



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2022 – 10:36 AM EDT

PDB ID : 7MHQ  
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 310 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 : 1.96 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](mailto: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.

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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	:	<b>FAILED</b>
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

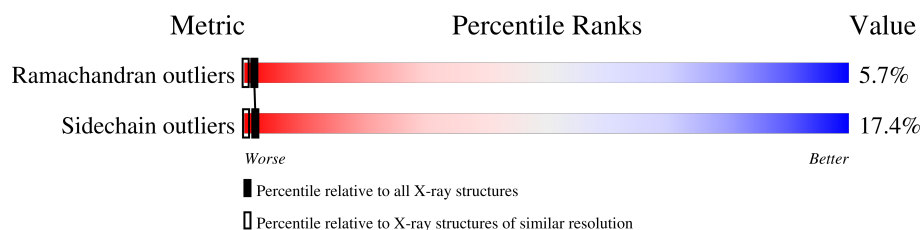
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)


























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  $\geq 3$ , 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	79% 18% .
1	10-A	306	78% 17% . .
1	11-A	306	75% 20% 5% .
1	12-A	306	80% 15% . .
1	13-A	306	81% 16% .
1	14-A	306	82% 14% .
1	15-A	306	79% 17% .
1	16-A	306	78% 18% .
1	17-A	306	76% 19% . .

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Mol	Chain	Length	Quality of chain
1	18-A	306	 74% 21% . .
1	19-A	306	 79% 18% . .
1	2-A	306	 82% 14% .
1	20-A	306	 77% 18% . .
1	21-A	306	 78% 17% .
1	22-A	306	 79% 18% .
1	23-A	306	 82% 15% .
1	24-A	306	 76% 19% 5% .
1	25-A	306	 75% 21% .
1	26-A	306	 80% 17% . .
1	27-A	306	 78% 17% . .
1	28-A	306	 76% 19% . .
1	29-A	306	 78% 19% .
1	3-A	306	 78% 18% . .
1	30-A	306	 82% 15% .
1	31-A	306	 79% 17% . .
1	32-A	306	 79% 15% . .
1	33-A	306	 79% 18% .
1	34-A	306	 80% 16% .
1	35-A	306	 78% 18% .
1	36-A	306	 77% 18% . .
1	4-A	306	 79% 19% .
1	5-A	306	 81% 17% . .
1	6-A	306	 79% 17% . .
1	7-A	306	 84% 13% .

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Mol	Chain	Length	Quality of chain
1	8-A	306	<div><div></div><div>81%</div><div>15%</div><div>.</div><div>.</div></div>
1	9-A	306	<div><div></div><div>80%</div><div>15%</div><div>.</div><div>.</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 170649 atoms, of which 83700 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			

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	36-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		

- 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		

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	45	Total 45	O 45	0	0
4	2-A	45	Total 45	O 45	0	0
4	3-A	46	Total 46	O 46	0	0
4	4-A	37	Total 37	O 37	0	0
4	5-A	42	Total 42	O 42	0	0
4	6-A	43	Total 43	O 43	0	0
4	7-A	35	Total 35	O 35	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	8-A	33	Total 33	O 33	0	0
4	9-A	39	Total 39	O 39	0	0
4	10-A	37	Total 37	O 37	0	0
4	11-A	41	Total 41	O 41	0	0
4	12-A	42	Total 42	O 42	0	0
4	13-A	45	Total 45	O 45	0	0
4	14-A	43	Total 43	O 43	0	0
4	15-A	38	Total 38	O 38	0	0
4	16-A	30	Total 30	O 30	0	0
4	17-A	34	Total 34	O 34	0	0
4	18-A	46	Total 46	O 46	0	0
4	19-A	41	Total 41	O 41	0	0
4	20-A	38	Total 38	O 38	0	0
4	21-A	42	Total 42	O 42	0	0
4	22-A	44	Total 44	O 44	0	0
4	23-A	40	Total 40	O 40	0	0
4	24-A	33	Total 33	O 33	0	0
4	25-A	36	Total 36	O 36	0	0
4	26-A	41	Total 41	O 41	0	0
4	27-A	38	Total 38	O 38	0	0
4	28-A	39	Total 39	O 39	0	0

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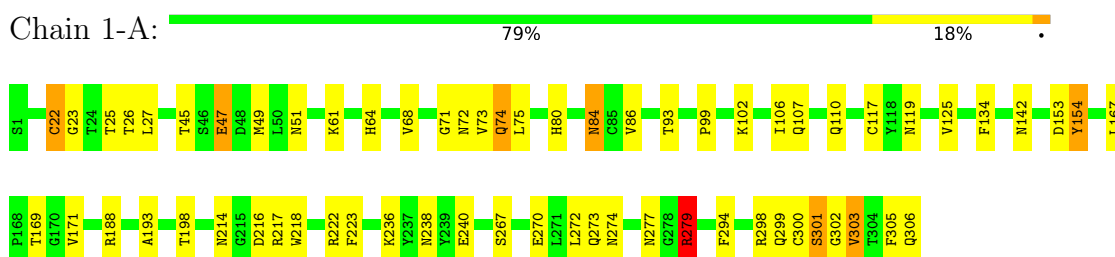
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	29-A	38	Total	O	0	0
			38	38		
4	30-A	37	Total	O	0	0
			37	37		
4	31-A	34	Total	O	0	0
			34	34		
4	32-A	34	Total	O	0	0
			34	34		
4	33-A	39	Total	O	0	0
			39	39		
4	34-A	48	Total	O	0	0
			48	48		
4	35-A	37	Total	O	0	0
			37	37		
4	36-A	33	Total	O	0	0
			33	33		

