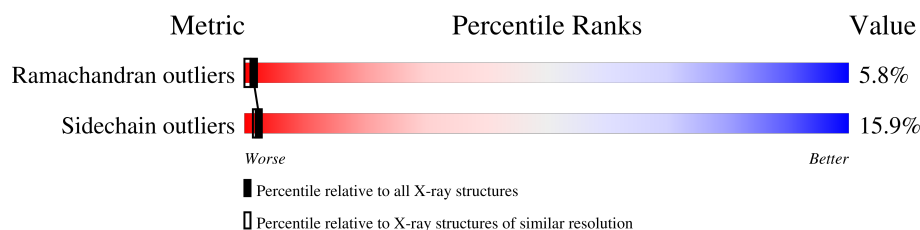
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)












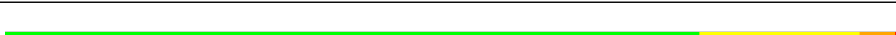

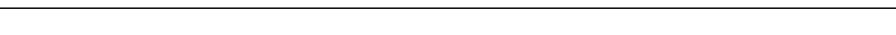
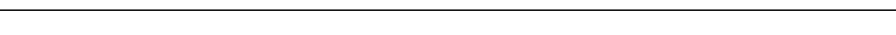
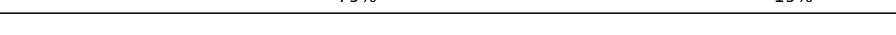

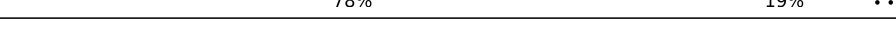







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	78% 19% .
1	10-A	306	83% 14% . .
1	11-A	306	81% 16% .
1	12-A	306	80% 16% .
1	13-A	306	80% 18% .
1	14-A	306	79% 17% .
1	15-A	306	79% 18% .
1	16-A	306	82% 16% .
1	17-A	306	80% 15% 5%

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Mol	Chain	Length	Quality of chain
1	18-A	306	 78%19%.
1	19-A	306	 78%19%..
1	2-A	306	 80%16%..
1	20-A	306	 80%16%..
1	21-A	306	 79%17%.
1	22-A	306	 80%17%..
1	23-A	306	 81%16%..
1	24-A	306	 81%16%.
1	25-A	306	 79%18%.
1	26-A	306	 82%16%.
1	27-A	306	 76%22%.
1	28-A	306	 78%18%..
1	29-A	306	 77%18%.
1	3-A	306	 80%17%.
1	30-A	306	 79%19%.
1	31-A	306	 81%16%.
1	32-A	306	 78%19%..
1	33-A	306	 84%12%..
1	34-A	306	 79%18%..
1	35-A	306	 77%19%.
1	36-A	306	 79%18%.
1	37-A	306	 77%18%..
1	38-A	306	 82%13%..
1	39-A	306	 78%19%.
1	4-A	306	 80%17%..

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Mol	Chain	Length	Quality of chain
1	40-A	306	 78% 19% ..
1	41-A	306	 81% 16% .
1	42-A	306	 85% 12% .
1	43-A	306	 82% 15% .
1	44-A	306	 82% 14% .
1	45-A	306	 81% 15% .
1	5-A	306	 77% 21% ..
1	6-A	306	 82% 16% ..
1	7-A	306	 82% 16% .
1	8-A	306	 79% 17% .
1	9-A	306	 80% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 213552 atoms, of which 104625 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
			4680	1499	2313	402	444	22			
1	2-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	3-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	4-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	5-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	6-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	7-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	8-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	9-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	10-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	11-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	12-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	13-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	14-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	15-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	16-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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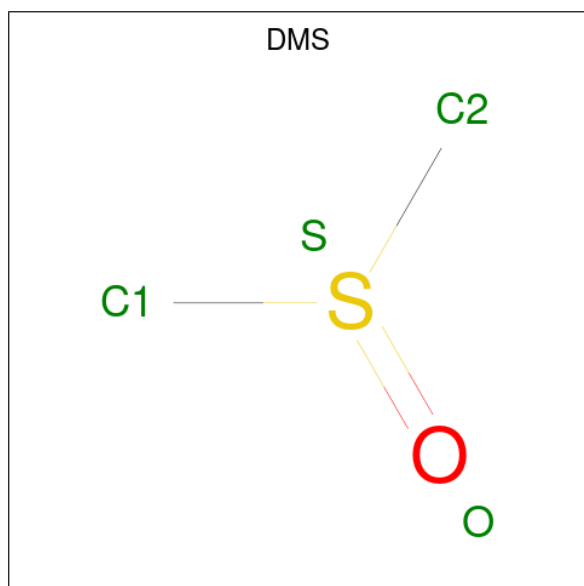
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	18-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	19-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	20-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	21-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	22-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	23-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	24-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	25-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	26-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	27-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	28-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	29-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	30-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	31-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	32-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	33-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	34-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	35-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	36-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	37-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	39-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	40-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	41-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	42-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	43-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	44-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	45-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	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		

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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	44-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	45-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	44-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	45-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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	17-A	1	Total 1	Zn 1	0	0
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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	38-A	1	Total 1	Zn 1	0	0
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
3	44-A	1	Total 1	Zn 1	0	0
3	45-A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	45	Total 45	O 45	0	0
4	2-A	38	Total 38	O 38	0	0
4	3-A	37	Total 37	O 37	0	0
4	4-A	44	Total 44	O 44	0	0
4	5-A	47	Total 47	O 47	0	0
4	6-A	45	Total 45	O 45	0	0
4	7-A	44	Total 44	O 44	0	0
4	8-A	37	Total 37	O 37	0	0
4	9-A	46	Total 46	O 46	0	0
4	10-A	50	Total 50	O 50	0	0
4	11-A	50	Total 50	O 50	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	12-A	48	Total 48	O 48	0	0
4	13-A	48	Total 48	O 48	0	0
4	14-A	42	Total 42	O 42	0	0
4	15-A	41	Total 41	O 41	0	0
4	16-A	42	Total 42	O 42	0	0
4	17-A	42	Total 42	O 42	0	0
4	18-A	44	Total 44	O 44	0	0
4	19-A	41	Total 41	O 41	0	0
4	20-A	48	Total 48	O 48	0	0
4	21-A	42	Total 42	O 42	0	0
4	22-A	46	Total 46	O 46	0	0
4	23-A	55	Total 55	O 55	0	0
4	24-A	49	Total 49	O 49	0	0
4	25-A	54	Total 54	O 54	0	0
4	26-A	41	Total 41	O 41	0	0
4	27-A	39	Total 39	O 39	0	0
4	28-A	40	Total 40	O 40	0	0
4	29-A	47	Total 47	O 47	0	0
4	30-A	46	Total 46	O 46	0	0
4	31-A	47	Total 47	O 47	0	0
4	32-A	45	Total 45	O 45	0	0

