wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 07:26 AM EDT

PDB ID	:	7MHO
Title	:	Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 298 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	:	1.88 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

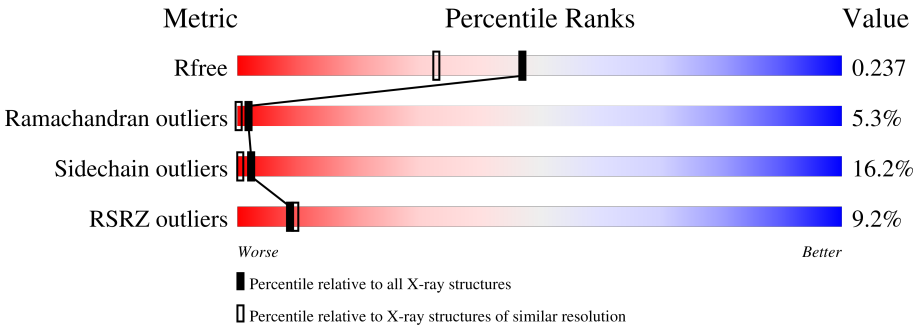
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	306	10% 81% 15% ·
1	10-A	306	10% 80% 16% ·
1	11-A	306	10% 78% 18% ·
1	12-A	306	10% 81% 16% · ·
1	13-A	306	10% 83% 15% ·
1	14-A	306	10% 79% 16% · ·
1	15-A	306	10% 82% 15% ·

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Mol	Chain	Length	Quality of chain
1	16-A	306	10% 83% 14%
1	17-A	306	10% 82% 14%
1	18-A	306	10% 77% 21%
1	19-A	306	10% 81% 16%
1	2-A	306	10% 80% 17%
1	20-A	306	10% 83% 14%
1	21-A	306	10% 80% 18%
1	22-A	306	10% 81% 18%
1	23-A	306	10% 86% 11%
1	24-A	306	10% 85% 12%
1	25-A	306	10% 83% 14%
1	26-A	306	10% 82% 14%
1	27-A	306	10% 80% 18%
1	28-A	306	10% 85% 12%
1	29-A	306	10% 84% 12%
1	3-A	306	10% 80% 17%
1	30-A	306	10% 85% 12%
1	31-A	306	10% 80% 16%
1	32-A	306	10% 81% 17%
1	33-A	306	10% 84% 13%
1	34-A	306	10% 78% 19%
1	35-A	306	10% 79% 18%
1	36-A	306	10% 81% 17%
1	37-A	306	10% 78% 18%
1	38-A	306	10% 78% 19%

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Mol	Chain	Length	Quality of chain
1	39-A	306	10% 76% 19% 5%
1	4-A	306	10% 83% 12%
1	40-A	306	10% 81% 15%
1	41-A	306	10% 79% 18%
1	42-A	306	10% 78% 18%
1	43-A	306	10% 77% 19%
1	44-A	306	10% 78% 18%
1	45-A	306	10% 79% 17%
1	46-A	306	10% 77% 18%
1	47-A	306	10% 81% 15%
1	48-A	306	10% 82% 13% 5%
1	49-A	306	10% 80% 18%
1	5-A	306	10% 82% 14%
1	50-A	306	10% 80% 17%
1	51-A	306	10% 82% 15%
1	52-A	306	10% 83% 15%
1	53-A	306	10% 79% 16%
1	54-A	306	10% 81% 15%
1	55-A	306	10% 81% 16%
1	56-A	306	10% 80% 15%
1	57-A	306	10% 79% 16%
1	58-A	306	10% 83% 16%
1	59-A	306	10% 80% 17%
1	6-A	306	10% 79% 17%
1	60-A	306	10% 79% 17%

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Mol	Chain	Length	Quality of chain
1	61-A	306	10% 79% 19%
1	62-A	306	10% 79% 17%
1	63-A	306	10% 82% 15%
1	64-A	306	10% 80% 16%
1	65-A	306	10% 82% 15%
1	66-A	306	10% 82% 14%
1	67-A	306	10% 79% 18%
1	68-A	306	10% 81% 16%
1	69-A	306	10% 82% 15%
1	7-A	306	10% 78% 19%
1	70-A	306	10% 77% 19%
1	71-A	306	10% 76% 18% 5%
1	72-A	306	10% 80% 18%
1	73-A	306	10% 79% 16%
1	74-A	306	10% 77% 19%
1	75-A	306	10% 79% 15% 5%
1	8-A	306	10% 79% 16%
1	9-A	306	10% 80% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	1-A	401	-	-	-	X
2	DMS	1-A	402	-	-	-	X
2	DMS	10-A	401	-	-	-	X
2	DMS	10-A	402	-	-	-	X
2	DMS	11-A	401	-	-	-	X
2	DMS	11-A	402	-	-	-	X
2	DMS	12-A	401	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	12-A	402	-	-	-	X
2	DMS	13-A	401	-	-	-	X
2	DMS	13-A	402	-	-	-	X
2	DMS	14-A	401	-	-	-	X
2	DMS	14-A	402	-	-	-	X
2	DMS	15-A	401	-	-	-	X
2	DMS	15-A	402	-	-	-	X
2	DMS	16-A	401	-	-	-	X
2	DMS	16-A	402	-	-	-	X
2	DMS	17-A	401	-	-	-	X
2	DMS	17-A	402	-	-	-	X
2	DMS	18-A	401	-	-	-	X
2	DMS	18-A	402	-	-	-	X
2	DMS	19-A	401	-	-	-	X
2	DMS	19-A	402	-	-	-	X
2	DMS	2-A	401	-	-	-	X
2	DMS	2-A	402	-	-	-	X
2	DMS	20-A	401	-	-	-	X
2	DMS	20-A	402	-	-	-	X
2	DMS	21-A	401	-	-	-	X
2	DMS	21-A	402	-	-	-	X
2	DMS	22-A	401	-	-	-	X
2	DMS	22-A	402	-	-	-	X
2	DMS	23-A	401	-	-	-	X
2	DMS	23-A	402	-	-	-	X
2	DMS	24-A	401	-	-	-	X
2	DMS	24-A	402	-	-	-	X
2	DMS	25-A	401	-	-	-	X
2	DMS	25-A	402	-	-	-	X
2	DMS	26-A	401	-	-	-	X
2	DMS	26-A	402	-	-	-	X
2	DMS	27-A	401	-	-	-	X
2	DMS	27-A	402	-	-	-	X
2	DMS	28-A	401	-	-	-	X
2	DMS	28-A	402	-	-	-	X
2	DMS	29-A	401	-	-	-	X
2	DMS	29-A	402	-	-	-	X
2	DMS	3-A	401	-	-	-	X
2	DMS	3-A	402	-	-	-	X
2	DMS	30-A	401	-	-	-	X
2	DMS	30-A	402	-	-	-	X
2	DMS	31-A	401	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	31-A	402	-	-	-	X
2	DMS	32-A	401	-	-	-	X
2	DMS	32-A	402	-	-	-	X
2	DMS	33-A	401	-	-	-	X
2	DMS	33-A	402	-	-	-	X
2	DMS	34-A	401	-	X	-	X
2	DMS	34-A	402	-	-	-	X
2	DMS	35-A	401	-	-	-	X
2	DMS	35-A	402	-	-	-	X
2	DMS	36-A	401	-	-	-	X
2	DMS	36-A	402	-	-	-	X
2	DMS	37-A	401	-	-	-	X
2	DMS	37-A	402	-	-	-	X
2	DMS	38-A	401	-	-	-	X
2	DMS	38-A	402	-	-	-	X
2	DMS	39-A	401	-	-	-	X
2	DMS	39-A	402	-	-	-	X
2	DMS	4-A	401	-	-	-	X
2	DMS	4-A	402	-	-	-	X
2	DMS	40-A	401	-	-	-	X
2	DMS	40-A	402	-	-	-	X
2	DMS	41-A	401	-	-	-	X
2	DMS	41-A	402	-	-	-	X
2	DMS	42-A	401	-	-	-	X
2	DMS	42-A	402	-	-	-	X
2	DMS	43-A	401	-	-	-	X
2	DMS	43-A	402	-	-	-	X
2	DMS	44-A	401	-	-	-	X
2	DMS	44-A	402	-	-	-	X
2	DMS	45-A	401	-	-	-	X
2	DMS	45-A	402	-	-	-	X
2	DMS	46-A	401	-	-	-	X
2	DMS	46-A	402	-	-	-	X
2	DMS	47-A	401	-	-	-	X
2	DMS	47-A	402	-	-	-	X
2	DMS	48-A	401	-	-	-	X
2	DMS	48-A	402	-	-	-	X
2	DMS	49-A	401	-	-	-	X
2	DMS	49-A	402	-	-	-	X
2	DMS	5-A	401	-	-	-	X
2	DMS	5-A	402	-	-	-	X
2	DMS	50-A	401	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	50-A	402	-	-	-	X
2	DMS	51-A	401	-	-	-	X
2	DMS	51-A	402	-	-	-	X
2	DMS	52-A	401	-	-	-	X
2	DMS	52-A	402	-	-	-	X
2	DMS	53-A	401	-	-	-	X
2	DMS	53-A	402	-	-	-	X
2	DMS	54-A	401	-	-	-	X
2	DMS	54-A	402	-	-	-	X
2	DMS	55-A	401	-	-	-	X
2	DMS	55-A	402	-	-	-	X
2	DMS	56-A	401	-	-	-	X
2	DMS	56-A	402	-	-	-	X
2	DMS	57-A	401	-	-	-	X
2	DMS	57-A	402	-	-	-	X
2	DMS	58-A	401	-	X	-	X
2	DMS	58-A	402	-	-	-	X
2	DMS	59-A	401	-	-	-	X
2	DMS	59-A	402	-	-	-	X
2	DMS	6-A	401	-	-	-	X
2	DMS	6-A	402	-	-	-	X
2	DMS	60-A	401	-	-	-	X
2	DMS	60-A	402	-	-	-	X
2	DMS	61-A	401	-	-	-	X
2	DMS	61-A	402	-	-	-	X
2	DMS	62-A	401	-	-	-	X
2	DMS	62-A	402	-	-	-	X
2	DMS	63-A	401	-	-	-	X
2	DMS	63-A	402	-	-	-	X
2	DMS	64-A	401	-	-	-	X
2	DMS	64-A	402	-	-	-	X
2	DMS	65-A	401	-	-	-	X
2	DMS	65-A	402	-	-	-	X
2	DMS	66-A	401	-	-	-	X
2	DMS	66-A	402	-	-	-	X
2	DMS	67-A	401	-	-	-	X
2	DMS	67-A	402	-	-	-	X
2	DMS	68-A	401	-	-	-	X
2	DMS	68-A	402	-	-	-	X
2	DMS	69-A	401	-	-	-	X
2	DMS	69-A	402	-	-	-	X
2	DMS	7-A	401	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	7-A	402	-	-	-	X
2	DMS	70-A	401	-	-	-	X
2	DMS	70-A	402	-	X	-	X
2	DMS	71-A	401	-	-	-	X
2	DMS	71-A	402	-	-	-	X
2	DMS	72-A	401	-	-	-	X
2	DMS	72-A	402	-	-	-	X
2	DMS	73-A	401	-	-	-	X
2	DMS	73-A	402	-	-	-	X
2	DMS	74-A	401	-	-	-	X
2	DMS	74-A	402	-	-	-	X
2	DMS	75-A	401	-	-	-	X
2	DMS	75-A	402	-	-	-	X
2	DMS	8-A	401	-	-	-	X
2	DMS	8-A	402	-	-	-	X
2	DMS	9-A	401	-	-	-	X
2	DMS	9-A	402	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 355880 atoms, of which 174375 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			
1	46-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	47-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	48-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	49-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	50-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	51-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	52-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	53-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	54-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	55-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	56-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	57-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	58-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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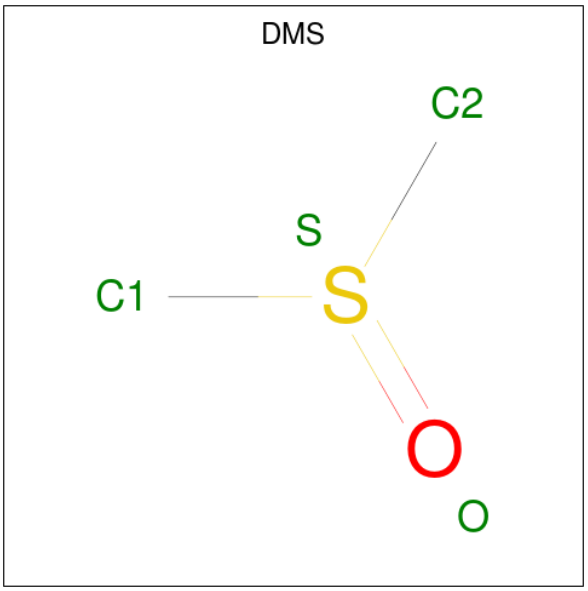
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	60-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	61-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	62-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	63-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	64-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	65-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	66-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	67-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	68-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	69-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	70-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	71-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	72-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	73-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	74-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	75-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_2H_6OS).