### 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.

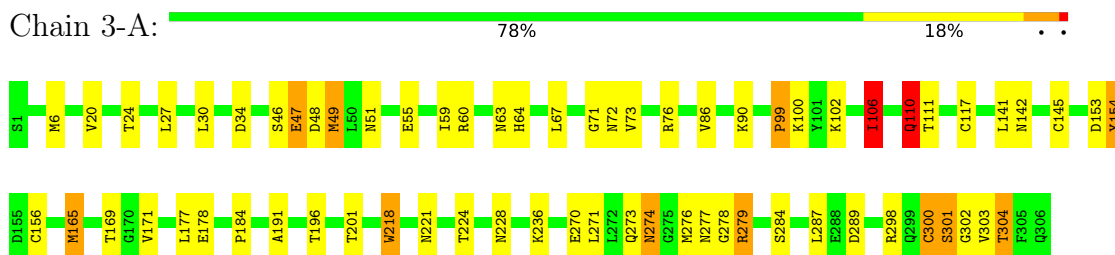
- Molecule 1: 3C-like proteinase



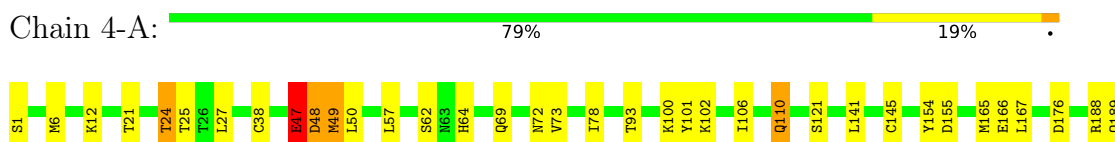
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase





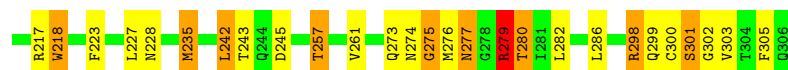
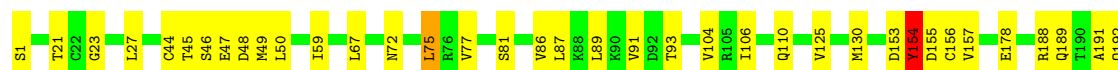
- Molecule 1: 3C-like proteinase

Chain 5-A: 81% 17% ..



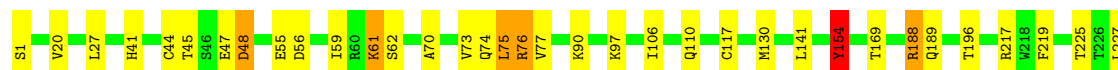
- Molecule 1: 3C-like proteinase

Chain 6-A: 79% 17% ..



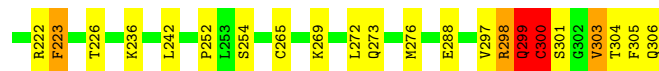
- Molecule 1: 3C-like proteinase

Chain 7-A: 84% 13% .



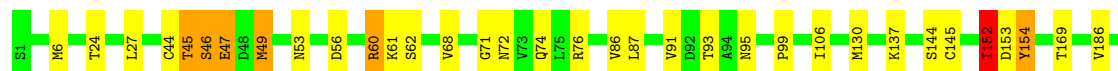
- Molecule 1: 3C-like proteinase

Chain 8-A: 81% 15% ..



- Molecule 1: 3C-like proteinase

Chain 9-A: 80% 15% ..

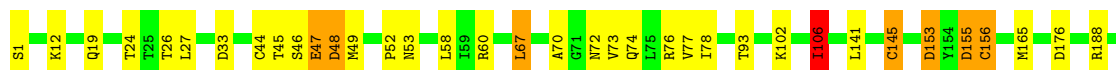






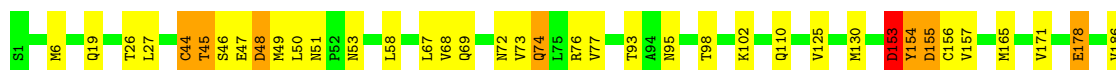
- Molecule 1: 3C-like proteinase

Chain 10-A: 78% 17% . .



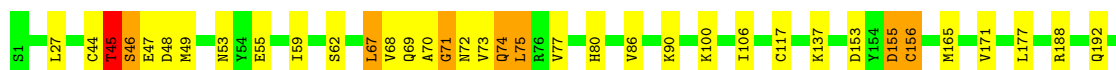
- Molecule 1: 3C-like proteinase

Chain 11-A: 75% 20% 5% . .



- Molecule 1: 3C-like proteinase

Chain 12-A: 80% 15% . .



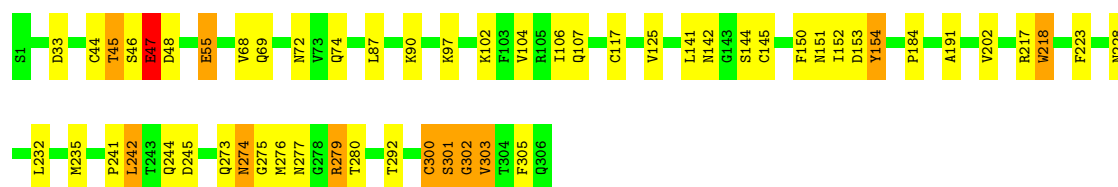
- Molecule 1: 3C-like proteinase

Chain 13-A: 81% 16% .