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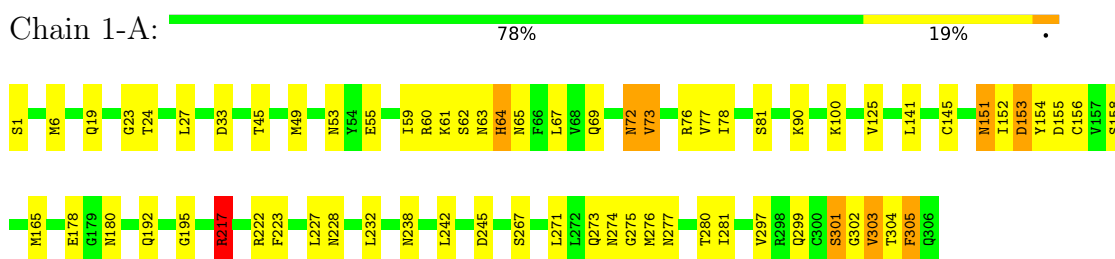
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	33-A	48	Total 48	O 48	0	0
4	34-A	43	Total 43	O 43	0	0
4	35-A	38	Total 38	O 38	0	0
4	36-A	37	Total 37	O 37	0	0
4	37-A	41	Total 41	O 41	0	0
4	38-A	47	Total 47	O 47	0	0
4	39-A	49	Total 49	O 49	0	0
4	40-A	48	Total 48	O 48	0	0
4	41-A	42	Total 42	O 42	0	0
4	42-A	48	Total 48	O 48	0	0
4	43-A	45	Total 45	O 45	0	0
4	44-A	52	Total 52	O 52	0	0
4	45-A	39	Total 39	O 39	0	0

3 Residue-property plots

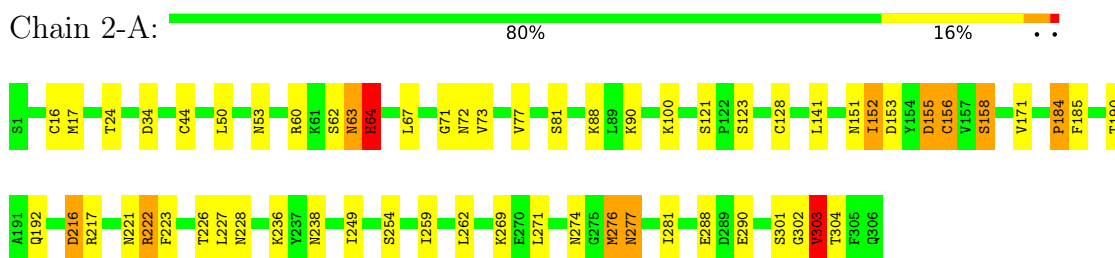
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

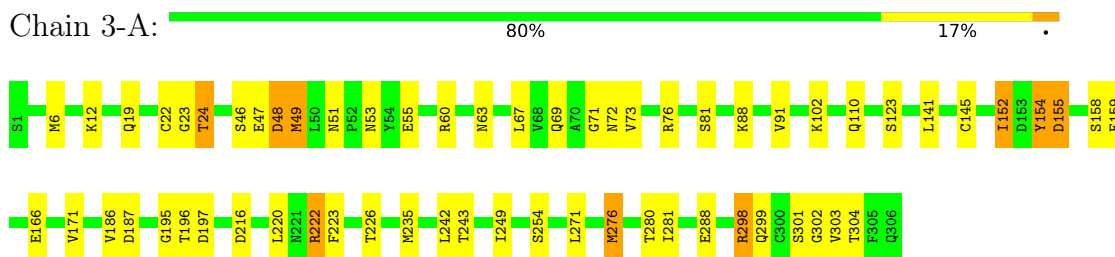
- Molecule 1: 3C-like proteinase



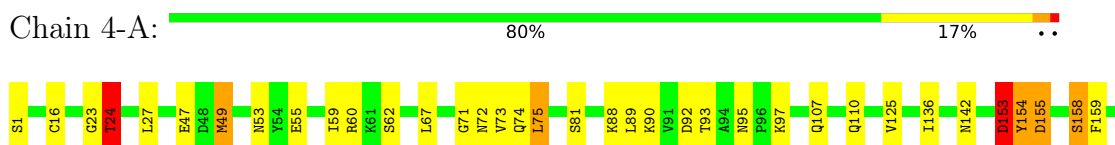
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



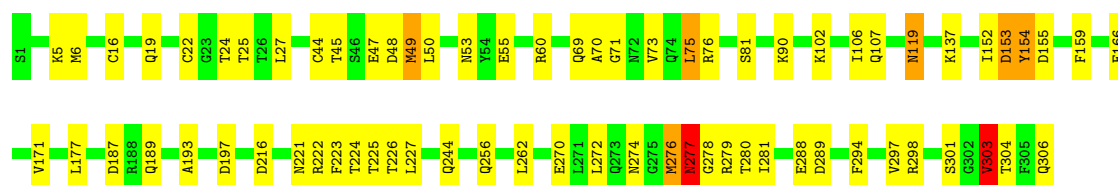
- Molecule 1: 3C-like proteinase





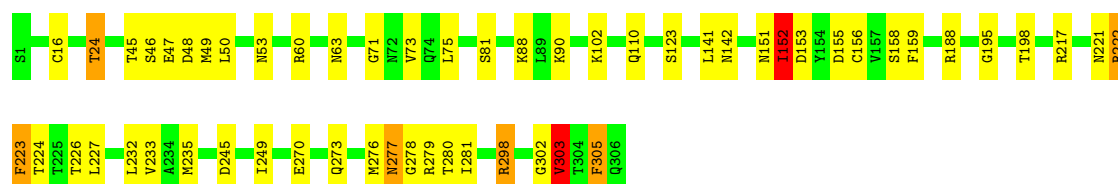
- Molecule 1: 3C-like proteinase

Chain 5-A: 77% 21% ..



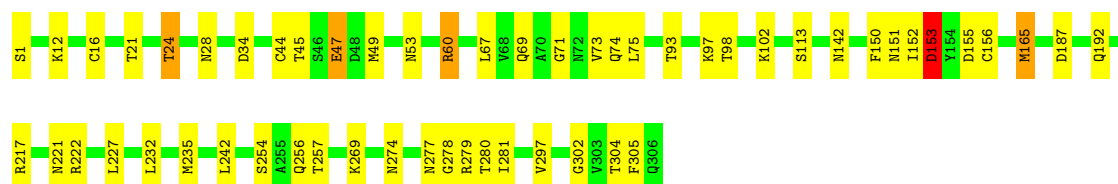
- Molecule 1: 3C-like proteinase

Chain 6-A: 82% 16% ..



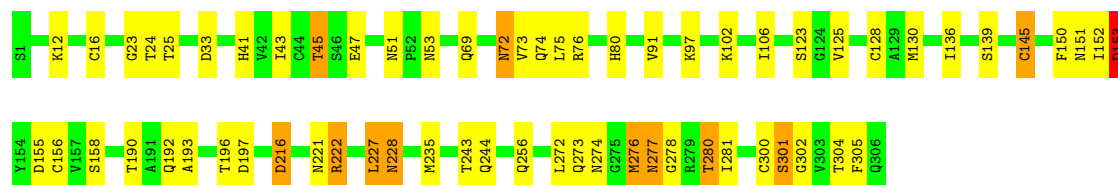
- Molecule 1: 3C-like proteinase

Chain 7-A: 82% 16% .



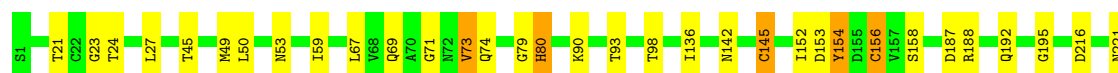
- Molecule 1: 3C-like proteinase

Chain 8-A: 79% 17% .