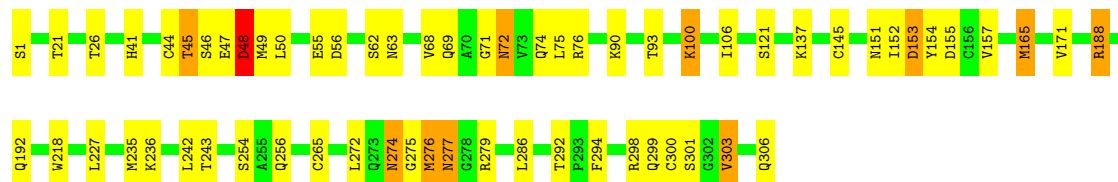
- Molecule 1: 3C-like proteinase

Chain 14-A: 82% 14% .



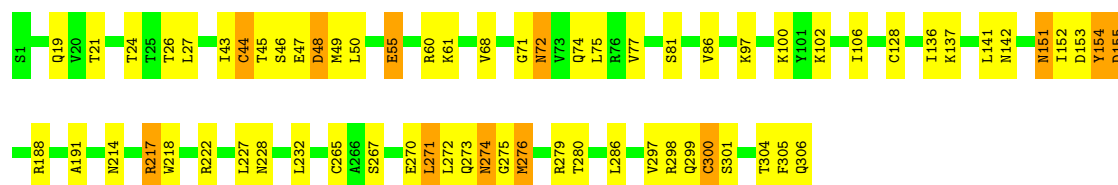
- Molecule 1: 3C-like proteinase

Chain 15-A: 79% 17% .



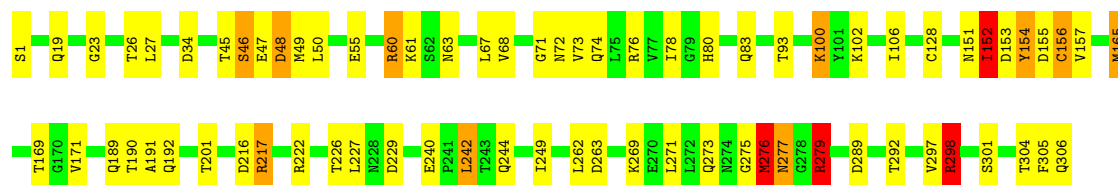
- Molecule 1: 3C-like proteinase

Chain 16-A: 78% 18% .



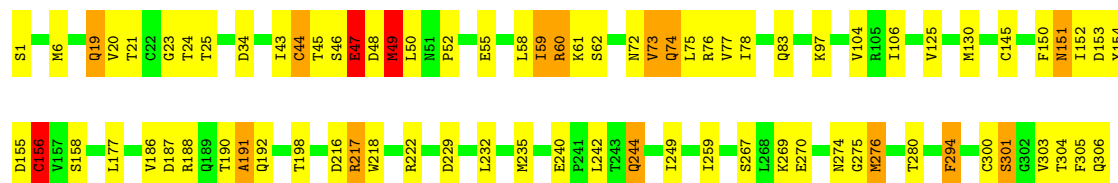
- Molecule 1: 3C-like proteinase

Chain 17-A: 76% 19% . .



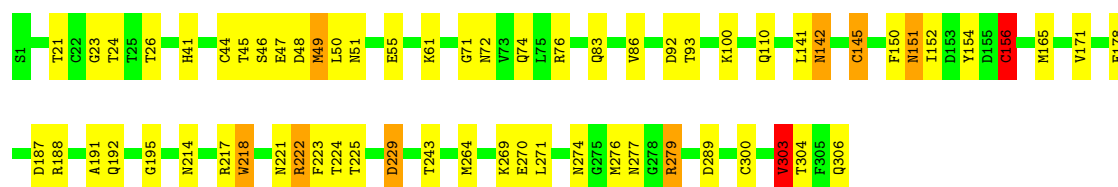
- Molecule 1: 3C-like proteinase

Chain 18-A: 74% 21% . .



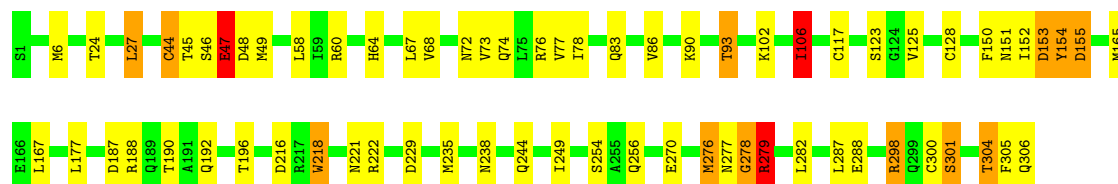
- Molecule 1: 3C-like proteinase

Chain 19-A: 79% 18% . .



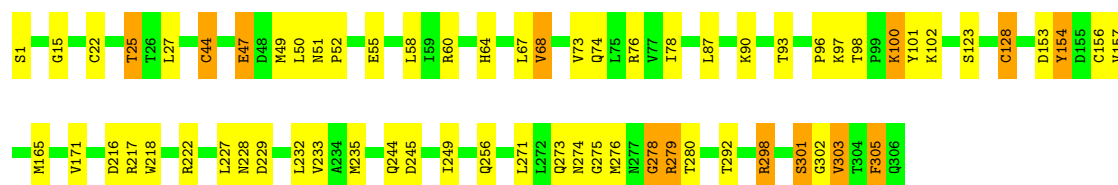
- Molecule 1: 3C-like proteinase

Chain 20-A: 77% 18% . .



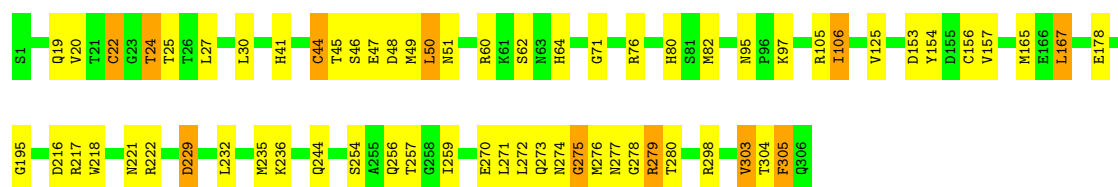
- Molecule 1: 3C-like proteinase

Chain 21-A: 78% 17% .



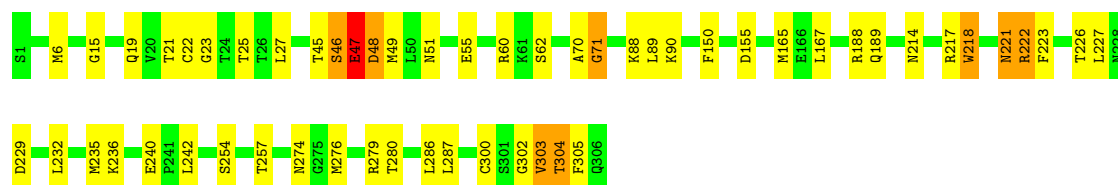
- Molecule 1: 3C-like proteinase

Chain 22-A: 79% 18% .



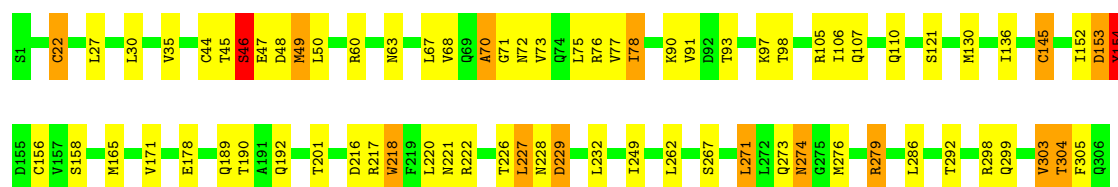
- Molecule 1: 3C-like proteinase

Chain 23-A: 82% 15% .



- Molecule 1: 3C-like proteinase

Chain 24-A: 76% 19% 5% .



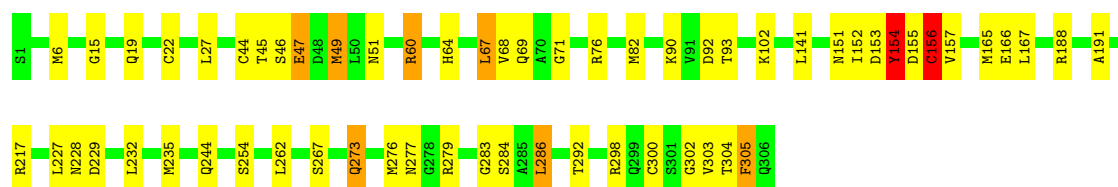
- Molecule 1: 3C-like proteinase

Chain 25-A: 75% 21% .



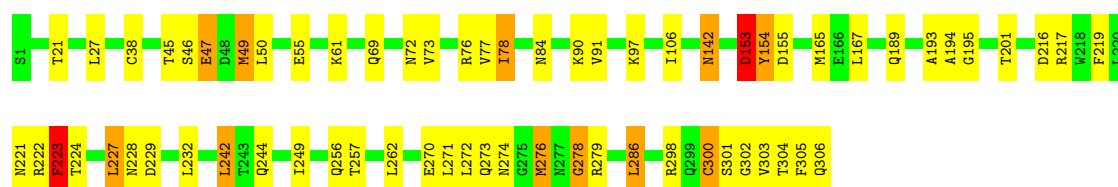
- Molecule 1: 3C-like proteinase

Chain 26-A: 80% 17% ..



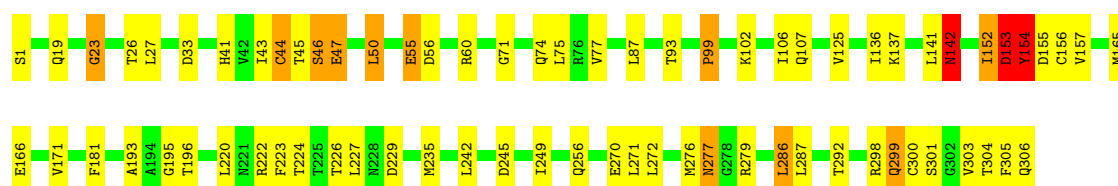
- Molecule 1: 3C-like proteinase

Chain 27-A: 78% 17% . .