- Molecule 1: 3C-like proteinase

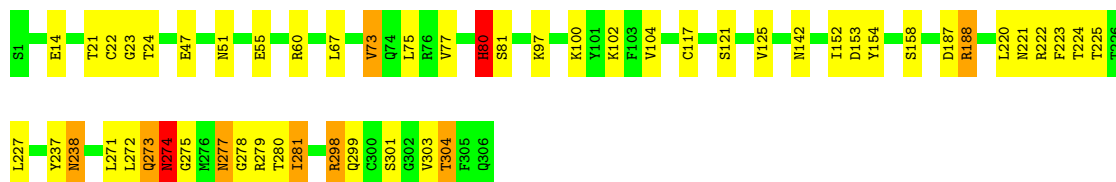
Chain 9-A: 80% 17% .





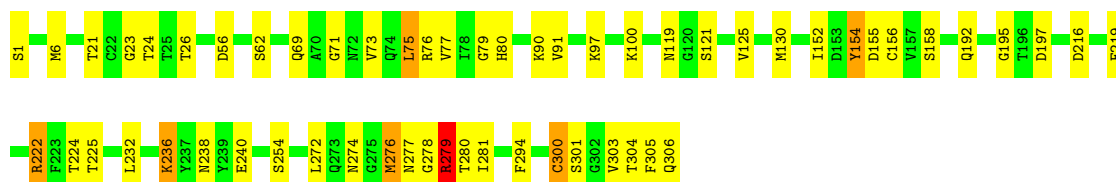
- Molecule 1: 3C-like proteinase

Chain 10-A: 83% 14% . .



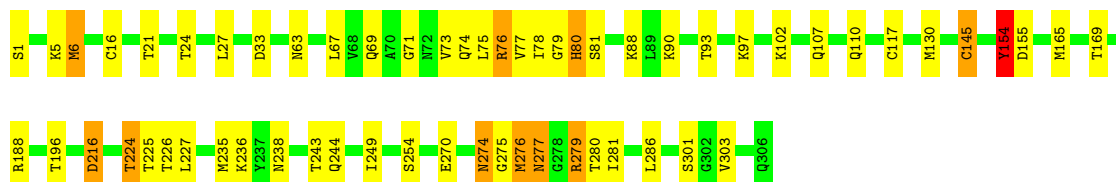
- Molecule 1: 3C-like proteinase

Chain 11-A: 81% 16% .



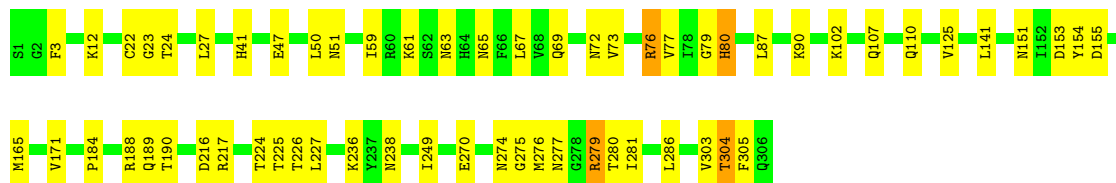
- Molecule 1: 3C-like proteinase

Chain 12-A: 80% 16% .



- Molecule 1: 3C-like proteinase

Chain 13-A: 80% 18% .



- Molecule 1: 3C-like proteinase

Chain 14-A: 79% 17% .





- Molecule 1: 3C-like proteinase

Chain 15-A: 79% 18%



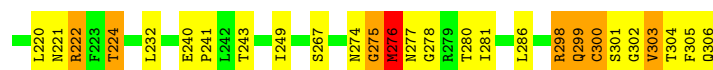
- Molecule 1: 3C-like proteinase

Chain 16-A: 82% 16%



- Molecule 1: 3C-like proteinase

Chain 17-A: 80% 15% 5%



- Molecule 1: 3C-like proteinase

Chain 18-A: 78% 19%



- Molecule 1: 3C-like proteinase

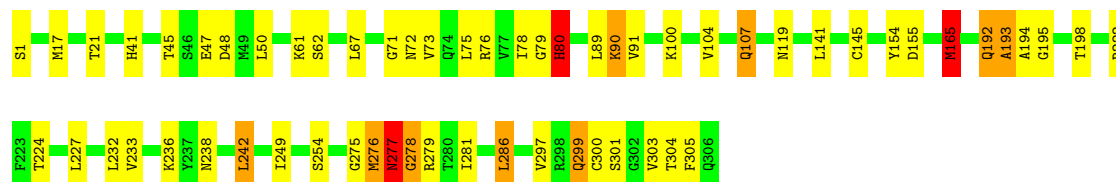
Chain 19-A: 78% 19%





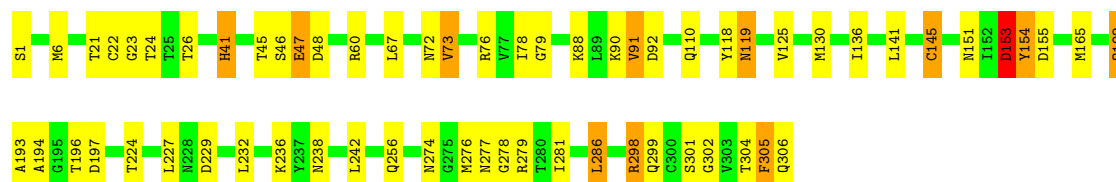
- Molecule 1: 3C-like proteinase

Chain 20-A: 80% 16% ..



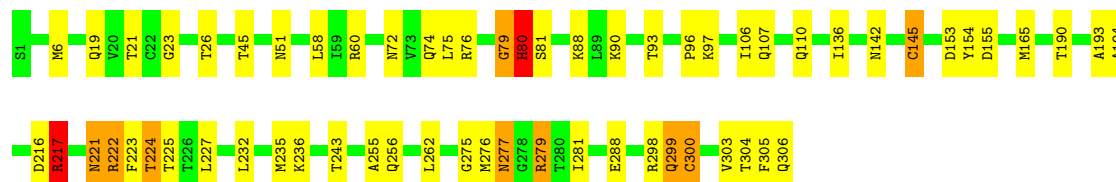
- Molecule 1: 3C-like proteinase

Chain 21-A: 79% 17% .



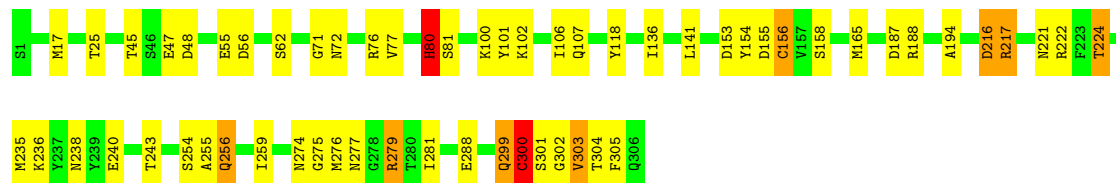
- Molecule 1: 3C-like proteinase

Chain 22-A: 80% 17% ..



- Molecule 1: 3C-like proteinase

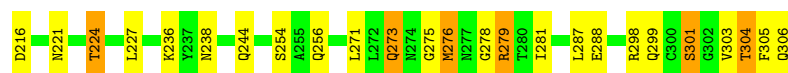
Chain 23-A: 81% 16% ..