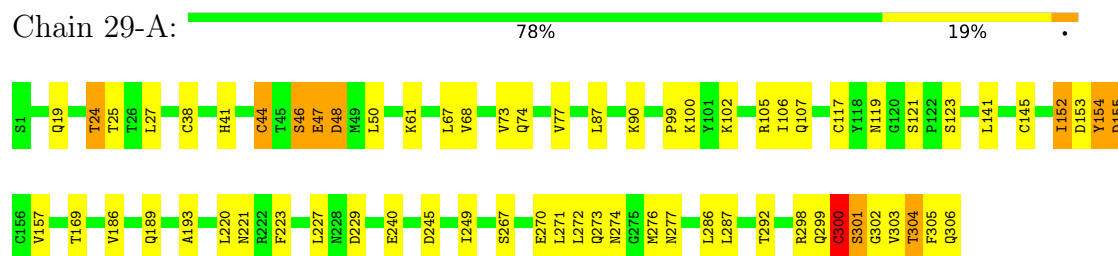


- Molecule 1: 3C-like proteinase

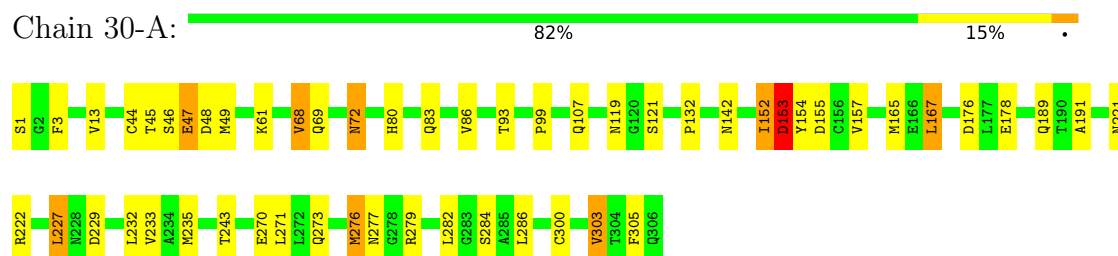
Chain 28-A: 76% 19% . .



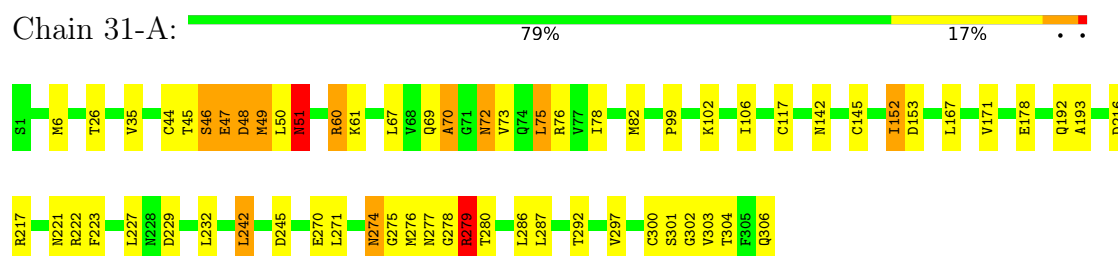
- Molecule 1: 3C-like proteinase



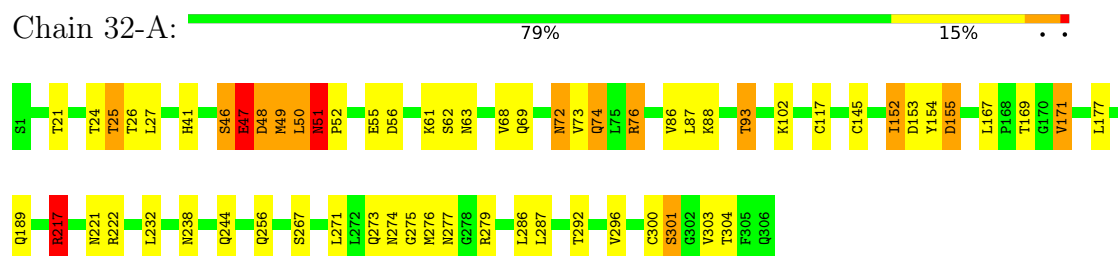
- Molecule 1: 3C-like proteinase



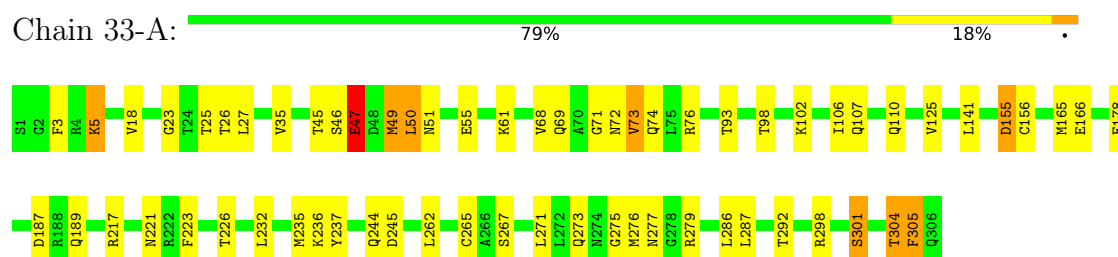
- Molecule 1: 3C-like proteinase



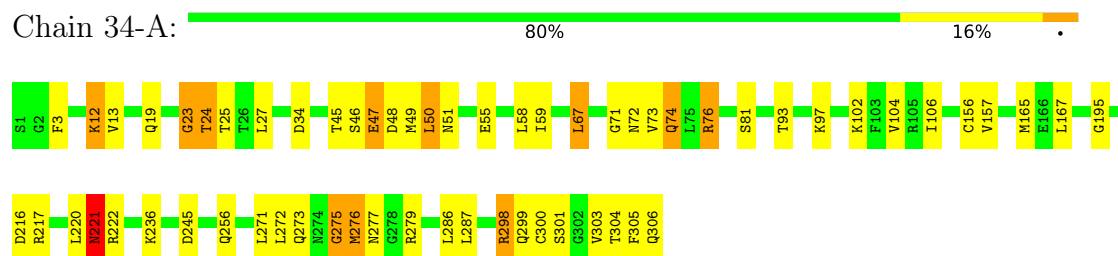
- Molecule 1: 3C-like proteinase



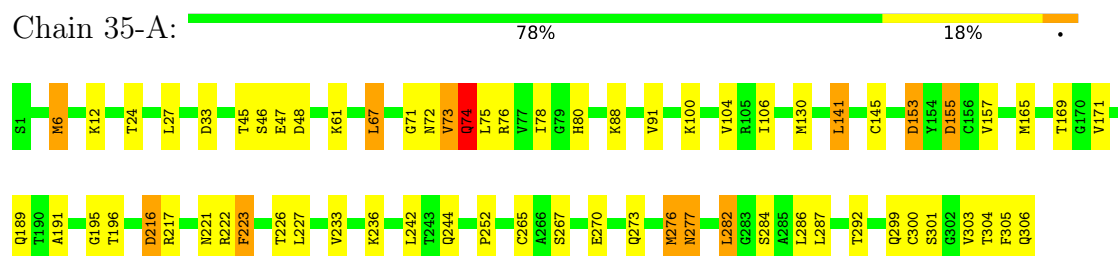
- Molecule 1: 3C-like proteinase



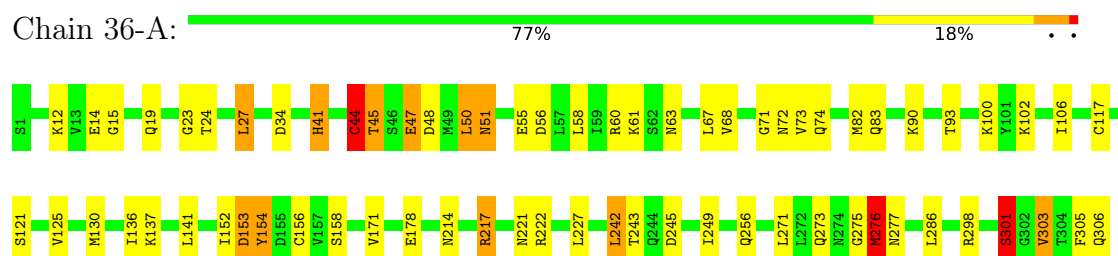
- Molecule 1: 3C-like proteinase



- 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, $\alpha$ , $\beta$ , $\gamma$	114.30Å 54.29Å 44.97Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	43.97 – 1.96	Depositor
% Data completeness (in resolution range)	99.8 (43.97-1.96)	Depositor
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.55 (at 1.97Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, $R_{free}$	0.171 , 0.235	Depositor
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.246	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	170649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.76	2/2420 (0.1%)	0.87	3/3289 (0.1%)
1	2-A	0.78	4/2420 (0.2%)	0.87	1/3289 (0.0%)
1	3-A	0.78	4/2420 (0.2%)	0.88	4/3289 (0.1%)
1	4-A	0.79	4/2420 (0.2%)	0.88	0/3289
1	5-A	0.75	2/2420 (0.1%)	0.87	1/3289 (0.0%)
1	6-A	0.79	3/2420 (0.1%)	0.88	4/3289 (0.1%)
1	7-A	0.79	2/2420 (0.1%)	0.86	0/3289
1	8-A	0.81	5/2420 (0.2%)	0.88	0/3289
1	9-A	0.82	2/2420 (0.1%)	0.92	5/3289 (0.2%)
1	10-A	0.81	2/2420 (0.1%)	0.89	5/3289 (0.2%)
1	11-A	0.79	5/2420 (0.2%)	0.92	1/3289 (0.0%)
1	12-A	0.77	4/2420 (0.2%)	0.88	3/3289 (0.1%)
1	13-A	0.79	3/2420 (0.1%)	0.87	1/3289 (0.0%)
1	14-A	0.78	5/2420 (0.2%)	0.87	2/3289 (0.1%)
1	15-A	0.79	2/2420 (0.1%)	0.87	3/3289 (0.1%)
1	16-A	0.78	2/2420 (0.1%)	0.89	3/3289 (0.1%)
1	17-A	0.75	2/2420 (0.1%)	0.90	3/3289 (0.1%)
1	18-A	0.87	6/2420 (0.2%)	0.89	7/3289 (0.2%)
1	19-A	0.82	4/2420 (0.2%)	0.87	2/3289 (0.1%)
1	20-A	0.77	2/2420 (0.1%)	0.93	10/3289 (0.3%)
1	21-A	0.83	4/2420 (0.2%)	0.88	1/3289 (0.0%)
1	22-A	0.83	4/2420 (0.2%)	0.88	1/3289 (0.0%)
1	23-A	0.75	3/2420 (0.1%)	0.87	0/3289
1	24-A	0.80	4/2420 (0.2%)	0.91	4/3289 (0.1%)
1	25-A	0.76	4/2420 (0.2%)	0.90	6/3289 (0.2%)
1	26-A	0.80	4/2420 (0.2%)	0.89	5/3289 (0.2%)
1	27-A	0.80	3/2420 (0.1%)	0.88	4/3289 (0.1%)
1	28-A	0.77	5/2420 (0.2%)	0.88	3/3289 (0.1%)
1	29-A	0.77	3/2420 (0.1%)	0.88	1/3289 (0.0%)
1	30-A	0.72	1/2420 (0.0%)	0.85	1/3289 (0.0%)
1	31-A	0.77	3/2420 (0.1%)	0.88	2/3289 (0.1%)
1	32-A	0.80	4/2420 (0.2%)	0.87	3/3289 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	33-A	0.75	3/2420 (0.1%)	0.87	3/3289 (0.1%)
1	34-A	0.75	1/2420 (0.0%)	0.86	3/3289 (0.1%)
1	35-A	0.79	3/2420 (0.1%)	0.88	5/3289 (0.2%)
1	36-A	0.76	3/2420 (0.1%)	0.89	4/3289 (0.1%)
All	All	0.78	117/87120 (0.1%)	0.88	104/118404 (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	6
1	3-A	0	5
1	4-A	0	7
1	5-A	0	9
1	6-A	0	9
1	7-A	0	8
1	8-A	0	6
1	9-A	0	13
1	10-A	0	10
1	11-A	0	18
1	12-A	0	12
1	13-A	0	11
1	14-A	0	10
1	15-A	0	7
1	16-A	0	7
1	17-A	0	15
1	18-A	0	13
1	19-A	0	12
1	20-A	0	12
1	21-A	0	15
1	22-A	0	8
1	23-A	0	6
1	24-A	0	16
1	25-A	0	10
1	26-A	0	9
1	27-A	0	10
1	28-A	0	17
1	29-A	0	12
1	30-A	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	31-A	0	14
1	32-A	0	9
1	33-A	0	3
1	34-A	0	11
1	35-A	0	6
1	36-A	0	8
All	All	0	360