- Molecule 1: 3C-like proteinase

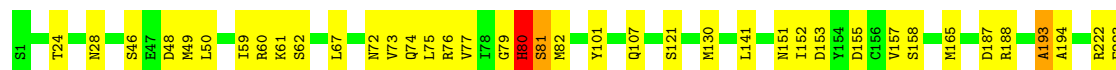
Chain 24-A: 81% 16% .





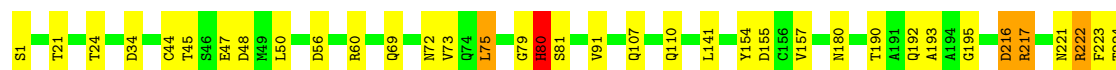
- Molecule 1: 3C-like proteinase

Chain 25-A: 79% 18% .



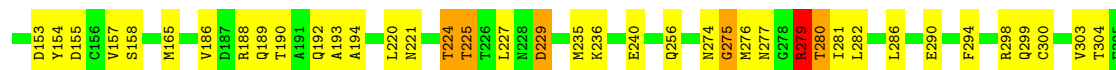
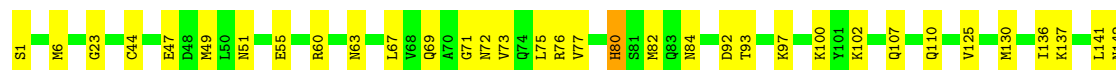
- Molecule 1: 3C-like proteinase

Chain 26-A: 82% 16% .



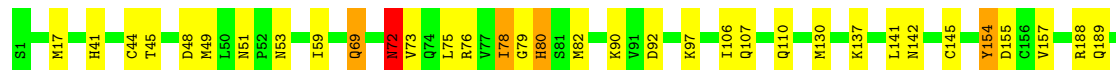
- Molecule 1: 3C-like proteinase

Chain 27-A: 76% 22% .



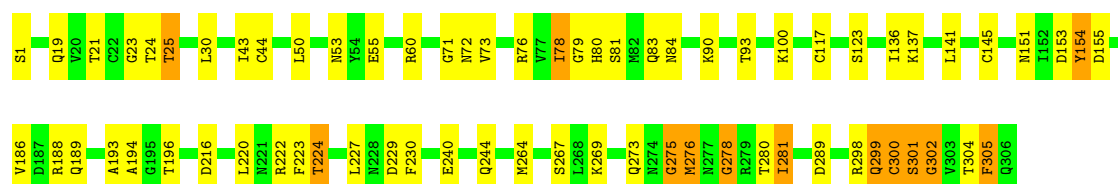
- Molecule 1: 3C-like proteinase

Chain 28-A: 78% 18% . .



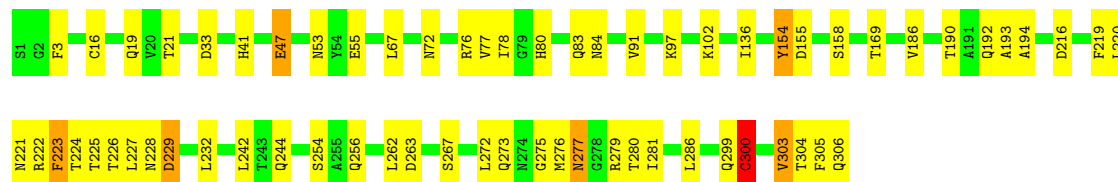
- Molecule 1: 3C-like proteinase

Chain 29-A: 77% 18% .



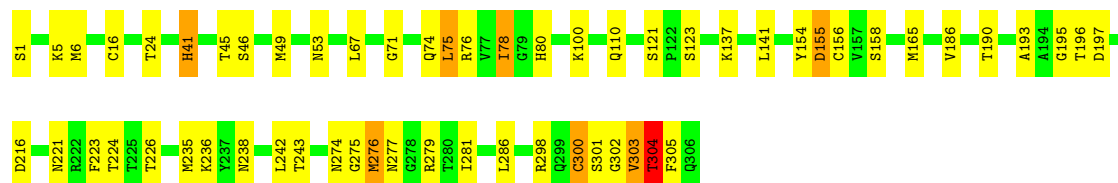
- Molecule 1: 3C-like proteinase

Chain 30-A: 79% 19% .



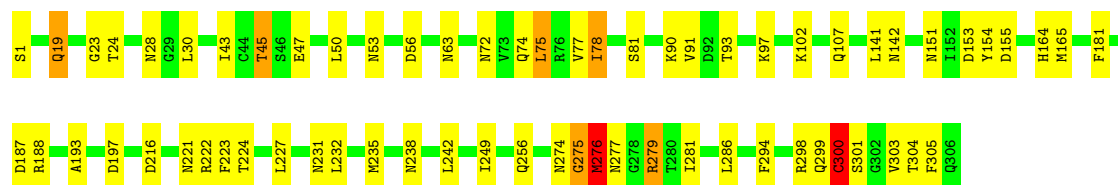
- Molecule 1: 3C-like proteinase

Chain 31-A: 81% 16% .



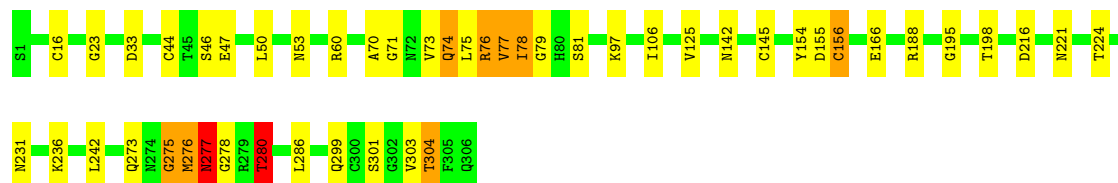
- Molecule 1: 3C-like proteinase

Chain 32-A: 78% 19% ..



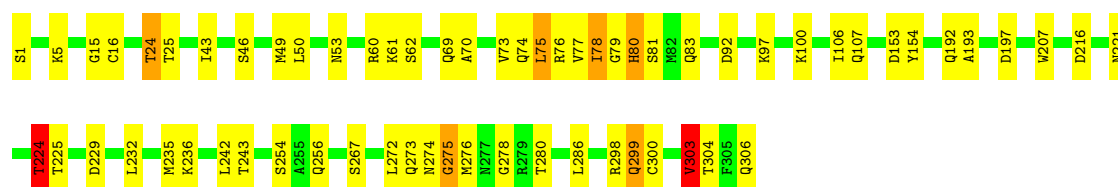
- Molecule 1: 3C-like proteinase

Chain 33-A: 84% 12% ..



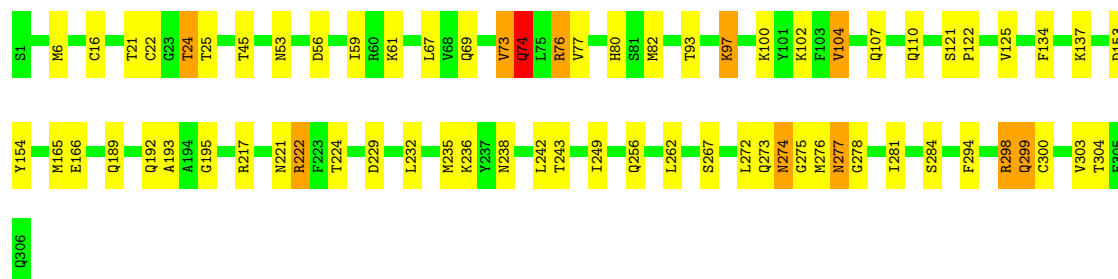
- Molecule 1: 3C-like proteinase

Chain 34-A: 79% 18% ..