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	21-A	128	CYS	CB-SG	-16.74	1.53	1.82
1	10-A	145	CYS	CB-SG	13.64	2.05	1.82
1	18-A	145	CYS	CB-SG	-13.28	1.59	1.82
1	9-A	145	CYS	CB-SG	12.55	2.03	1.82
1	8-A	145	CYS	CB-SG	11.95	2.02	1.82

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	20-A	128	CYS	CA-CB-SG	-13.80	89.17	114.00
1	10-A	218	TRP	CA-CB-CG	8.09	129.07	113.70
1	27-A	300	CYS	CA-CB-SG	-7.84	99.89	114.00
1	1-A	22	CYS	CA-CB-SG	-7.60	100.33	114.00
1	20-A	44	CYS	CA-CB-SG	-7.46	100.58	114.00

There are no chirality outliers.

5 of 360 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	154	TYR	Peptide
1	1-A	279	ARG	Sidechain,Peptide
1	1-A	64	HIS	Peptide
1	1-A	74	GLN	Peptide
1	2-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	2313	2313	0	0
1	2-A	2367	2313	2312	0	0
1	3-A	2367	2313	2313	0	0
1	4-A	2367	2313	2312	0	0
1	5-A	2367	2313	2313	0	0
1	6-A	2367	2313	2313	0	0
1	7-A	2367	2313	2311	0	0
1	8-A	2367	2313	2313	0	0
1	9-A	2367	2313	2313	0	0
1	10-A	2367	2313	2312	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	2312	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	2310	0	0
1	21-A	2367	2313	2313	0	0
1	22-A	2367	2313	2312	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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
4	1-A	45	0	0	0	0
4	2-A	45	0	0	0	0
4	3-A	46	0	0	0	0
4	4-A	37	0	0	0	0
4	5-A	42	0	0	0	0
4	6-A	43	0	0	0	0
4	7-A	35	0	0	0	0
4	8-A	33	0	0	0	0
4	9-A	39	0	0	0	0
4	10-A	37	0	0	0	0
4	11-A	41	0	0	0	0
4	12-A	42	0	0	0	0
4	13-A	45	0	0	0	0
4	14-A	43	0	0	0	0
4	15-A	38	0	0	0	0
4	16-A	30	0	0	0	0
4	17-A	34	0	0	0	0
4	18-A	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	19-A	41	0	0	0	0
4	20-A	38	0	0	0	0
4	21-A	42	0	0	0	0
4	22-A	44	0	0	0	0
4	23-A	40	0	0	0	0
4	24-A	33	0	0	0	0
4	25-A	36	0	0	0	0
4	26-A	41	0	0	0	0
4	27-A	38	0	0	0	0
4	28-A	39	0	0	0	0
4	29-A	38	0	0	0	0
4	30-A	37	0	0	0	0
4	31-A	34	0	0	0	0
4	32-A	34	0	0	0	0
4	33-A	39	0	0	0	0
4	34-A	48	0	0	0	0
4	35-A	37	0	0	0	0
4	36-A	33	0	0	0	0
All	All	86949	83700	83690	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%)	249 (82%)	35 (12%)	20 (7%)	1	0
1	2-A	304/306 (99%)	255 (84%)	33 (11%)	16 (5%)	2	0
1	3-A	304/306 (99%)	257 (84%)	23 (8%)	24 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-A	304/306 (99%)	255 (84%)	32 (10%)	17 (6%)	2	0
1	5-A	304/306 (99%)	250 (82%)	43 (14%)	11 (4%)	3	0
1	6-A	304/306 (99%)	255 (84%)	28 (9%)	21 (7%)	1	0
1	7-A	304/306 (99%)	256 (84%)	37 (12%)	11 (4%)	3	0
1	8-A	304/306 (99%)	254 (84%)	32 (10%)	18 (6%)	1	0
1	9-A	304/306 (99%)	258 (85%)	24 (8%)	22 (7%)	1	0
1	10-A	304/306 (99%)	254 (84%)	32 (10%)	18 (6%)	1	0
1	11-A	304/306 (99%)	244 (80%)	36 (12%)	24 (8%)	1	0
1	12-A	304/306 (99%)	257 (84%)	31 (10%)	16 (5%)	2	0
1	13-A	304/306 (99%)	262 (86%)	31 (10%)	11 (4%)	3	0
1	14-A	304/306 (99%)	272 (90%)	20 (7%)	12 (4%)	3	0
1	15-A	304/306 (99%)	262 (86%)	28 (9%)	14 (5%)	2	0
1	16-A	304/306 (99%)	249 (82%)	42 (14%)	13 (4%)	2	0
1	17-A	304/306 (99%)	248 (82%)	35 (12%)	21 (7%)	1	0
1	18-A	304/306 (99%)	245 (81%)	39 (13%)	20 (7%)	1	0
1	19-A	304/306 (99%)	260 (86%)	28 (9%)	16 (5%)	2	0
1	20-A	304/306 (99%)	261 (86%)	28 (9%)	15 (5%)	2	0
1	21-A	304/306 (99%)	247 (81%)	43 (14%)	14 (5%)	2	0
1	22-A	304/306 (99%)	251 (83%)	33 (11%)	20 (7%)	1	0
1	23-A	304/306 (99%)	257 (84%)	31 (10%)	16 (5%)	2	0
1	24-A	304/306 (99%)	247 (81%)	41 (14%)	16 (5%)	2	0
1	25-A	304/306 (99%)	248 (82%)	33 (11%)	23 (8%)	1	0
1	26-A	304/306 (99%)	272 (90%)	20 (7%)	12 (4%)	3	0
1	27-A	304/306 (99%)	257 (84%)	27 (9%)	20 (7%)	1	0
1	28-A	304/306 (99%)	246 (81%)	40 (13%)	18 (6%)	1	0
1	29-A	304/306 (99%)	252 (83%)	34 (11%)	18 (6%)	1	0
1	30-A	304/306 (99%)	253 (83%)	37 (12%)	14 (5%)	2	0
1	31-A	304/306 (99%)	259 (85%)	25 (8%)	20 (7%)	1	0
1	32-A	304/306 (99%)	251 (83%)	32 (10%)	21 (7%)	1	0
1	33-A	304/306 (99%)	258 (85%)	26 (9%)	20 (7%)	1	0
1	34-A	304/306 (99%)	256 (84%)	27 (9%)	21 (7%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	35-A	304/306 (99%)	257 (84%)	32 (10%)	15 (5%)	2	0
1	36-A	304/306 (99%)	257 (84%)	28 (9%)	19 (6%)	1	0
All	All	10944/11016 (99%)	9171 (84%)	1146 (10%)	627 (6%)	1	0