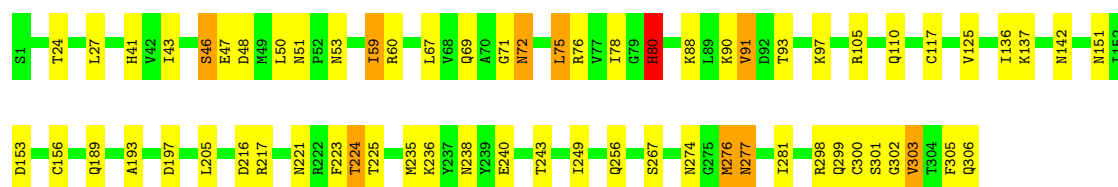
- Molecule 1: 3C-like proteinase

Chain 35-A:



- Molecule 1: 3C-like proteinase

Chain 36-A:



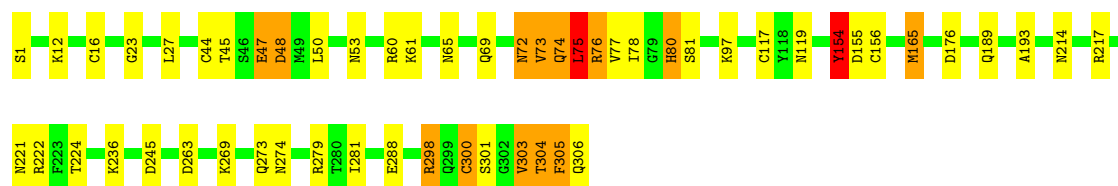
- Molecule 1: 3C-like proteinase

Chain 37-A:

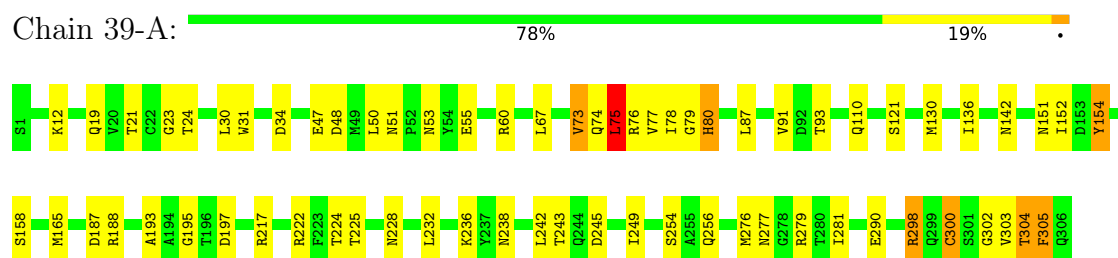


- Molecule 1: 3C-like proteinase

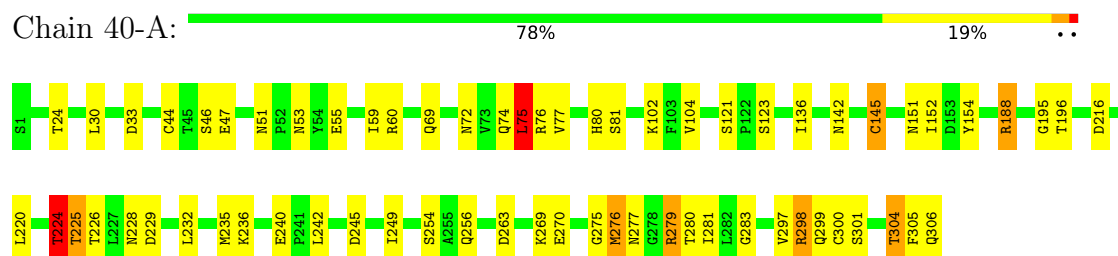
Chain 38-A:



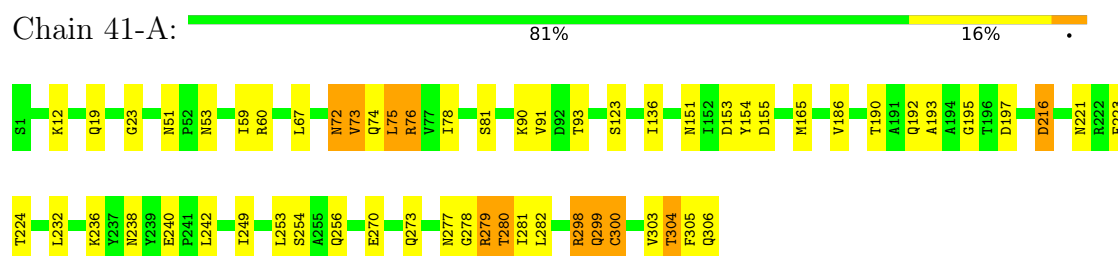
• Molecule 1: 3C-like proteinase



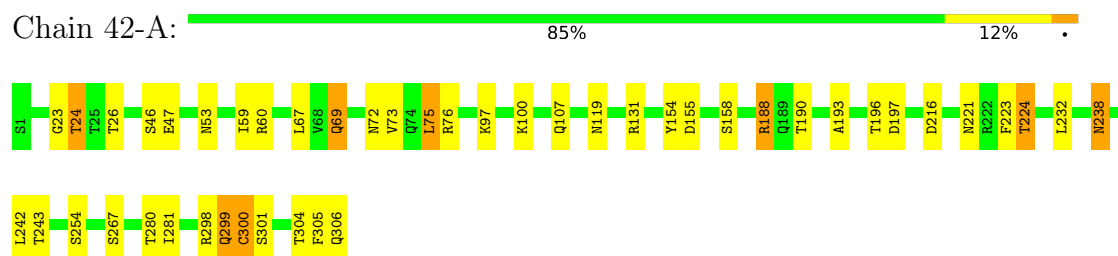
• Molecule 1: 3C-like proteinase



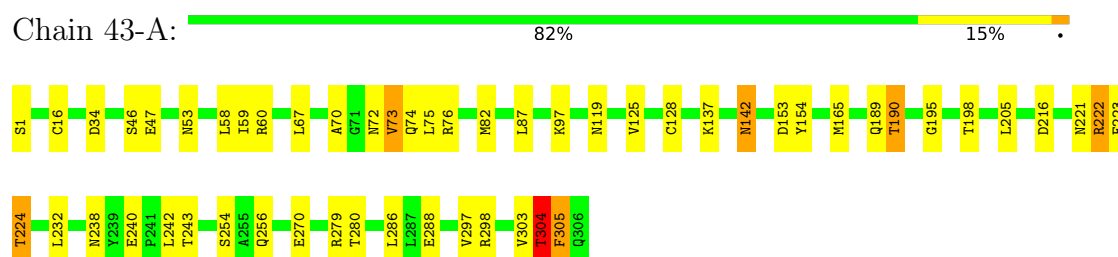
• Molecule 1: 3C-like proteinase




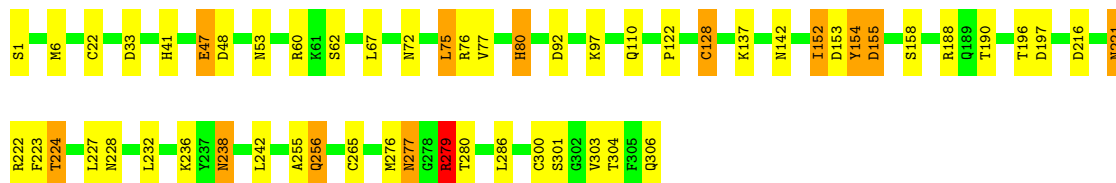
• Molecule 1: 3C-like proteinase




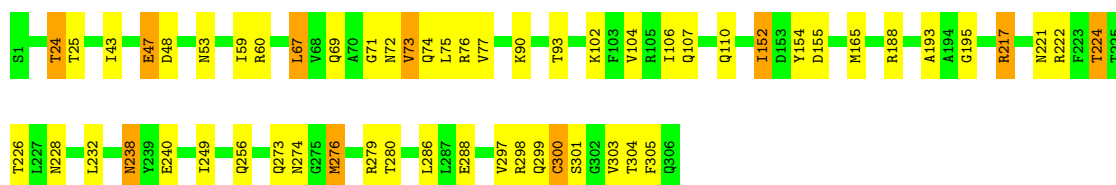
• Molecule 1: 3C-like proteinase



• Molecule 1: 3C-like proteinase

Chain 44-A:  82% 14% .

• Molecule 1: 3C-like proteinase

Chain 45-A:  81% 15% .

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	115.02Å 54.36Å 44.97Å 90.00° 101.50° 90.00°	Depositor
Resolution (Å)	48.96 – 2.19	Depositor
% Data completeness (in resolution range)	99.3 (48.96-2.19)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.153 , 0.215	Depositor
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.312	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	213552	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.17% 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	0.77	3/2420 (0.1%)	0.87	3/3289 (0.1%)
1	2-A	0.77	5/2420 (0.2%)	0.81	0/3289
1	3-A	0.75	1/2420 (0.0%)	0.90	7/3289 (0.2%)
1	4-A	0.74	1/2420 (0.0%)	0.89	5/3289 (0.2%)
1	5-A	0.77	3/2420 (0.1%)	0.90	6/3289 (0.2%)
1	6-A	0.81	1/2420 (0.0%)	0.87	1/3289 (0.0%)
1	7-A	0.78	4/2420 (0.2%)	0.86	3/3289 (0.1%)
1	8-A	0.80	3/2420 (0.1%)	0.86	2/3289 (0.1%)
1	9-A	0.72	0/2420	0.84	2/3289 (0.1%)
1	10-A	0.73	3/2420 (0.1%)	0.84	1/3289 (0.0%)
1	11-A	0.81	2/2420 (0.1%)	0.89	2/3289 (0.1%)
1	12-A	0.74	3/2420 (0.1%)	0.87	4/3289 (0.1%)
1	13-A	0.72	0/2420	0.83	1/3289 (0.0%)
1	14-A	0.74	3/2420 (0.1%)	0.88	4/3289 (0.1%)
1	15-A	0.78	3/2420 (0.1%)	0.84	3/3289 (0.1%)
1	16-A	0.73	2/2420 (0.1%)	0.86	0/3289
1	17-A	0.77	4/2420 (0.2%)	0.85	3/3289 (0.1%)
1	18-A	0.76	3/2420 (0.1%)	0.86	2/3289 (0.1%)
1	19-A	0.77	3/2420 (0.1%)	0.89	1/3289 (0.0%)
1	20-A	0.77	3/2420 (0.1%)	0.87	5/3289 (0.2%)
1	21-A	0.76	2/2420 (0.1%)	0.87	3/3289 (0.1%)
1	22-A	0.78	1/2420 (0.0%)	0.84	3/3289 (0.1%)
1	23-A	0.80	4/2420 (0.2%)	0.87	4/3289 (0.1%)
1	24-A	0.75	2/2420 (0.1%)	0.85	0/3289
1	25-A	0.81	3/2420 (0.1%)	0.86	5/3289 (0.2%)
1	26-A	0.76	2/2420 (0.1%)	0.90	3/3289 (0.1%)
1	27-A	0.76	1/2420 (0.0%)	0.85	2/3289 (0.1%)
1	28-A	0.77	2/2420 (0.1%)	0.86	4/3289 (0.1%)
1	29-A	0.85	3/2420 (0.1%)	0.89	2/3289 (0.1%)
1	30-A	0.77	2/2420 (0.1%)	0.87	1/3289 (0.0%)
1	31-A	0.77	1/2420 (0.0%)	0.87	0/3289
1	32-A	0.75	2/2420 (0.1%)	0.84	4/3289 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.77	5/2420 (0.2%)	0.86	0/3289
1	34-A	0.82	4/2420 (0.2%)	0.85	2/3289 (0.1%)
1	35-A	0.80	3/2420 (0.1%)	0.86	2/3289 (0.1%)
1	36-A	0.76	1/2420 (0.0%)	0.86	0/3289
1	37-A	0.79	2/2420 (0.1%)	0.85	0/3289
1	38-A	0.79	4/2420 (0.2%)	0.88	4/3289 (0.1%)
1	39-A	0.76	2/2420 (0.1%)	0.89	7/3289 (0.2%)
1	40-A	0.73	2/2420 (0.1%)	0.87	1/3289 (0.0%)
1	41-A	0.72	0/2420	0.82	2/3289 (0.1%)
1	42-A	0.71	0/2420	0.79	1/3289 (0.0%)
1	43-A	0.74	1/2420 (0.0%)	0.83	0/3289
1	44-A	0.79	2/2420 (0.1%)	0.83	1/3289 (0.0%)
1	45-A	0.74	0/2420	0.84	2/3289 (0.1%)
All	All	0.77	101/108900 (0.1%)	0.86	108/148005 (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	7
1	2-A	0	9
1	3-A	0	6
1	4-A	0	10
1	5-A	0	5
1	6-A	0	9
1	7-A	0	8
1	8-A	0	11
1	9-A	0	8
1	10-A	0	11
1	11-A	0	8
1	12-A	0	8
1	13-A	0	5
1	14-A	0	7
1	15-A	0	9
1	16-A	0	6
1	17-A	0	13
1	18-A	0	10
1	19-A	0	10
1	20-A	0	10
1	21-A	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	22-A	0	6
1	23-A	0	8
1	24-A	0	4
1	25-A	0	10
1	26-A	0	12
1	27-A	0	10
1	28-A	0	14
1	29-A	0	10
1	30-A	0	9
1	31-A	0	11
1	32-A	0	9
1	33-A	0	9
1	34-A	0	8
1	35-A	0	13
1	36-A	0	11
1	37-A	0	9
1	38-A	0	4
1	39-A	0	4
1	40-A	0	12
1	41-A	0	10
1	42-A	0	5
1	43-A	0	4
1	44-A	0	11
1	45-A	0	10
All	All	0	391

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	29-A	145	CYS	CB-SG	13.56	2.05	1.82
1	44-A	128	CYS	CB-SG	-13.36	1.59	1.82
1	8-A	145	CYS	CB-SG	12.69	2.03	1.82
1	37-A	156	CYS	CB-SG	12.57	2.03	1.82
1	8-A	156	CYS	CB-SG	-10.76	1.64	1.82

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	155	ASP	CB-CG-OD2	-9.87	109.42	118.30
1	26-A	305	PHE	CB-CG-CD1	8.76	126.93	120.80
1	18-A	67	LEU	CA-CB-CG	7.82	133.28	115.30
1	14-A	300	CYS	CA-CB-SG	-7.47	100.55	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	155	ASP	CB-CG-OD2	-7.42	111.63	118.30

There are no chirality outliers.