5 of 627 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	22	CYS
1	1-A	47	GLU
1	1-A	51	ASN
1	1-A	72	ASN
1	1-A	73	VAL

### 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%)	219 (83%)	44 (17%)	2	0
1	2-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	3-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	4-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	5-A	263/263 (100%)	217 (82%)	46 (18%)	2	0
1	6-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	7-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	8-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	9-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	10-A	263/263 (100%)	213 (81%)	50 (19%)	1	0
1	11-A	263/263 (100%)	212 (81%)	51 (19%)	1	0
1	12-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
1	13-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	14-A	263/263 (100%)	224 (85%)	39 (15%)	3	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	15-A	263/263 (100%)	213 (81%)	50 (19%)	1	0
1	16-A	263/263 (100%)	209 (80%)	54 (20%)	1	0
1	17-A	263/263 (100%)	212 (81%)	51 (19%)	1	0
1	18-A	263/263 (100%)	208 (79%)	55 (21%)	1	0
1	19-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	20-A	263/263 (100%)	211 (80%)	52 (20%)	1	0
1	21-A	263/263 (100%)	217 (82%)	46 (18%)	2	0
1	22-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
1	23-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	24-A	263/263 (100%)	210 (80%)	53 (20%)	1	0
1	25-A	263/263 (100%)	214 (81%)	49 (19%)	1	0
1	26-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	27-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	28-A	263/263 (100%)	215 (82%)	48 (18%)	1	0
1	29-A	263/263 (100%)	215 (82%)	48 (18%)	1	0
1	30-A	263/263 (100%)	226 (86%)	37 (14%)	3	0
1	31-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	32-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	33-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	34-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	35-A	263/263 (100%)	211 (80%)	52 (20%)	1	0
1	36-A	263/263 (100%)	211 (80%)	52 (20%)	1	0
All	All	9468/9468 (100%)	7824 (83%)	1644 (17%)	2	0

5 of 1644 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	21-A	58	LEU
1	25-A	297	VAL
1	36-A	47	GLU
1	21-A	244	GLN
1	21-A	55	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 290 such sidechains are listed below:

Mol	Chain	Res	Type
1	29-A	221	ASN
1	36-A	65	ASN
1	30-A	80	HIS
1	32-A	299	GLN
1	13-A	163	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 36 are monoatomic - leaving 72 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	2-A	502	-	3,3,3	0.81	0	3,3,3	0.55	0
2	DMS	1-A	501	-	3,3,3	0.77	0	3,3,3	2.23	2 (66%)
2	DMS	2-A	501	-	3,3,3	0.71	0	3,3,3	1.24	0
2	DMS	1-A	502	-	3,3,3	0.84	0	3,3,3	0.88	0
2	DMS	3-A	501	-	3,3,3	0.70	0	3,3,3	0.46	0

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	501	DMS	C2-S-C1	2.69	112.28	98.44
2	1-A	501	DMS	O-S-C1	2.06	117.06	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	4-A	1
1	22-A	1
1	10-A	1
1	15-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
4	A	106:ILE	C	107:GLN	N	1.17
22	A	106:ILE	C	107:GLN	N	1.15
10	A	106:ILE	C	107:GLN	N	1.13
15	A	106:ILE	C	107:GLN	N	1.11

## 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.