5 of 391 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	151	ASN	Peptide
1	1-A	195	GLY	Peptide
1	1-A	217	ARG	Sidechain
1	1-A	72	ASN	Peptide
1	1-A	73	VAL	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	2313	2313	0	0
1	2-A	2367	2313	2313	0	0
1	3-A	2367	2313	2313	0	0
1	4-A	2367	2313	2313	0	0
1	5-A	2367	2313	2313	0	0
1	6-A	2367	2313	2313	0	0
1	7-A	2367	2313	2313	0	0
1	8-A	2367	2313	2313	0	0
1	9-A	2367	2313	2313	0	0
1	10-A	2367	2313	2313	0	0
1	11-A	2367	2313	2313	0	0
1	12-A	2367	2313	2313	0	0
1	13-A	2367	2313	2313	0	0
1	14-A	2367	2313	2313	0	0
1	15-A	2367	2313	2313	0	0
1	16-A	2367	2313	2313	0	0
1	17-A	2367	2313	2313	0	0
1	18-A	2367	2313	2313	0	0
1	19-A	2367	2313	2313	0	0
1	20-A	2367	2313	2313	0	0
1	21-A	2367	2313	2313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	22-A	2367	2313	2313	0	0
1	23-A	2367	2313	2313	0	0
1	24-A	2367	2313	2313	0	0
1	25-A	2367	2313	2313	0	0
1	26-A	2367	2313	2313	0	0
1	27-A	2367	2313	2313	0	0
1	28-A	2367	2313	2313	0	0
1	29-A	2367	2313	2313	0	0
1	30-A	2367	2313	2313	0	0
1	31-A	2367	2313	2313	0	0
1	32-A	2367	2313	2313	0	0
1	33-A	2367	2313	2313	0	0
1	34-A	2367	2313	2313	0	0
1	35-A	2367	2313	2313	0	0
1	36-A	2367	2313	2311	0	0
1	37-A	2367	2313	2313	0	0
1	38-A	2367	2313	2313	0	0
1	39-A	2367	2313	2313	0	0
1	40-A	2367	2313	2313	0	0
1	41-A	2367	2313	2313	0	0
1	42-A	2367	2313	2313	0	0
1	43-A	2367	2313	2313	0	0
1	44-A	2367	2313	2313	0	0
1	45-A	2367	2313	2313	0	0
2	1-A	8	12	12	0	0
2	2-A	8	12	12	0	0
2	3-A	8	12	12	0	0
2	4-A	8	12	12	0	0
2	5-A	8	12	12	0	0
2	6-A	8	12	12	0	0
2	7-A	8	12	12	0	0
2	8-A	8	12	12	0	0
2	9-A	8	12	12	0	0
2	10-A	8	12	12	0	0
2	11-A	8	12	12	0	0
2	12-A	8	12	12	0	0
2	13-A	8	12	12	0	0
2	14-A	8	12	12	0	0
2	15-A	8	12	12	0	0
2	16-A	8	12	12	0	0
2	17-A	8	12	12	0	0
2	18-A	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	19-A	8	12	12	0	0
2	20-A	8	12	12	0	0
2	21-A	8	12	12	0	0
2	22-A	8	12	12	0	0
2	23-A	8	12	12	0	0
2	24-A	8	12	12	0	0
2	25-A	8	12	12	0	0
2	26-A	8	12	12	0	0
2	27-A	8	12	12	0	0
2	28-A	8	12	12	0	0
2	29-A	8	12	12	0	0
2	30-A	8	12	12	0	0
2	31-A	8	12	12	0	0
2	32-A	8	12	12	0	0
2	33-A	8	12	12	0	0
2	34-A	8	12	12	0	0
2	35-A	8	12	12	0	0
2	36-A	8	12	12	0	0
2	37-A	8	12	12	0	0
2	38-A	8	12	12	0	0
2	39-A	8	12	12	0	0
2	40-A	8	12	12	0	0
2	41-A	8	12	12	0	0
2	42-A	8	12	12	0	0
2	43-A	8	12	12	0	0
2	44-A	8	12	12	0	0
2	45-A	8	12	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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
3	44-A	1	0	0	0	0
3	45-A	1	0	0	0	0
4	1-A	45	0	0	0	0
4	2-A	38	0	0	0	0
4	3-A	37	0	0	0	0
4	4-A	44	0	0	0	0
4	5-A	47	0	0	0	0
4	6-A	45	0	0	0	0
4	7-A	44	0	0	0	0
4	8-A	37	0	0	0	0
4	9-A	46	0	0	0	0
4	10-A	50	0	0	0	0
4	11-A	50	0	0	0	0
4	12-A	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	13-A	48	0	0	0	0
4	14-A	42	0	0	0	0
4	15-A	41	0	0	0	0
4	16-A	42	0	0	0	0
4	17-A	42	0	0	0	0
4	18-A	44	0	0	0	0
4	19-A	41	0	0	0	0
4	20-A	48	0	0	0	0
4	21-A	42	0	0	0	0
4	22-A	46	0	0	0	0
4	23-A	55	0	0	0	0
4	24-A	49	0	0	0	0
4	25-A	54	0	0	0	0
4	26-A	41	0	0	0	0
4	27-A	39	0	0	0	0
4	28-A	40	0	0	0	0
4	29-A	47	0	0	0	0
4	30-A	46	0	0	0	0
4	31-A	47	0	0	0	0
4	32-A	45	0	0	0	0
4	33-A	48	0	0	0	0
4	34-A	43	0	0	0	0
4	35-A	38	0	0	0	0
4	36-A	37	0	0	0	0
4	37-A	41	0	0	0	0
4	38-A	47	0	0	0	0
4	39-A	49	0	0	0	0
4	40-A	48	0	0	0	0
4	41-A	42	0	0	0	0
4	42-A	48	0	0	0	0
4	43-A	45	0	0	0	0
4	44-A	52	0	0	0	0
4	45-A	39	0	0	0	0
All	All	108927	104625	104623	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	259 (85%)	22 (7%)	23 (8%)	1	0
1	2-A	304/306 (99%)	258 (85%)	29 (10%)	17 (6%)	2	0
1	3-A	304/306 (99%)	263 (86%)	24 (8%)	17 (6%)	2	0
1	4-A	304/306 (99%)	266 (88%)	20 (7%)	18 (6%)	1	0
1	5-A	304/306 (99%)	255 (84%)	29 (10%)	20 (7%)	1	0
1	6-A	304/306 (99%)	258 (85%)	29 (10%)	17 (6%)	2	0
1	7-A	304/306 (99%)	261 (86%)	32 (10%)	11 (4%)	3	1
1	8-A	304/306 (99%)	256 (84%)	26 (9%)	22 (7%)	1	0
1	9-A	304/306 (99%)	254 (84%)	31 (10%)	19 (6%)	1	0
1	10-A	304/306 (99%)	257 (84%)	28 (9%)	19 (6%)	1	0
1	11-A	304/306 (99%)	260 (86%)	29 (10%)	15 (5%)	2	1
1	12-A	304/306 (99%)	262 (86%)	26 (9%)	16 (5%)	2	0
1	13-A	304/306 (99%)	259 (85%)	28 (9%)	17 (6%)	2	0
1	14-A	304/306 (99%)	256 (84%)	32 (10%)	16 (5%)	2	0
1	15-A	304/306 (99%)	257 (84%)	24 (8%)	23 (8%)	1	0
1	16-A	304/306 (99%)	261 (86%)	25 (8%)	18 (6%)	1	0
1	17-A	304/306 (99%)	253 (83%)	30 (10%)	21 (7%)	1	0
1	18-A	304/306 (99%)	252 (83%)	30 (10%)	22 (7%)	1	0
1	19-A	304/306 (99%)	259 (85%)	27 (9%)	18 (6%)	1	0
1	20-A	304/306 (99%)	260 (86%)	25 (8%)	19 (6%)	1	0
1	21-A	304/306 (99%)	244 (80%)	43 (14%)	17 (6%)	2	0
1	22-A	304/306 (99%)	258 (85%)	26 (9%)	20 (7%)	1	0
1	23-A	304/306 (99%)	252 (83%)	33 (11%)	19 (6%)	1	0
1	24-A	304/306 (99%)	254 (84%)	32 (10%)	18 (6%)	1	0
1	25-A	304/306 (99%)	256 (84%)	32 (10%)	16 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	26-A	304/306 (99%)	261 (86%)	31 (10%)	12 (4%)	3	1
1	27-A	304/306 (99%)	254 (84%)	32 (10%)	18 (6%)	1	0
1	28-A	304/306 (99%)	247 (81%)	38 (12%)	19 (6%)	1	0
1	29-A	304/306 (99%)	259 (85%)	23 (8%)	22 (7%)	1	0
1	30-A	304/306 (99%)	259 (85%)	30 (10%)	15 (5%)	2	1
1	31-A	304/306 (99%)	261 (86%)	29 (10%)	14 (5%)	2	1
1	32-A	304/306 (99%)	254 (84%)	32 (10%)	18 (6%)	1	0
1	33-A	304/306 (99%)	260 (86%)	24 (8%)	20 (7%)	1	0
1	34-A	304/306 (99%)	250 (82%)	33 (11%)	21 (7%)	1	0
1	35-A	304/306 (99%)	260 (86%)	26 (9%)	18 (6%)	1	0
1	36-A	304/306 (99%)	260 (86%)	30 (10%)	14 (5%)	2	1
1	37-A	304/306 (99%)	252 (83%)	30 (10%)	22 (7%)	1	0
1	38-A	304/306 (99%)	254 (84%)	29 (10%)	21 (7%)	1	0
1	39-A	304/306 (99%)	249 (82%)	39 (13%)	16 (5%)	2	0
1	40-A	304/306 (99%)	256 (84%)	34 (11%)	14 (5%)	2	1
1	41-A	304/306 (99%)	263 (86%)	24 (8%)	17 (6%)	2	0
1	42-A	304/306 (99%)	272 (90%)	20 (7%)	12 (4%)	3	1
1	43-A	304/306 (99%)	258 (85%)	32 (10%)	14 (5%)	2	1
1	44-A	304/306 (99%)	255 (84%)	32 (10%)	17 (6%)	2	0
1	45-A	304/306 (99%)	263 (86%)	25 (8%)	16 (5%)	2	0
All	All	13680/13770 (99%)	11577 (85%)	1305 (10%)	798 (6%)	1	0

5 of 798 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	24	THR
1	1-A	63	ASN
1	1-A	72	ASN
1	1-A	73	VAL
1	1-A	152	ILE

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%)	220 (84%)	43 (16%)	2	2
1	2-A	263/263 (100%)	219 (83%)	44 (17%)	2	1
1	3-A	263/263 (100%)	222 (84%)	41 (16%)	2	2
1	4-A	263/263 (100%)	221 (84%)	42 (16%)	2	2
1	5-A	263/263 (100%)	214 (81%)	49 (19%)	1	1
1	6-A	263/263 (100%)	225 (86%)	38 (14%)	3	2
1	7-A	263/263 (100%)	227 (86%)	36 (14%)	3	3
1	8-A	263/263 (100%)	222 (84%)	41 (16%)	2	2
1	9-A	263/263 (100%)	221 (84%)	42 (16%)	2	2
1	10-A	263/263 (100%)	232 (88%)	31 (12%)	5	4
1	11-A	263/263 (100%)	224 (85%)	39 (15%)	3	2
1	12-A	263/263 (100%)	221 (84%)	42 (16%)	2	2
1	13-A	263/263 (100%)	222 (84%)	41 (16%)	2	2
1	14-A	263/263 (100%)	220 (84%)	43 (16%)	2	2
1	15-A	263/263 (100%)	226 (86%)	37 (14%)	3	2
1	16-A	263/263 (100%)	226 (86%)	37 (14%)	3	2
1	17-A	263/263 (100%)	227 (86%)	36 (14%)	3	3
1	18-A	263/263 (100%)	220 (84%)	43 (16%)	2	2
1	19-A	263/263 (100%)	220 (84%)	43 (16%)	2	2
1	20-A	263/263 (100%)	224 (85%)	39 (15%)	3	2
1	21-A	263/263 (100%)	217 (82%)	46 (18%)	2	1
1	22-A	263/263 (100%)	218 (83%)	45 (17%)	2	1
1	23-A	263/263 (100%)	226 (86%)	37 (14%)	3	2
1	24-A	263/263 (100%)	218 (83%)	45 (17%)	2	1
1	25-A	263/263 (100%)	220 (84%)	43 (16%)	2	2
1	26-A	263/263 (100%)	226 (86%)	37 (14%)	3	2
1	27-A	263/263 (100%)	212 (81%)	51 (19%)	1	1
1	28-A	263/263 (100%)	218 (83%)	45 (17%)	2	1
1	29-A	263/263 (100%)	218 (83%)	45 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	30-A	263/263 (100%)	217 (82%)	46 (18%)	2	1
1	31-A	263/263 (100%)	222 (84%)	41 (16%)	2	2
1	32-A	263/263 (100%)	218 (83%)	45 (17%)	2	1
1	33-A	263/263 (100%)	236 (90%)	27 (10%)	7	6
1	34-A	263/263 (100%)	224 (85%)	39 (15%)	3	2
1	35-A	263/263 (100%)	218 (83%)	45 (17%)	2	1
1	36-A	263/263 (100%)	213 (81%)	50 (19%)	1	1
1	37-A	263/263 (100%)	212 (81%)	51 (19%)	1	1
1	38-A	263/263 (100%)	224 (85%)	39 (15%)	3	2
1	39-A	263/263 (100%)	215 (82%)	48 (18%)	1	1
1	40-A	263/263 (100%)	215 (82%)	48 (18%)	1	1
1	41-A	263/263 (100%)	222 (84%)	41 (16%)	2	2
1	42-A	263/263 (100%)	227 (86%)	36 (14%)	3	3
1	43-A	263/263 (100%)	219 (83%)	44 (17%)	2	1
1	44-A	263/263 (100%)	224 (85%)	39 (15%)	3	2
1	45-A	263/263 (100%)	224 (85%)	39 (15%)	3	2
All	All	11835/11835 (100%)	9956 (84%)	1879 (16%)	2	2

5 of 1879 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	23-A	259	ILE
1	43-A	137	LYS
1	28-A	253	LEU
1	42-A	301	SER
1	39-A	77	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 413 such sidechains are listed below:

Mol	Chain	Res	Type
1	29-A	69	GLN
1	33-A	142	ASN
1	44-A	256	GLN
1	29-A	273	GLN
1	31-A	83	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 45 are monoatomic - leaving 90 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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.