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	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		
2	46-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	47-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	48-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	49-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	50-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	51-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	52-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	53-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	54-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	55-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	56-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	57-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	58-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	59-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	60-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	61-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	62-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	63-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	64-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	65-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	66-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	67-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	68-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	69-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	70-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	71-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	72-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	73-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	74-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	75-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	44-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	45-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	46-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	47-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	48-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	49-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	50-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	51-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	52-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	53-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	54-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	55-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	56-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	57-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	58-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	59-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	60-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	61-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	62-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	63-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	64-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	65-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	66-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	67-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	68-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	69-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	70-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	71-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	72-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	73-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	74-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	75-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		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	10-A	1	Total Zn 1 1	0	0
3	11-A	1	Total Zn 1 1	0	0
3	12-A	1	Total Zn 1 1	0	0
3	13-A	1	Total Zn 1 1	0	0
3	14-A	1	Total Zn 1 1	0	0
3	15-A	1	Total Zn 1 1	0	0
3	16-A	1	Total Zn 1 1	0	0
3	17-A	1	Total Zn 1 1	0	0
3	18-A	1	Total Zn 1 1	0	0
3	19-A	1	Total Zn 1 1	0	0
3	20-A	1	Total Zn 1 1	0	0
3	21-A	1	Total Zn 1 1	0	0
3	22-A	1	Total Zn 1 1	0	0
3	23-A	1	Total Zn 1 1	0	0
3	24-A	1	Total Zn 1 1	0	0
3	25-A	1	Total Zn 1 1	0	0
3	26-A	1	Total Zn 1 1	0	0
3	27-A	1	Total Zn 1 1	0	0
3	28-A	1	Total Zn 1 1	0	0
3	29-A	1	Total Zn 1 1	0	0
3	30-A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	31-A	1	Total Zn 1 1	0	0
3	32-A	1	Total Zn 1 1	0	0
3	33-A	1	Total Zn 1 1	0	0
3	34-A	1	Total Zn 1 1	0	0
3	35-A	1	Total Zn 1 1	0	0
3	36-A	1	Total Zn 1 1	0	0
3	37-A	1	Total Zn 1 1	0	0
3	38-A	1	Total Zn 1 1	0	0
3	39-A	1	Total Zn 1 1	0	0
3	40-A	1	Total Zn 1 1	0	0
3	41-A	1	Total Zn 1 1	0	0
3	42-A	1	Total Zn 1 1	0	0
3	43-A	1	Total Zn 1 1	0	0
3	44-A	1	Total Zn 1 1	0	0
3	45-A	1	Total Zn 1 1	0	0
3	46-A	1	Total Zn 1 1	0	0
3	47-A	1	Total Zn 1 1	0	0
3	48-A	1	Total Zn 1 1	0	0
3	49-A	1	Total Zn 1 1	0	0
3	50-A	1	Total Zn 1 1	0	0
3	51-A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	52-A	1	Total Zn 1 1	0	0
3	53-A	1	Total Zn 1 1	0	0
3	54-A	1	Total Zn 1 1	0	0
3	55-A	1	Total Zn 1 1	0	0
3	56-A	1	Total Zn 1 1	0	0
3	57-A	1	Total Zn 1 1	0	0
3	58-A	1	Total Zn 1 1	0	0
3	59-A	1	Total Zn 1 1	0	0
3	60-A	1	Total Zn 1 1	0	0
3	61-A	1	Total Zn 1 1	0	0
3	62-A	1	Total Zn 1 1	0	0
3	63-A	1	Total Zn 1 1	0	0
3	64-A	1	Total Zn 1 1	0	0
3	65-A	1	Total Zn 1 1	0	0
3	66-A	1	Total Zn 1 1	0	0
3	67-A	1	Total Zn 1 1	0	0
3	68-A	1	Total Zn 1 1	0	0
3	69-A	1	Total Zn 1 1	0	0
3	70-A	1	Total Zn 1 1	0	0
3	71-A	1	Total Zn 1 1	0	0
3	72-A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	73-A	1	Total Zn 1 1	0	0
3	74-A	1	Total Zn 1 1	0	0
3	75-A	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	40	Total O 40 40	0	0
4	2-A	38	Total O 38 38	0	0
4	3-A	50	Total O 50 50	0	0
4	4-A	44	Total O 44 44	0	0
4	5-A	37	Total O 37 37	0	0
4	6-A	41	Total O 41 41	0	0
4	7-A	37	Total O 37 37	0	0
4	8-A	33	Total O 33 33	0	0
4	9-A	38	Total O 38 38	0	0
4	10-A	38	Total O 38 38	0	0
4	11-A	43	Total O 43 43	0	0
4	12-A	48	Total O 48 48	0	0
4	13-A	48	Total O 48 48	0	0
4	14-A	49	Total O 49 49	0	0
4	15-A	47	Total O 47 47	0	0
4	16-A	49	Total O 49 49	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	17-A	39	Total O 39 39	0	0
4	18-A	43	Total O 43 43	0	0
4	19-A	39	Total O 39 39	0	0
4	20-A	48	Total O 48 48	0	0
4	21-A	45	Total O 45 45	0	0
4	22-A	49	Total O 49 49	0	0
4	23-A	44	Total O 44 44	0	0
4	24-A	51	Total O 51 51	0	0
4	25-A	52	Total O 52 52	0	0
4	26-A	48	Total O 48 48	0	0
4	27-A	43	Total O 43 43	0	0
4	28-A	41	Total O 41 41	0	0
4	29-A	43	Total O 43 43	0	0
4	30-A	43	Total O 43 43	0	0
4	31-A	44	Total O 44 44	0	0
4	32-A	46	Total O 46 46	0	0
4	33-A	47	Total O 47 47	0	0
4	34-A	39	Total O 39 39	0	0
4	35-A	41	Total O 41 41	0	0
4	36-A	41	Total O 41 41	0	0
4	37-A	43	Total O 43 43	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	38-A	44	Total O 44 44	0	0
4	39-A	45	Total O 45 45	0	0
4	40-A	41	Total O 41 41	0	0
4	41-A	43	Total O 43 43	0	0
4	42-A	39	Total O 39 39	0	0
4	43-A	49	Total O 49 49	0	0
4	44-A	47	Total O 47 47	0	0
4	45-A	51	Total O 51 51	0	0
4	46-A	54	Total O 54 54	0	0
4	47-A	47	Total O 47 47	0	0
4	48-A	44	Total O 44 44	0	0
4	49-A	39	Total O 39 39	0	0
4	50-A	46	Total O 46 46	0	0
4	51-A	41	Total O 41 41	0	0
4	52-A	43	Total O 43 43	0	0
4	53-A	42	Total O 42 42	0	0
4	54-A	56	Total O 56 56	0	0
4	55-A	52	Total O 52 52	0	0
4	56-A	46	Total O 46 46	0	0
4	57-A	46	Total O 46 46	0	0
4	58-A	39	Total O 39 39	0	0

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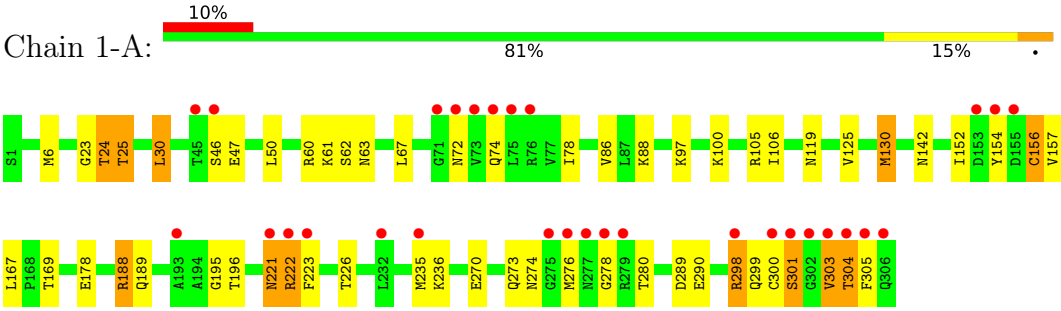
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	59-A	39	Total O 39 39	0	0
4	60-A	37	Total O 37 37	0	0
4	61-A	41	Total O 41 41	0	0
4	62-A	44	Total O 44 44	0	0
4	63-A	40	Total O 40 40	0	0
4	64-A	43	Total O 43 43	0	0
4	65-A	37	Total O 37 37	0	0
4	66-A	44	Total O 44 44	0	0
4	67-A	44	Total O 44 44	0	0
4	68-A	42	Total O 42 42	0	0
4	69-A	44	Total O 44 44	0	0
4	70-A	45	Total O 45 45	0	0
4	71-A	50	Total O 50 50	0	0
4	72-A	50	Total O 50 50	0	0
4	73-A	50	Total O 50 50	0	0
4	74-A	48	Total O 48 48	0	0
4	75-A	44	Total O 44 44	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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

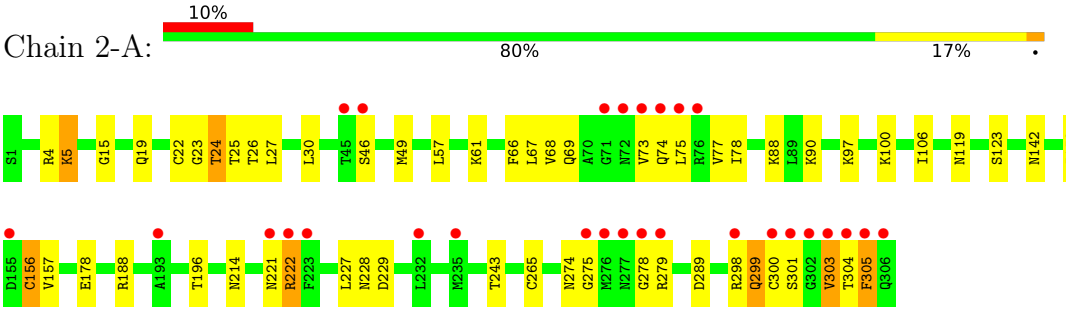
• Molecule 1: 3C-like proteinase

Chain 1-A:



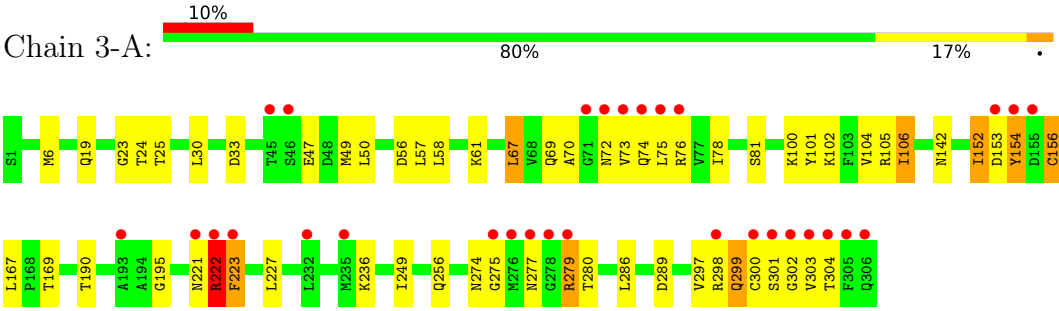
• Molecule 1: 3C-like proteinase

Chain 2-A:



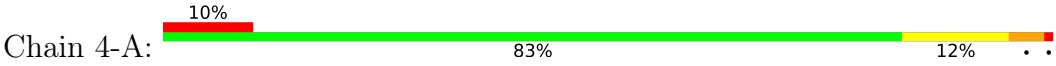
• Molecule 1: 3C-like proteinase

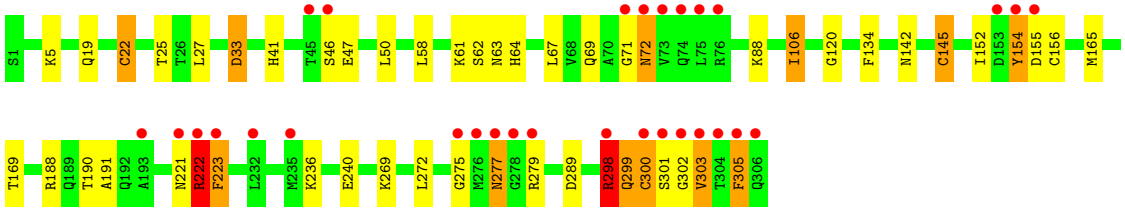
Chain 3-A:



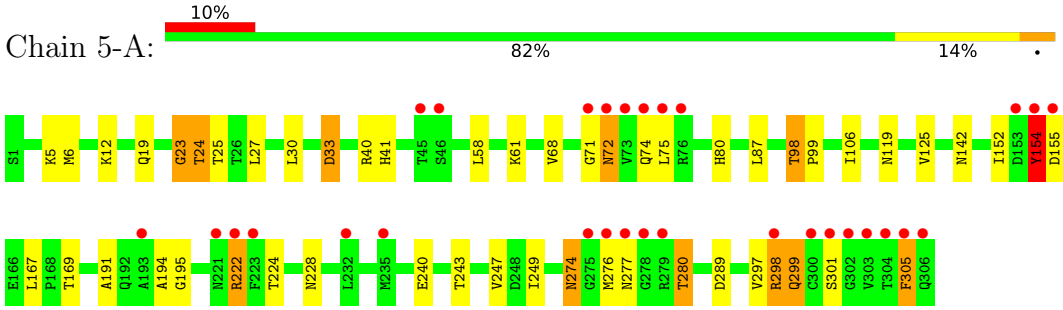
• Molecule 1: 3C-like proteinase

Chain 4-A:

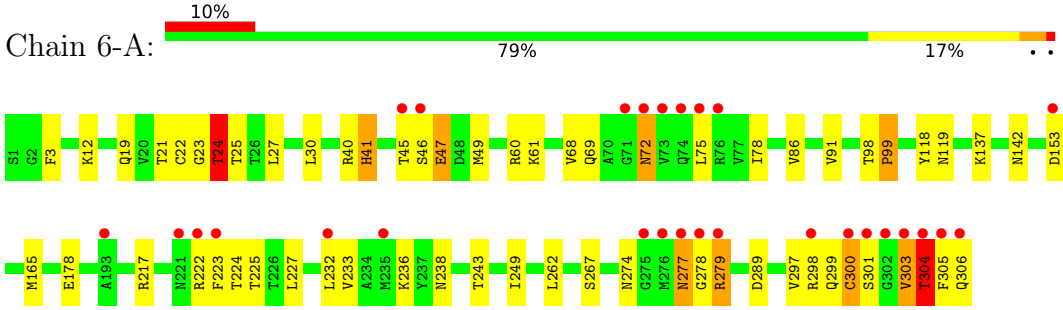




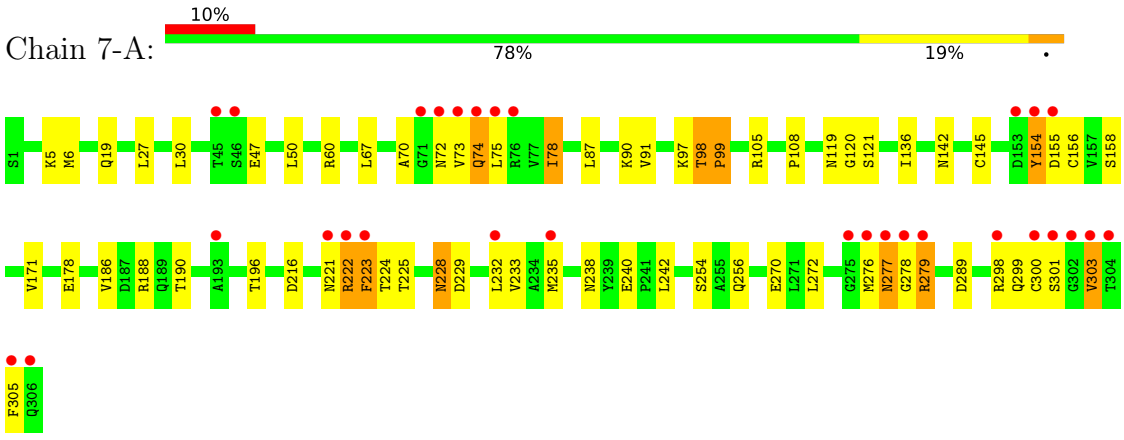
• Molecule 1: 3C-like proteinase



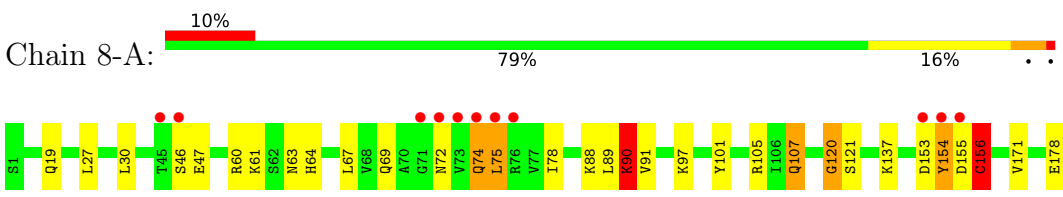
• Molecule 1: 3C-like proteinase



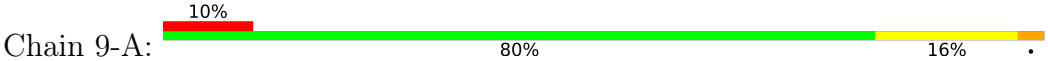
• Molecule 1: 3C-like proteinase

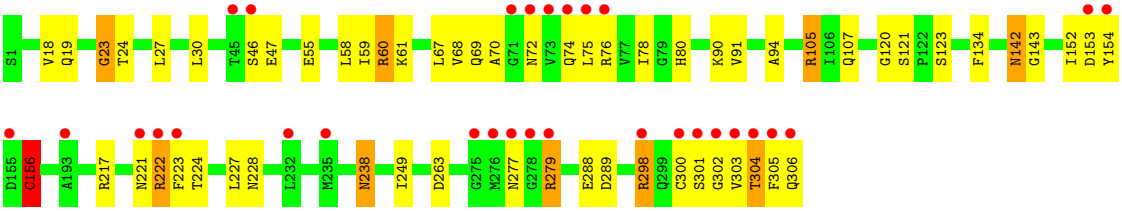


• Molecule 1: 3C-like proteinase

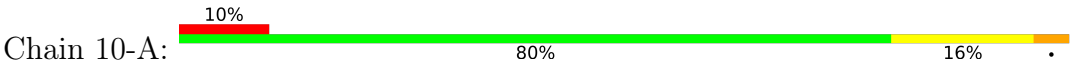


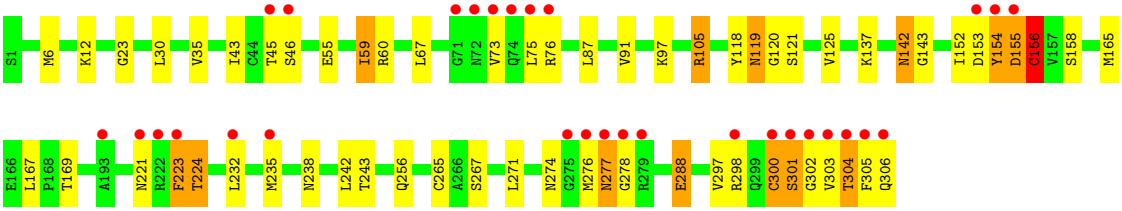
• Molecule 1: 3C-like proteinase



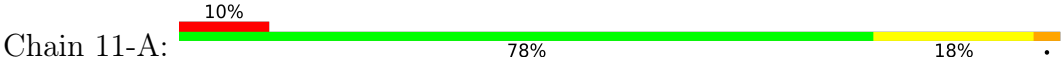


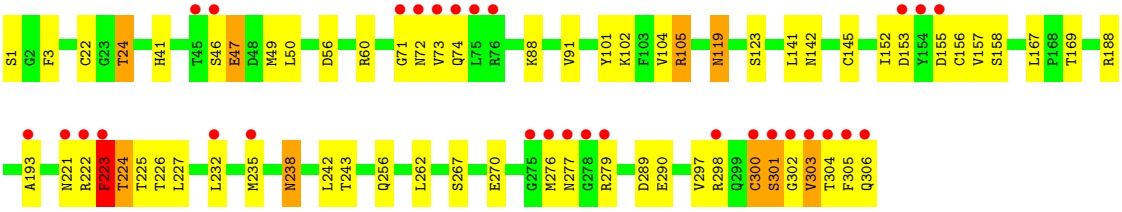
• Molecule 1: 3C-like proteinase



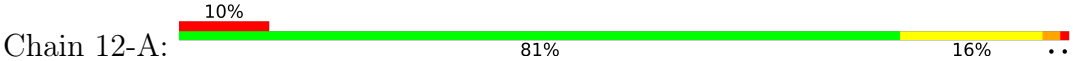


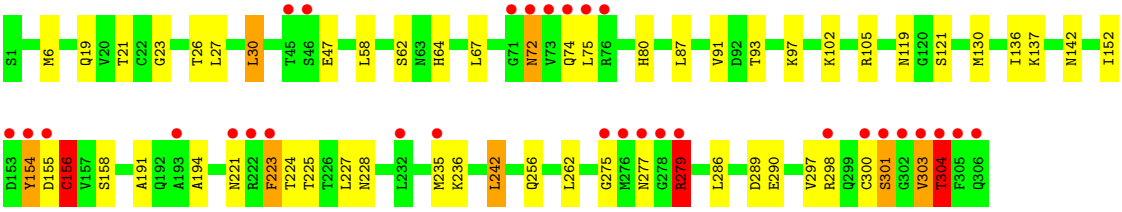
• Molecule 1: 3C-like proteinase



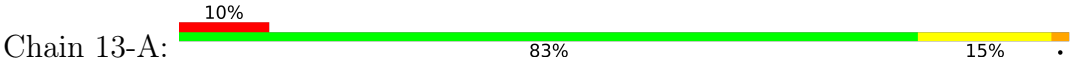


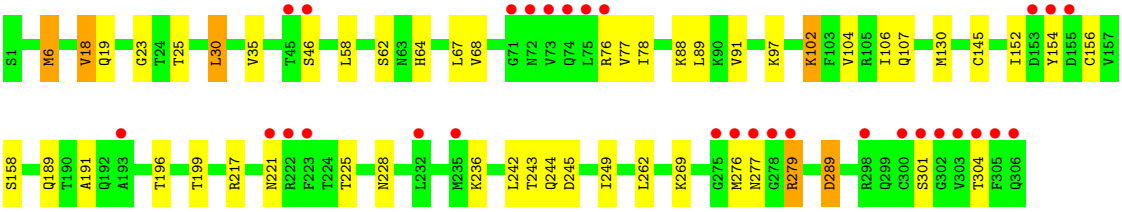
• Molecule 1: 3C-like proteinase



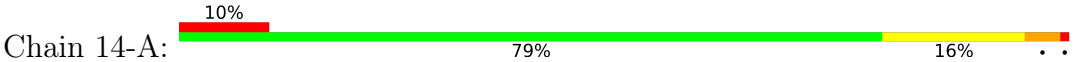


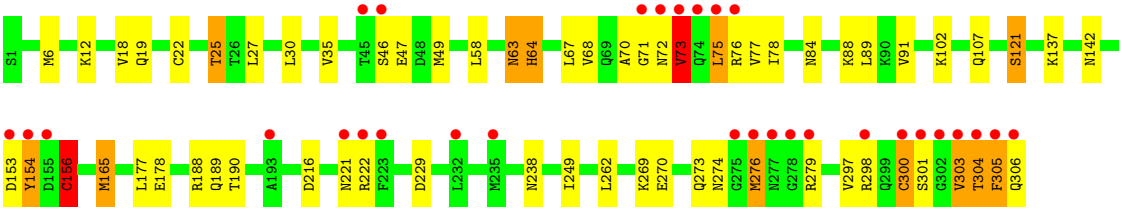
• Molecule 1: 3C-like proteinase



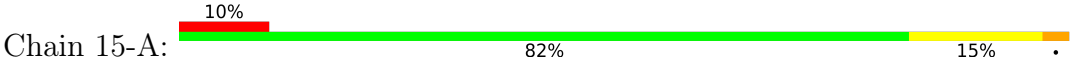


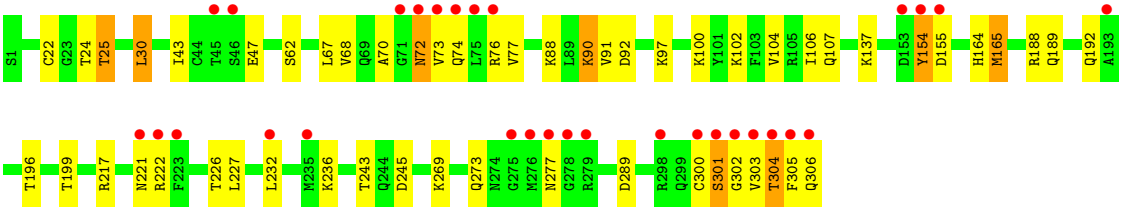
• Molecule 1: 3C-like proteinase



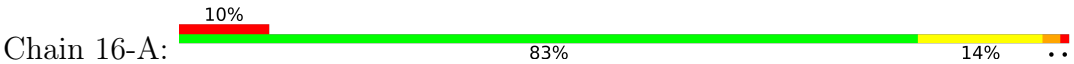


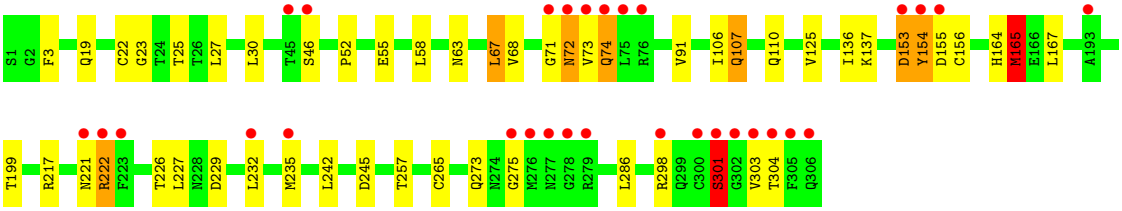
• Molecule 1: 3C-like proteinase



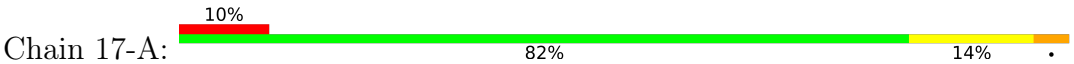


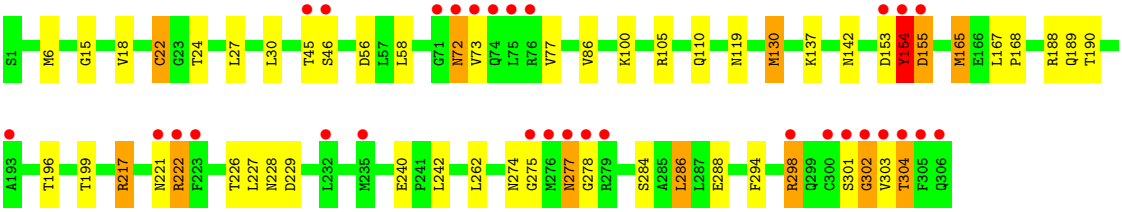
• Molecule 1: 3C-like proteinase





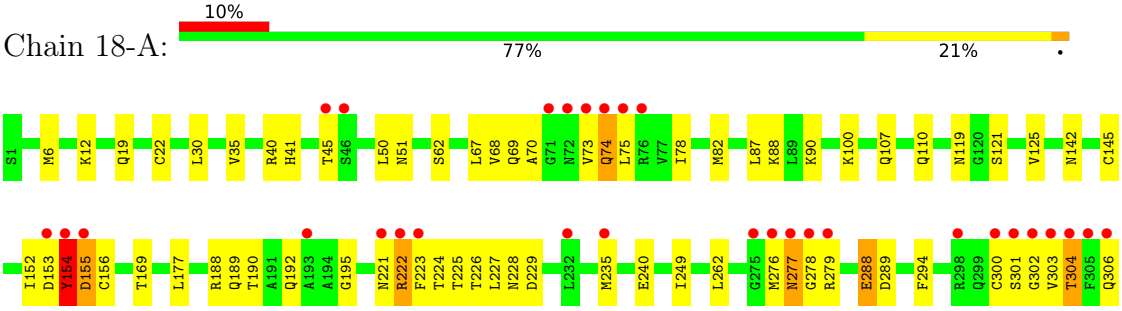
• Molecule 1: 3C-like proteinase





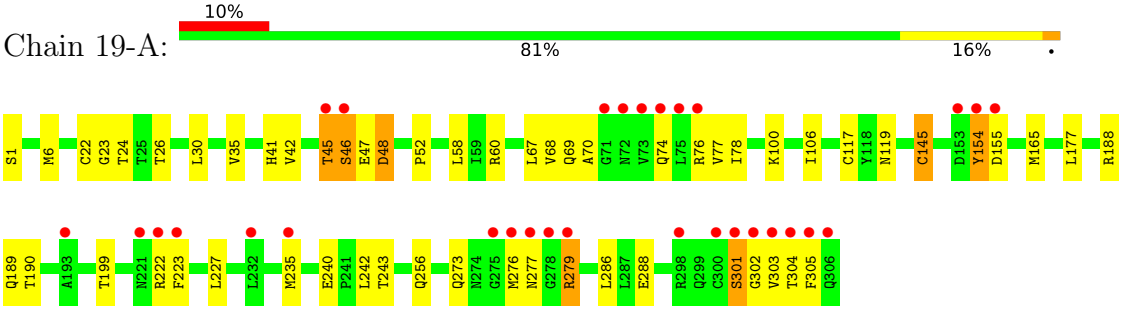
• Molecule 1: 3C-like proteinase

Chain 18-A:



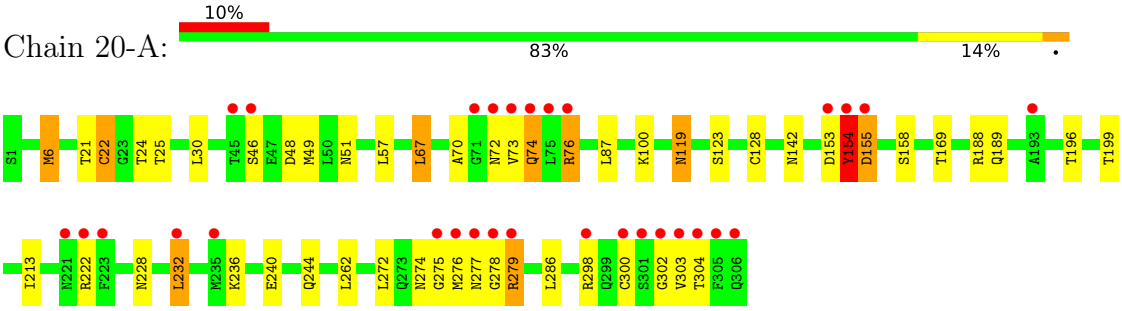
• Molecule 1: 3C-like proteinase

Chain 19-A:



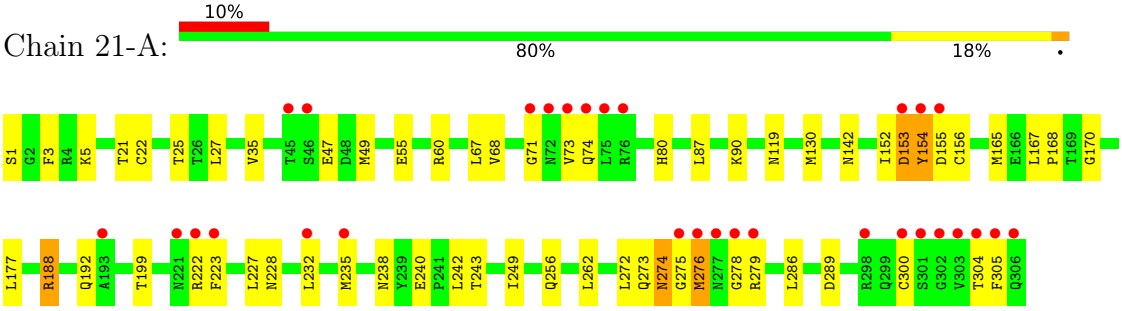
• Molecule 1: 3C-like proteinase

Chain 20-A:



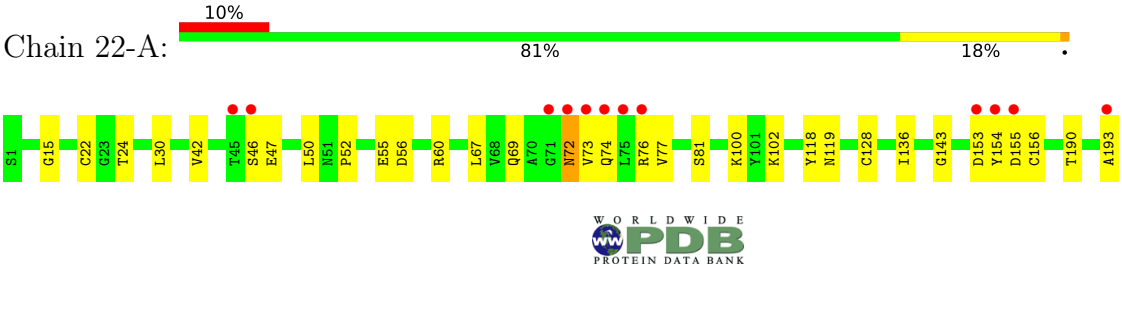
• Molecule 1: 3C-like proteinase

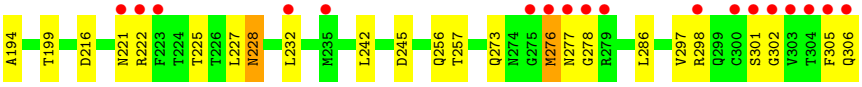
Chain 21-A:



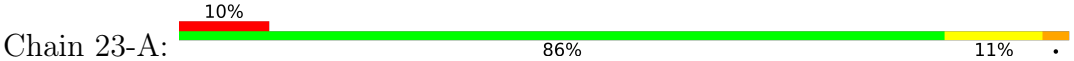
• Molecule 1: 3C-like proteinase

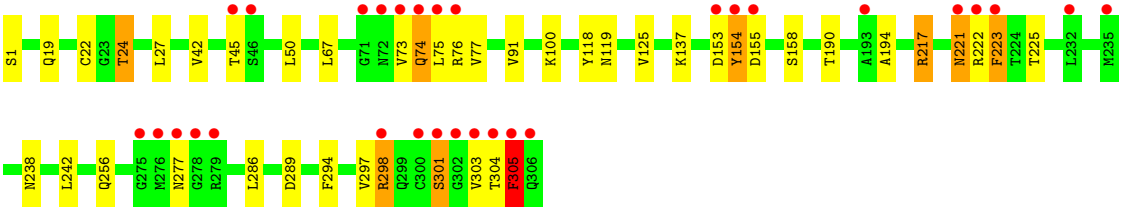
Chain 22-A:



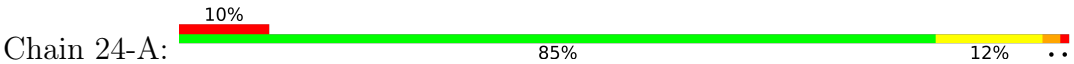


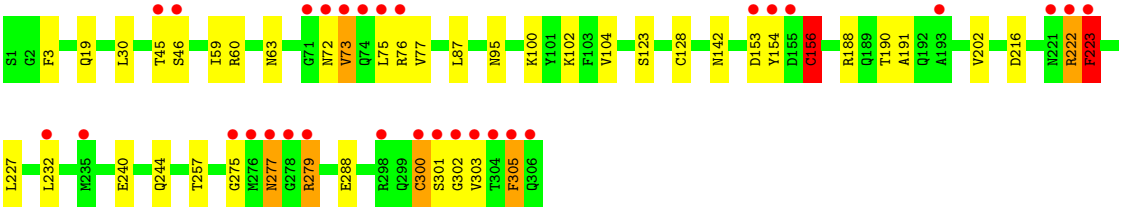
• Molecule 1: 3C-like proteinase



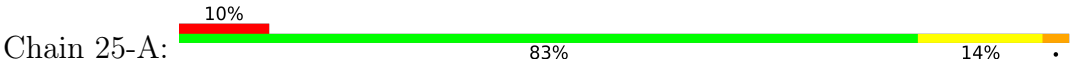


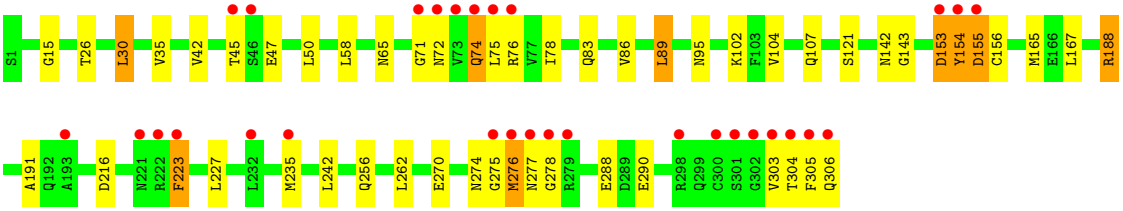
• Molecule 1: 3C-like proteinase



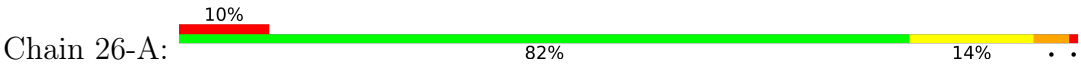


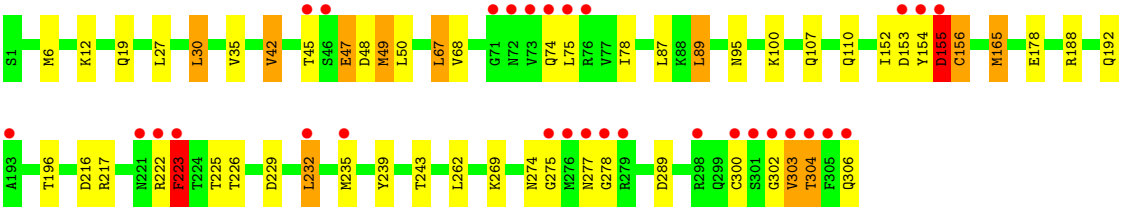
• Molecule 1: 3C-like proteinase



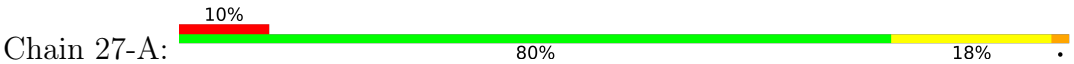


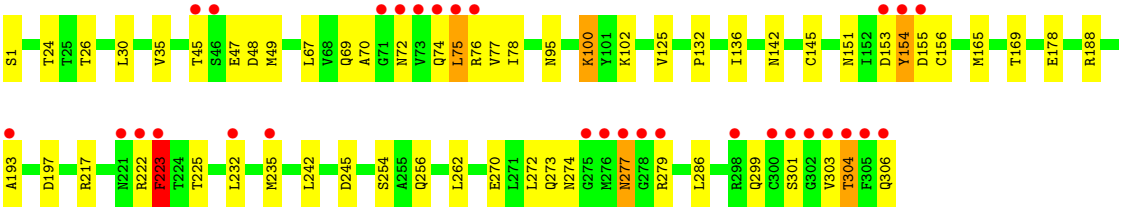
• Molecule 1: 3C-like proteinase



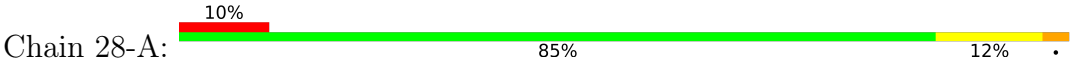


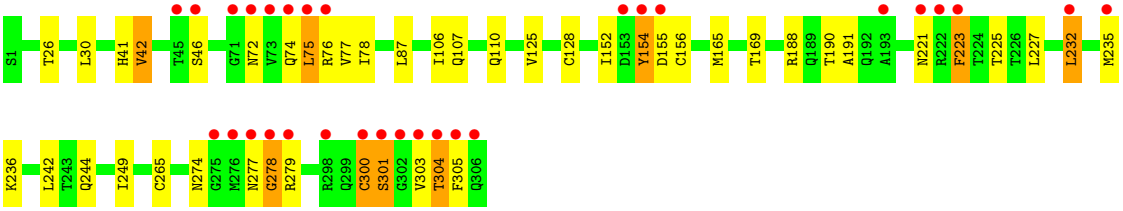
• Molecule 1: 3C-like proteinase



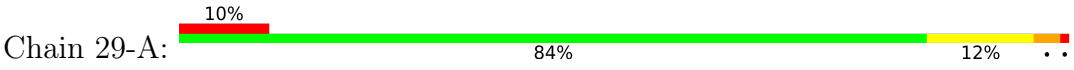


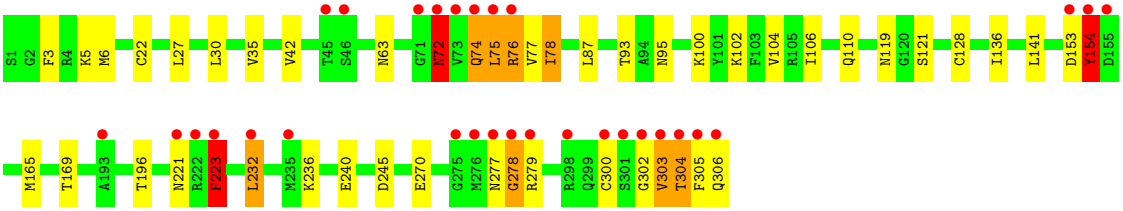
• Molecule 1: 3C-like proteinase



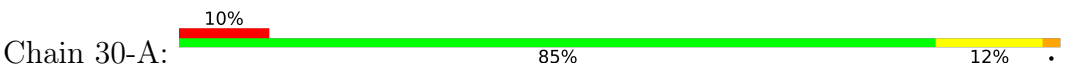


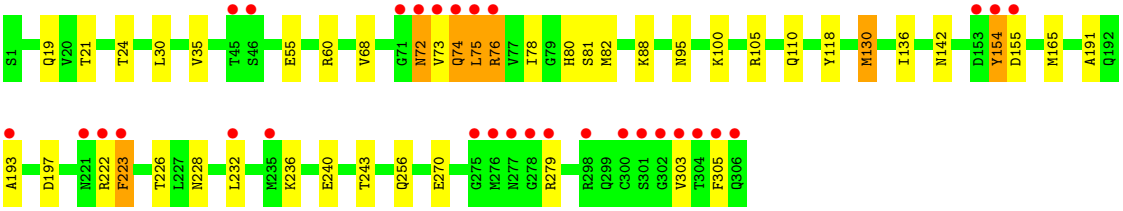
• Molecule 1: 3C-like proteinase



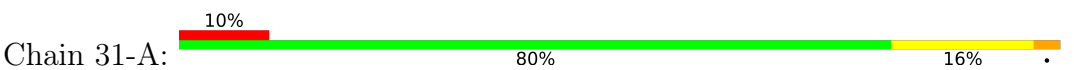


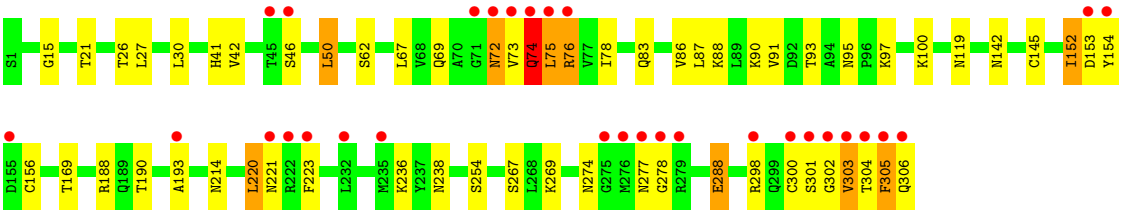
• Molecule 1: 3C-like proteinase





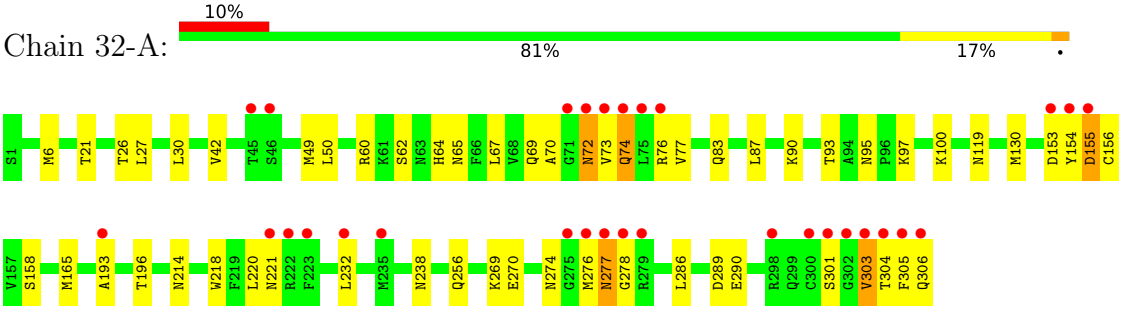
• Molecule 1: 3C-like proteinase





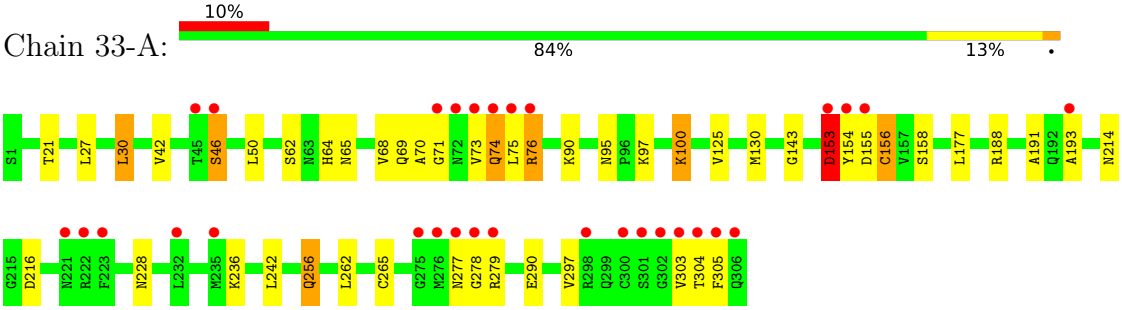
• Molecule 1: 3C-like proteinase

Chain 32-A:



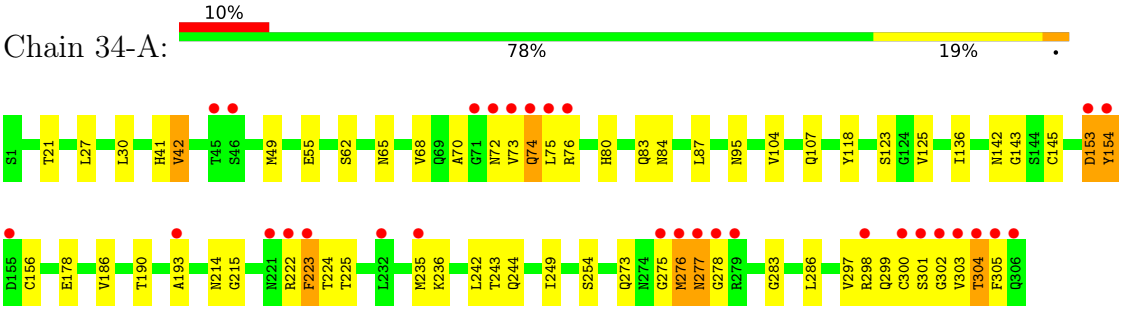
• Molecule 1: 3C-like proteinase

Chain 33-A:



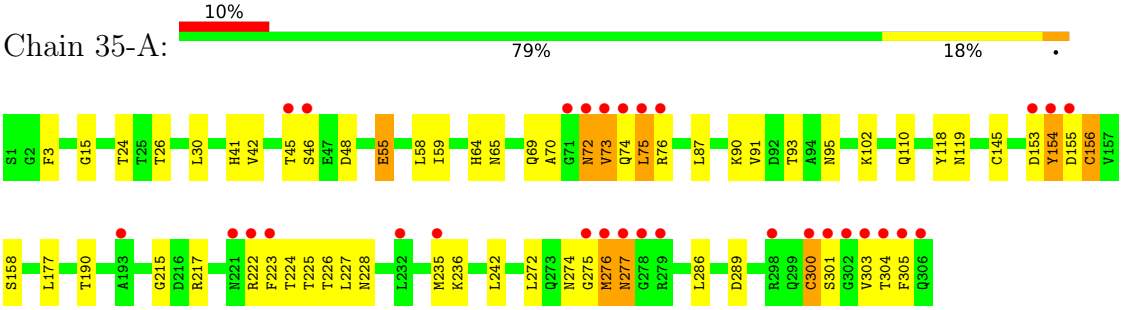
• Molecule 1: 3C-like proteinase

Chain 34-A:



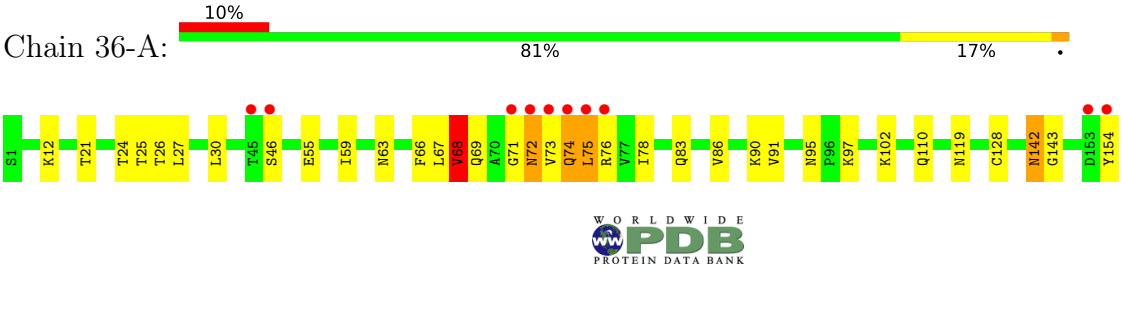
• Molecule 1: 3C-like proteinase

Chain 35-A:

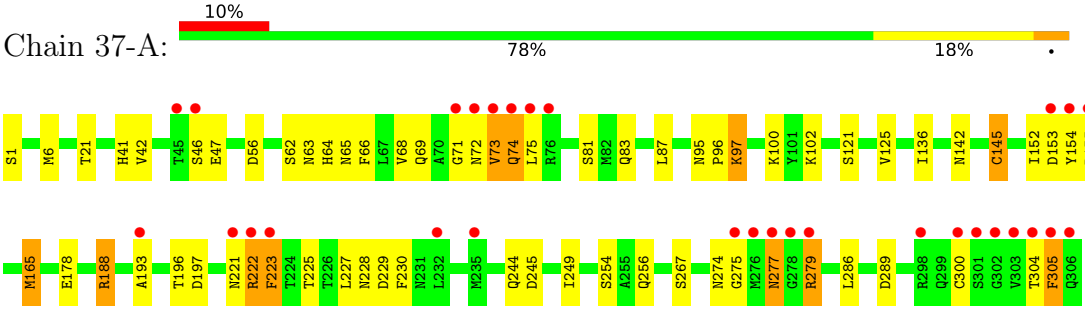


• Molecule 1: 3C-like proteinase

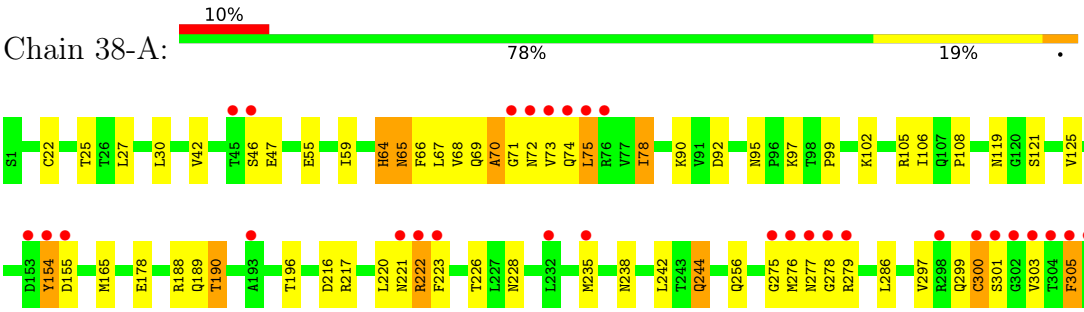
Chain 36-A:



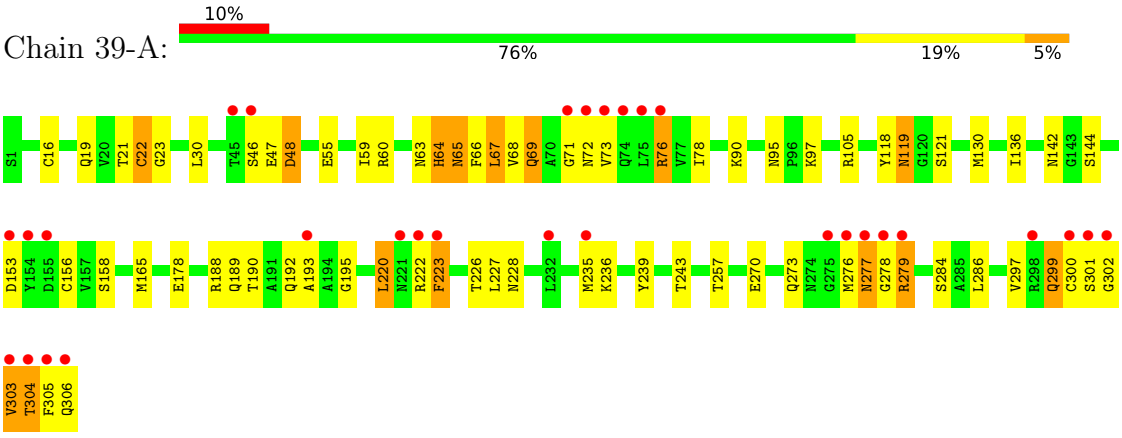
• Molecule 1: 3C-like proteinase



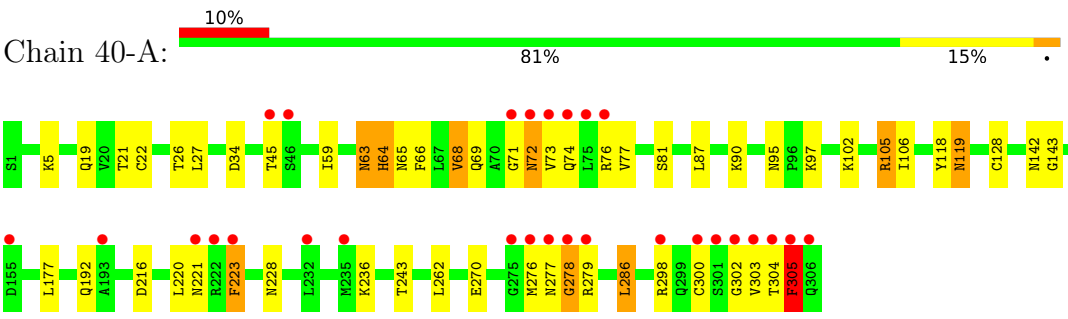
• Molecule 1: 3C-like proteinase



• Molecule 1: 3C-like proteinase

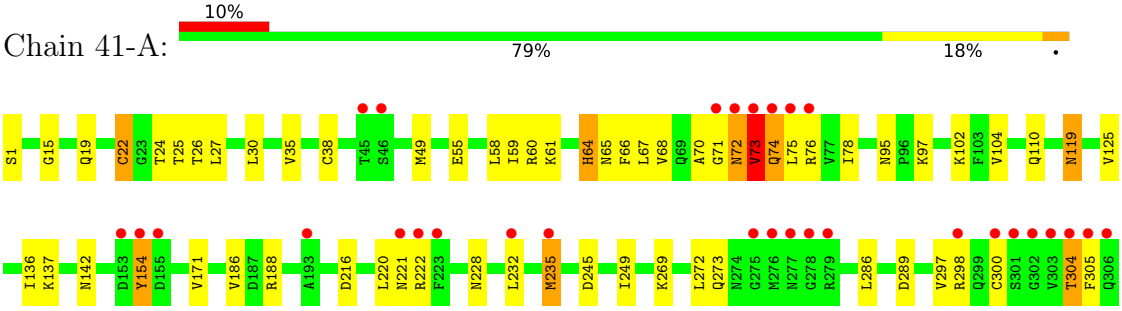


• Molecule 1: 3C-like proteinase



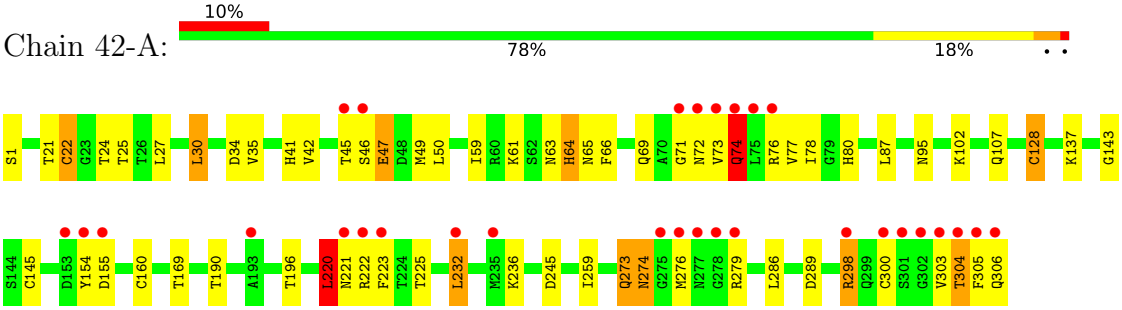
• Molecule 1: 3C-like proteinase

Chain 41-A:



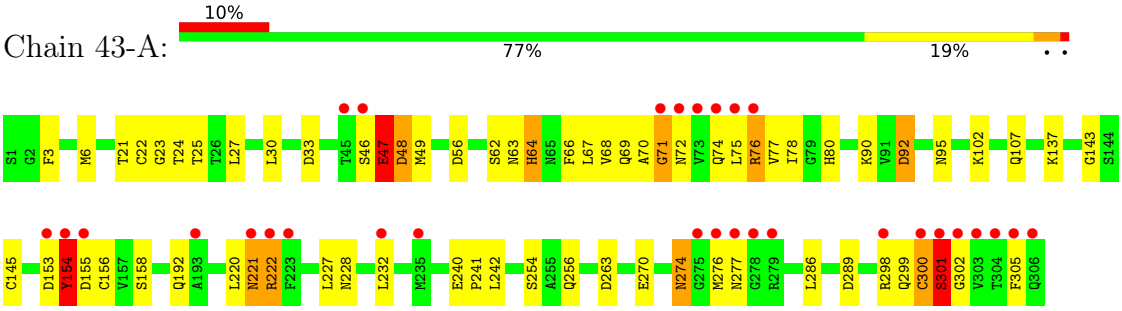
• Molecule 1: 3C-like proteinase

Chain 42-A:



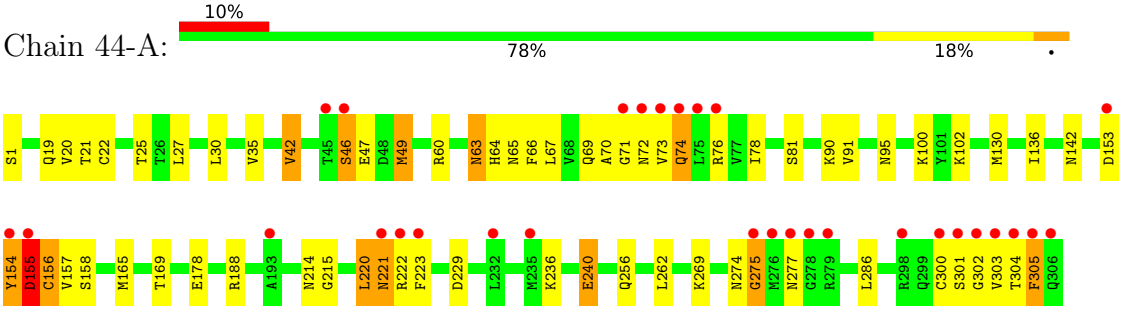
• Molecule 1: 3C-like proteinase

Chain 43-A:



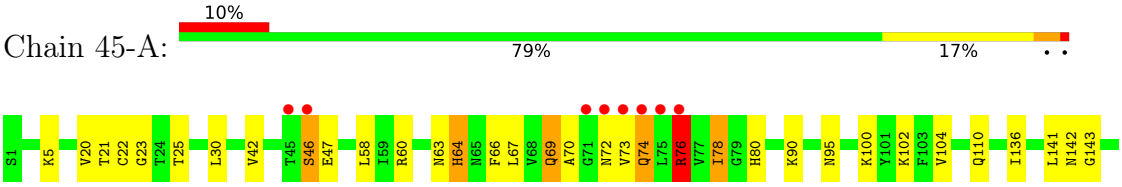
• Molecule 1: 3C-like proteinase

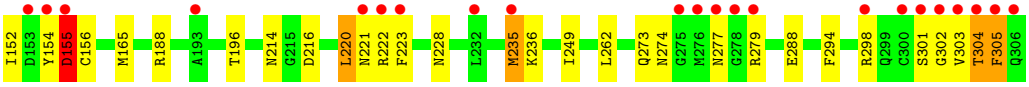
Chain 44-A:



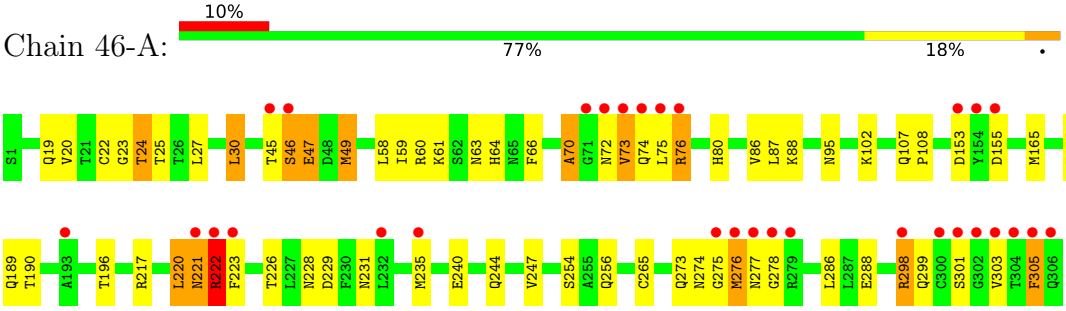
• Molecule 1: 3C-like proteinase

Chain 45-A:

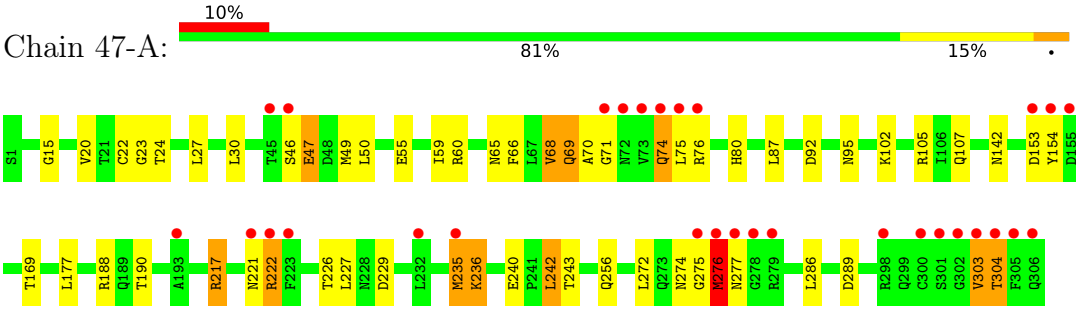




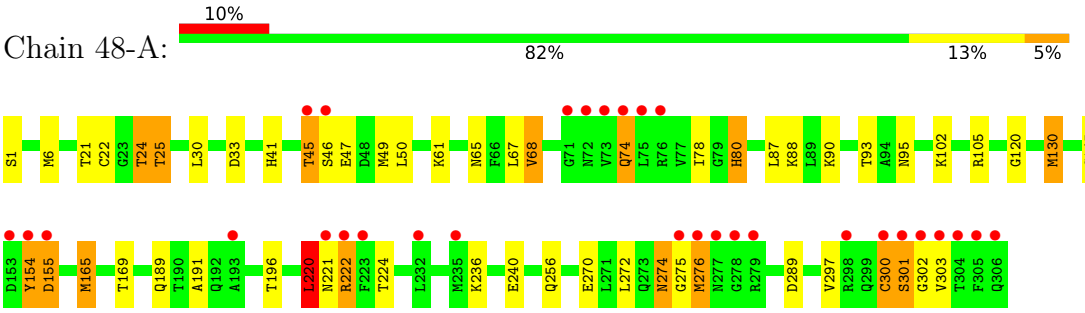
• Molecule 1: 3C-like proteinase



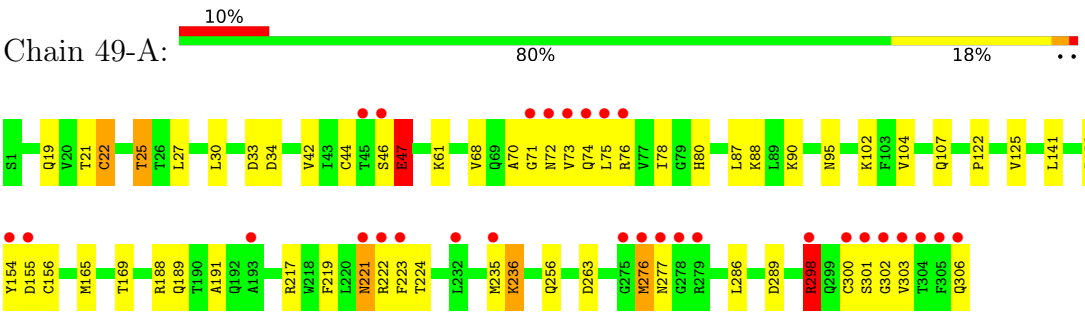
• Molecule 1: 3C-like proteinase



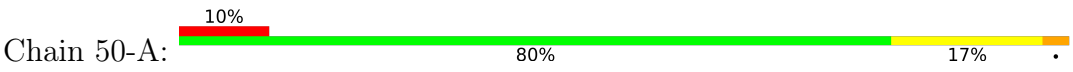
• Molecule 1: 3C-like proteinase

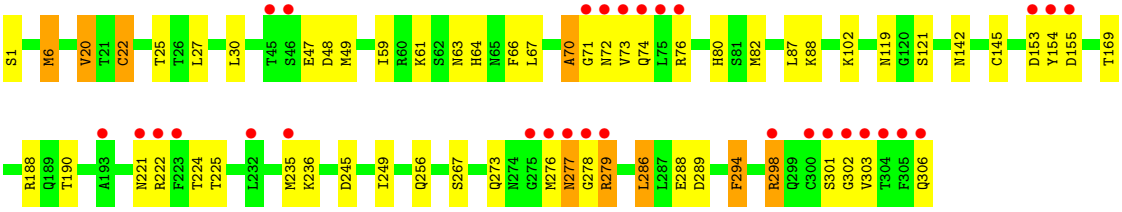


• Molecule 1: 3C-like proteinase

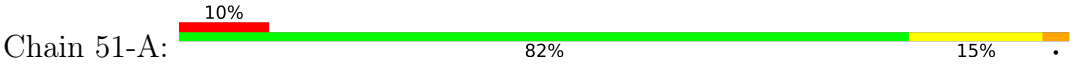


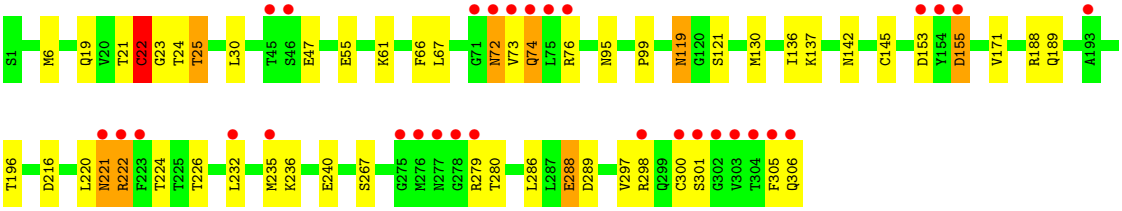
• Molecule 1: 3C-like proteinase



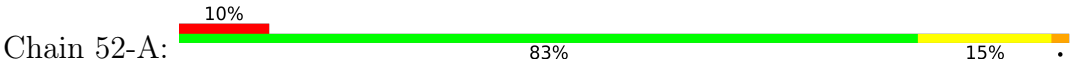


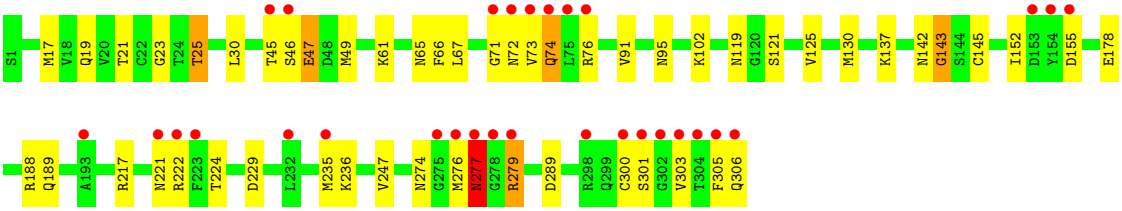
• Molecule 1: 3C-like proteinase



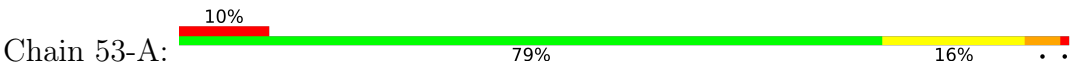


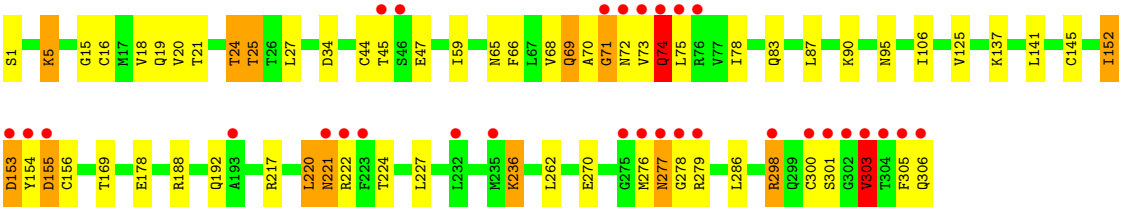
• Molecule 1: 3C-like proteinase



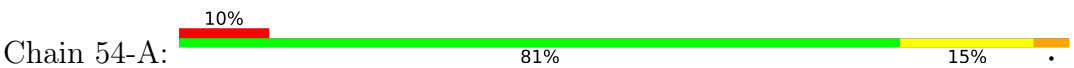


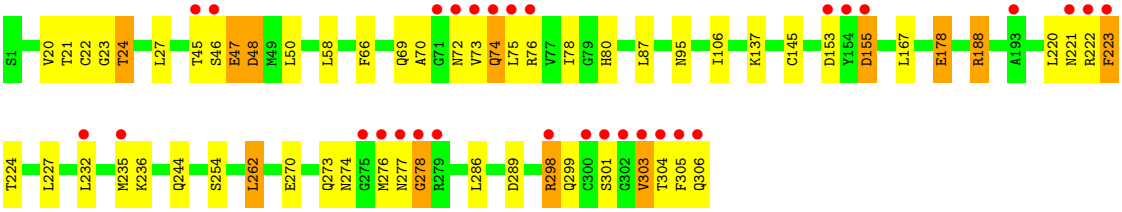
• Molecule 1: 3C-like proteinase





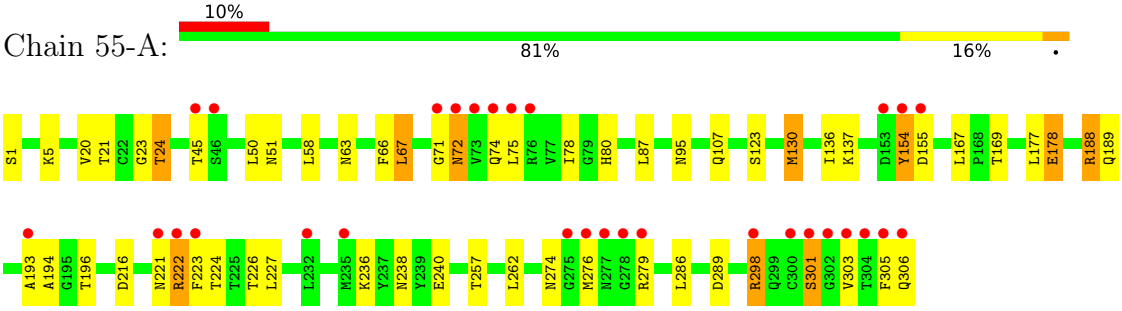
• Molecule 1: 3C-like proteinase





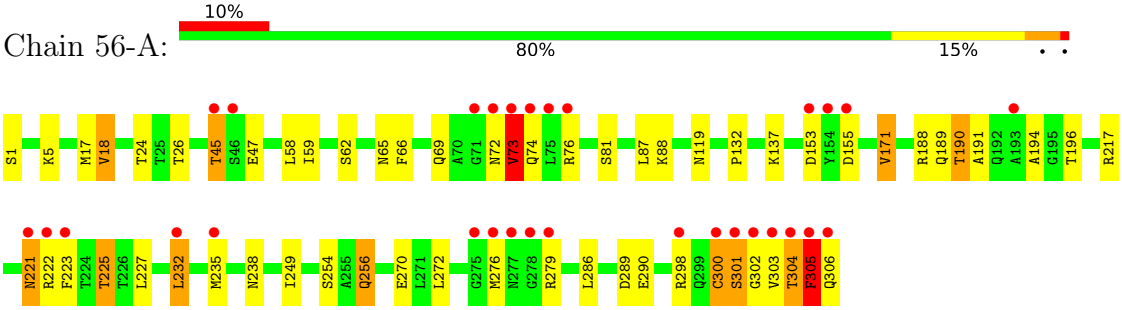
• Molecule 1: 3C-like proteinase

Chain 55-A:



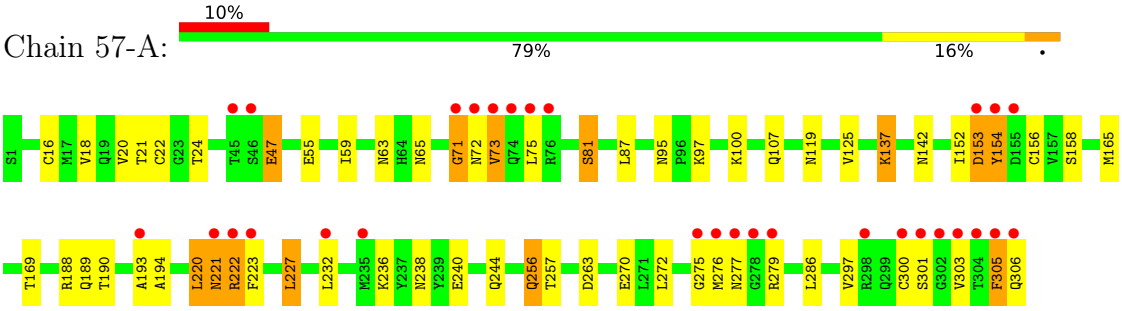
• Molecule 1: 3C-like proteinase

Chain 56-A:



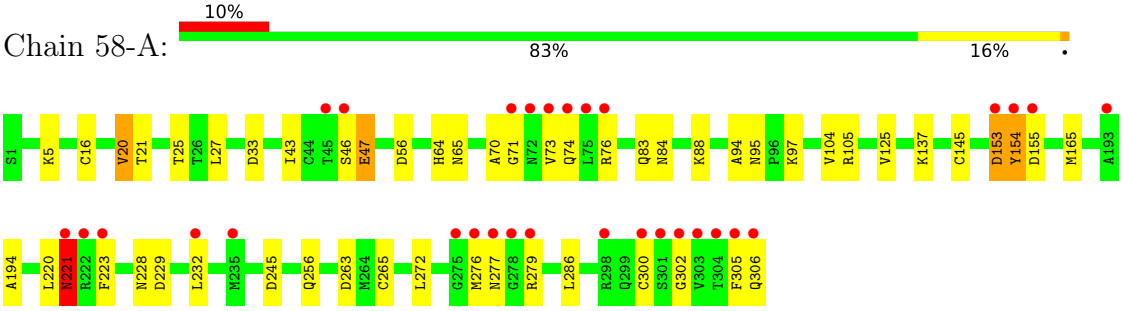
• Molecule 1: 3C-like proteinase

Chain 57-A:



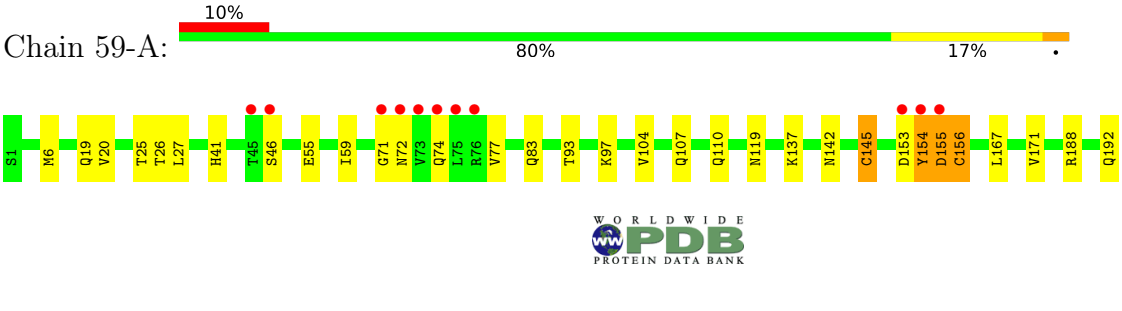
• Molecule 1: 3C-like proteinase

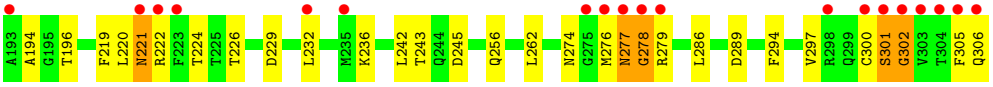
Chain 58-A:



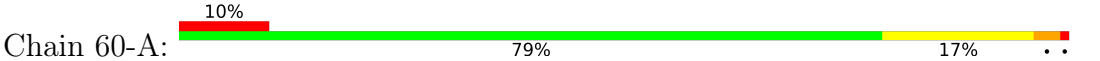
• Molecule 1: 3C-like proteinase

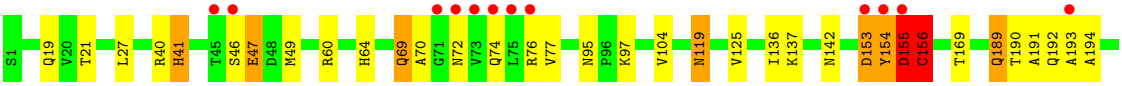
Chain 59-A:

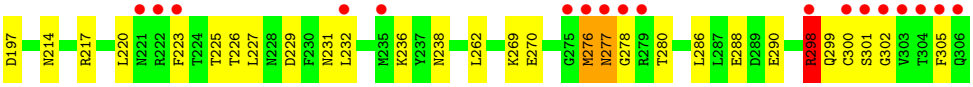




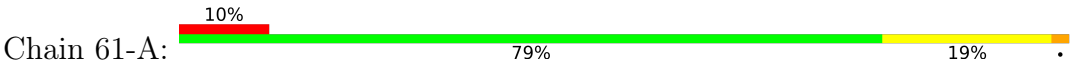
• Molecule 1: 3C-like proteinase

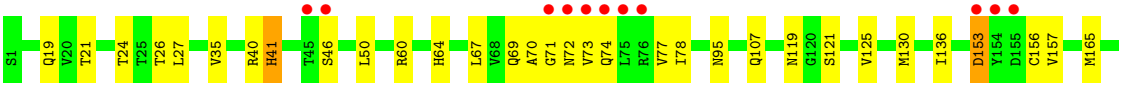


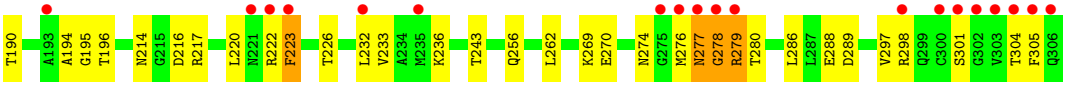




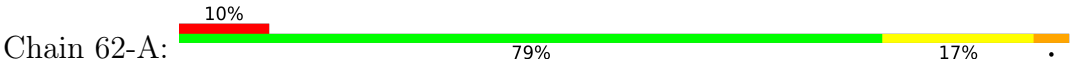
• Molecule 1: 3C-like proteinase

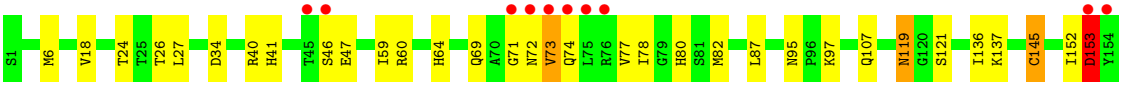




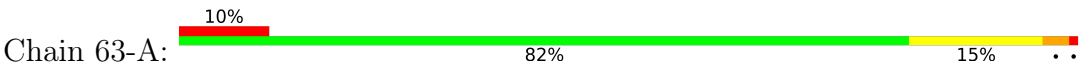


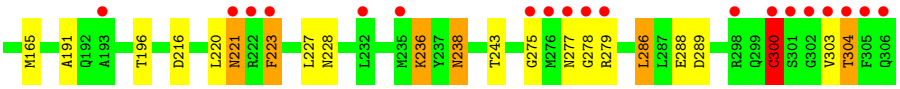
• Molecule 1: 3C-like proteinase



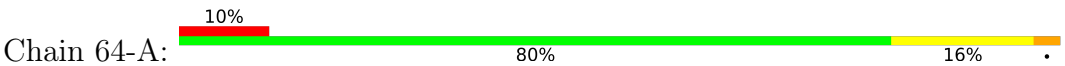


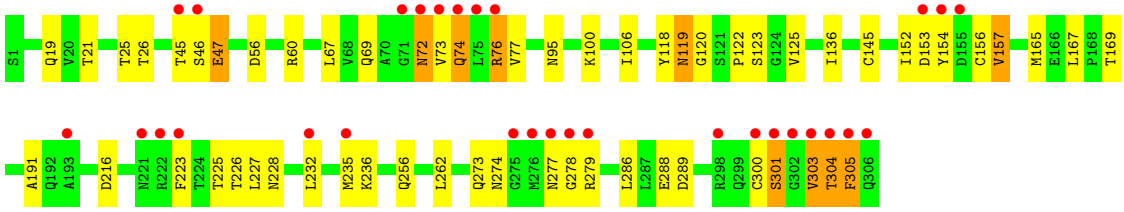
• Molecule 1: 3C-like proteinase





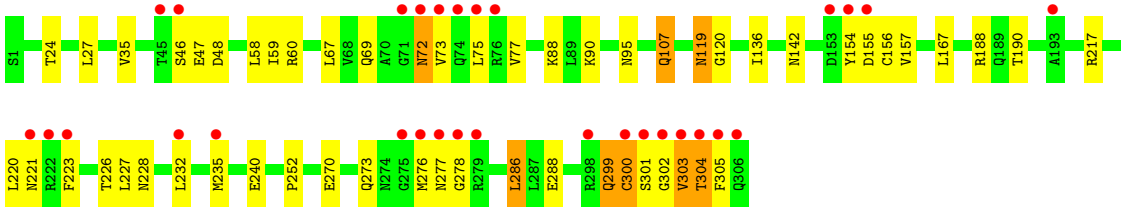
• Molecule 1: 3C-like proteinase





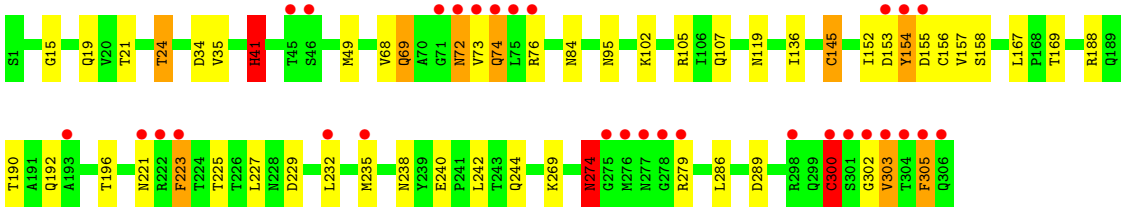
• Molecule 1: 3C-like proteinase

Chain 65-A:



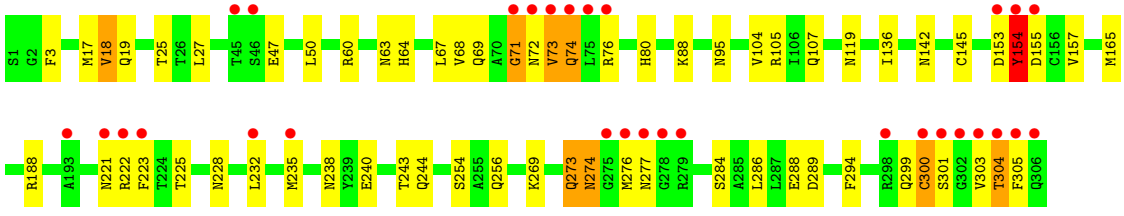
• Molecule 1: 3C-like proteinase

Chain 66-A:



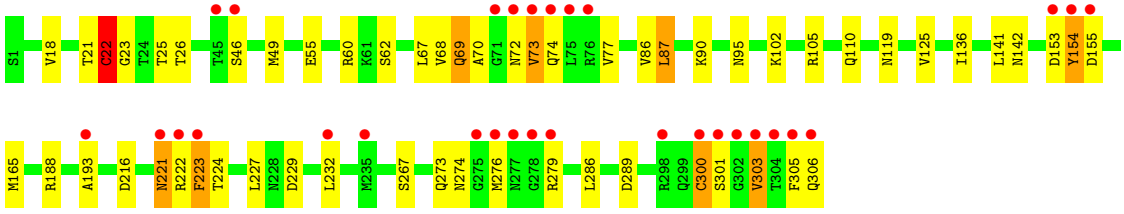
• Molecule 1: 3C-like proteinase

Chain 67-A:



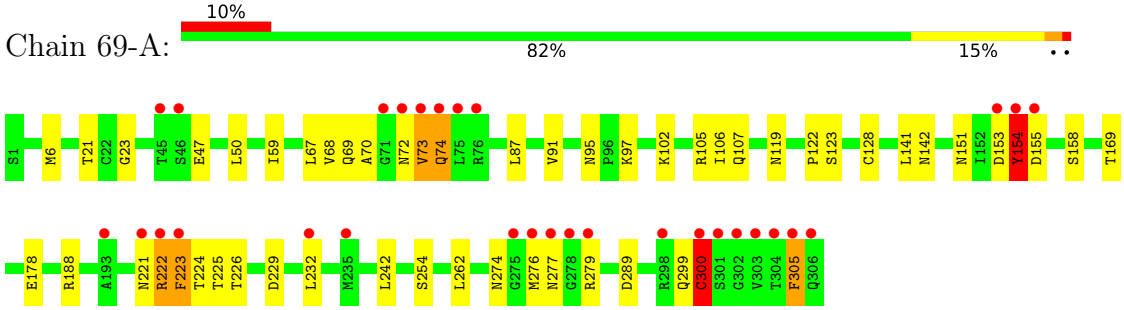
• Molecule 1: 3C-like proteinase

Chain 68-A:



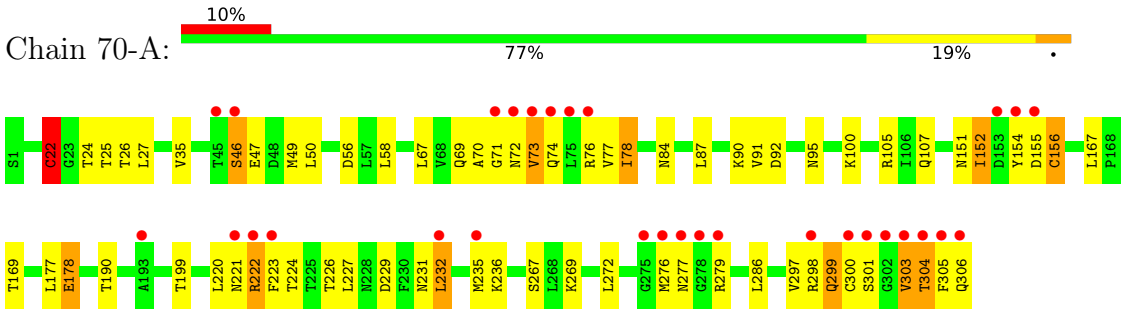
• Molecule 1: 3C-like proteinase

Chain 69-A:



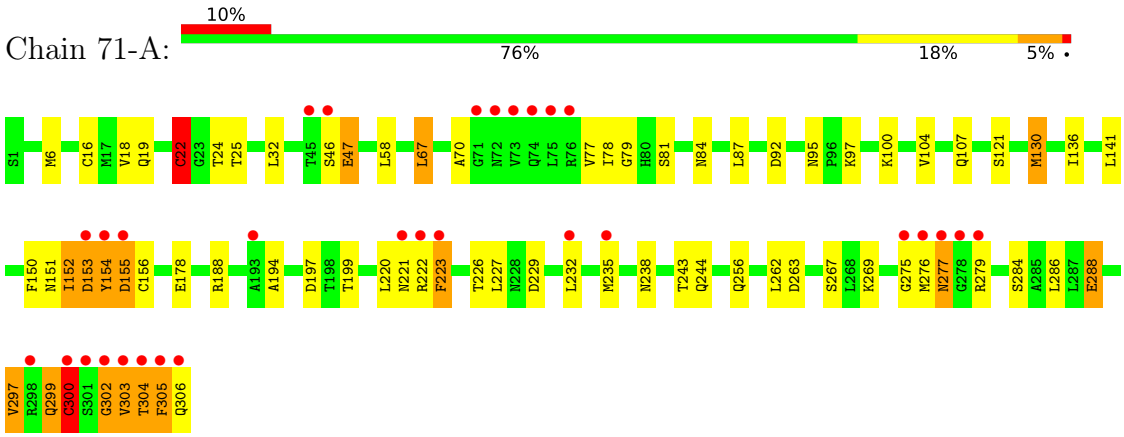
• Molecule 1: 3C-like proteinase

Chain 70-A:



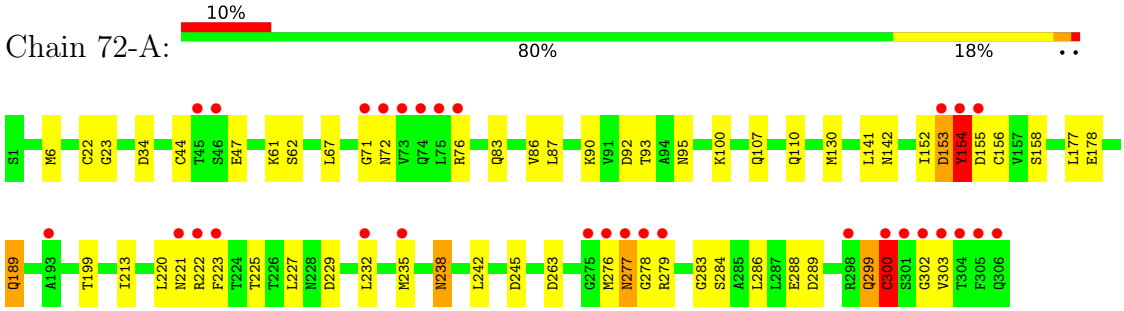
• Molecule 1: 3C-like proteinase

Chain 71-A:



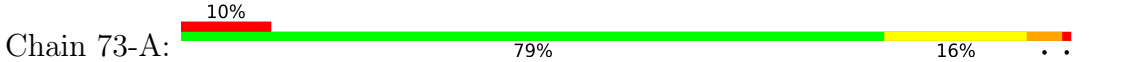
• Molecule 1: 3C-like proteinase

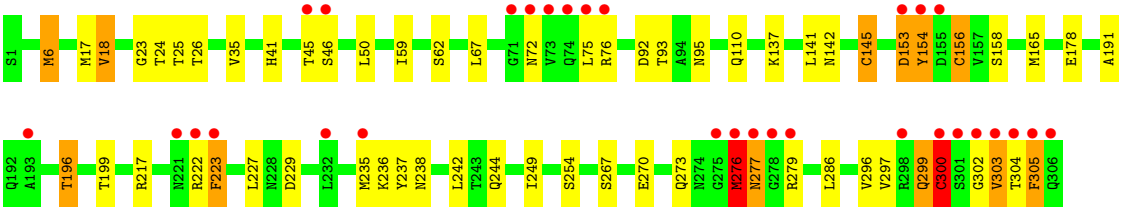
Chain 72-A:



• Molecule 1: 3C-like proteinase

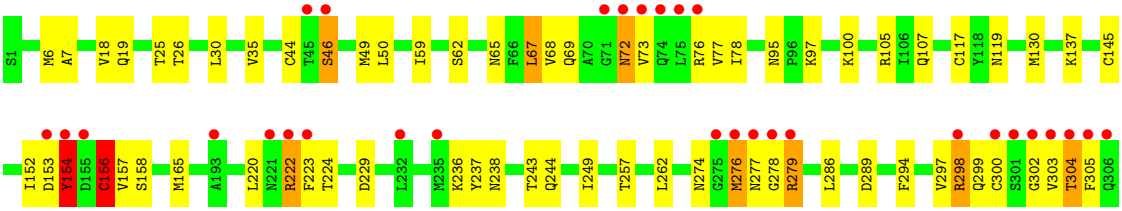
Chain 73-A:





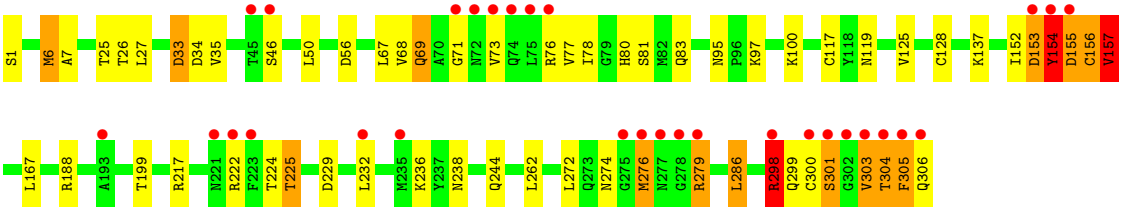
• Molecule 1: 3C-like proteinase

Chain 74-A:



• Molecule 1: 3C-like proteinase

Chain 75-A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.97Å 54.62Å 45.19Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	49.14 – 1.88 56.30 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.14-1.88) 90.6 (56.30-1.88)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.38 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.150 , 0.208 0.177 , 0.237	Depositor DCC
R_{free} test set	1107 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	355880	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.73	1/2420 (0.0%)	0.87	4/3289 (0.1%)
1	2-A	0.71	1/2420 (0.0%)	0.86	3/3289 (0.1%)
1	3-A	0.71	1/2420 (0.0%)	0.87	3/3289 (0.1%)
1	4-A	0.77	3/2420 (0.1%)	0.89	3/3289 (0.1%)
1	5-A	0.70	0/2420	0.87	2/3289 (0.1%)
1	6-A	0.72	2/2420 (0.1%)	0.87	7/3289 (0.2%)
1	7-A	0.73	1/2420 (0.0%)	0.85	2/3289 (0.1%)
1	8-A	0.75	4/2420 (0.2%)	0.89	4/3289 (0.1%)
1	9-A	0.74	2/2420 (0.1%)	0.85	1/3289 (0.0%)
1	10-A	0.73	4/2420 (0.2%)	0.90	4/3289 (0.1%)
1	11-A	0.89	4/2420 (0.2%)	0.83	1/3289 (0.0%)
1	12-A	0.75	3/2420 (0.1%)	0.86	6/3289 (0.2%)
1	13-A	0.73	1/2420 (0.0%)	0.86	3/3289 (0.1%)
1	14-A	0.77	5/2420 (0.2%)	0.87	7/3289 (0.2%)
1	15-A	0.71	2/2420 (0.1%)	0.86	4/3289 (0.1%)
1	16-A	0.73	2/2420 (0.1%)	0.84	2/3289 (0.1%)
1	17-A	0.69	3/2420 (0.1%)	0.86	4/3289 (0.1%)
1	18-A	0.76	4/2420 (0.2%)	0.84	2/3289 (0.1%)
1	19-A	0.85	2/2420 (0.1%)	0.84	2/3289 (0.1%)
1	20-A	0.69	3/2420 (0.1%)	0.86	4/3289 (0.1%)
1	21-A	0.71	2/2420 (0.1%)	0.86	3/3289 (0.1%)
1	22-A	0.71	1/2420 (0.0%)	0.81	0/3289
1	23-A	0.71	1/2420 (0.0%)	0.82	1/3289 (0.0%)
1	24-A	0.73	1/2420 (0.0%)	0.83	1/3289 (0.0%)
1	25-A	0.68	0/2420	0.84	2/3289 (0.1%)
1	26-A	0.71	2/2420 (0.1%)	0.89	7/3289 (0.2%)
1	27-A	0.71	2/2420 (0.1%)	0.84	1/3289 (0.0%)
1	28-A	0.73	4/2420 (0.2%)	0.86	3/3289 (0.1%)
1	29-A	0.76	3/2420 (0.1%)	0.87	2/3289 (0.1%)
1	30-A	0.69	0/2420	0.84	3/3289 (0.1%)
1	31-A	0.72	3/2420 (0.1%)	0.85	2/3289 (0.1%)
1	32-A	0.69	2/2420 (0.1%)	0.83	2/3289 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	33-A	0.71	4/2420 (0.2%)	0.85	3/3289 (0.1%)
1	34-A	0.75	3/2420 (0.1%)	0.87	2/3289 (0.1%)
1	35-A	0.74	4/2420 (0.2%)	0.85	2/3289 (0.1%)
1	36-A	0.68	2/2420 (0.1%)	0.82	1/3289 (0.0%)
1	37-A	0.73	1/2420 (0.0%)	0.87	3/3289 (0.1%)
1	38-A	0.77	5/2420 (0.2%)	0.87	2/3289 (0.1%)
1	39-A	0.74	6/2420 (0.2%)	0.86	2/3289 (0.1%)
1	40-A	0.74	1/2420 (0.0%)	0.85	3/3289 (0.1%)
1	41-A	0.81	2/2420 (0.1%)	0.86	2/3289 (0.1%)
1	42-A	0.76	2/2420 (0.1%)	0.88	7/3289 (0.2%)
1	43-A	0.77	3/2420 (0.1%)	0.88	3/3289 (0.1%)
1	44-A	0.77	5/2420 (0.2%)	0.89	4/3289 (0.1%)
1	45-A	0.73	1/2420 (0.0%)	0.87	3/3289 (0.1%)
1	46-A	0.72	3/2420 (0.1%)	0.90	3/3289 (0.1%)
1	47-A	0.70	0/2420	0.85	2/3289 (0.1%)
1	48-A	0.76	1/2420 (0.0%)	0.87	5/3289 (0.2%)
1	49-A	0.76	3/2420 (0.1%)	0.87	4/3289 (0.1%)
1	50-A	0.75	2/2420 (0.1%)	0.86	4/3289 (0.1%)
1	51-A	0.72	4/2420 (0.2%)	0.84	3/3289 (0.1%)
1	52-A	0.76	2/2420 (0.1%)	0.87	4/3289 (0.1%)
1	53-A	0.75	5/2420 (0.2%)	0.88	3/3289 (0.1%)
1	54-A	0.78	4/2420 (0.2%)	0.91	4/3289 (0.1%)
1	55-A	0.70	0/2420	0.87	3/3289 (0.1%)
1	56-A	0.72	2/2420 (0.1%)	0.85	1/3289 (0.0%)
1	57-A	0.74	4/2420 (0.2%)	0.85	3/3289 (0.1%)
1	58-A	0.74	3/2420 (0.1%)	0.84	1/3289 (0.0%)
1	59-A	0.74	3/2420 (0.1%)	0.86	3/3289 (0.1%)
1	60-A	0.75	4/2420 (0.2%)	0.87	6/3289 (0.2%)
1	61-A	0.73	0/2420	0.86	3/3289 (0.1%)
1	62-A	0.71	1/2420 (0.0%)	0.87	3/3289 (0.1%)
1	63-A	0.73	2/2420 (0.1%)	0.82	3/3289 (0.1%)
1	64-A	0.72	2/2420 (0.1%)	0.87	2/3289 (0.1%)
1	65-A	0.73	2/2420 (0.1%)	0.86	2/3289 (0.1%)
1	66-A	0.77	2/2420 (0.1%)	0.88	4/3289 (0.1%)
1	67-A	0.80	2/2420 (0.1%)	0.86	4/3289 (0.1%)
1	68-A	0.73	2/2420 (0.1%)	0.87	5/3289 (0.2%)
1	69-A	0.73	2/2420 (0.1%)	0.85	3/3289 (0.1%)
1	70-A	0.71	3/2420 (0.1%)	0.84	2/3289 (0.1%)
1	71-A	0.72	4/2420 (0.2%)	0.88	7/3289 (0.2%)
1	72-A	0.71	3/2420 (0.1%)	0.86	3/3289 (0.1%)
1	73-A	0.77	2/2420 (0.1%)	0.89	3/3289 (0.1%)
1	74-A	0.78	5/2420 (0.2%)	0.91	5/3289 (0.2%)
1	75-A	0.72	2/2420 (0.1%)	0.85	1/3289 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.74	182/181500 (0.1%)	0.86	231/246675 (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	4
1	2-A	0	4
1	3-A	0	6
1	4-A	0	11
1	5-A	0	9
1	6-A	0	4
1	7-A	0	4
1	8-A	0	10
1	9-A	0	10
1	10-A	0	8
1	11-A	0	11
1	12-A	0	7
1	13-A	0	5
1	14-A	0	7
1	15-A	0	6
1	16-A	0	6
1	17-A	0	9
1	18-A	0	7
1	19-A	0	4
1	20-A	0	5
1	21-A	0	5
1	22-A	0	6
1	23-A	0	9
1	24-A	0	9
1	25-A	0	7
1	26-A	0	7
1	27-A	0	4
1	28-A	0	4
1	29-A	0	8
1	30-A	0	2
1	31-A	0	7
1	32-A	0	4
1	33-A	0	3
1	34-A	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	35-A	0	7
1	36-A	0	8
1	37-A	0	9
1	38-A	0	7
1	39-A	0	12
1	40-A	0	9
1	41-A	0	6
1	42-A	0	10
1	43-A	0	15
1	44-A	0	10
1	45-A	0	11
1	46-A	0	13
1	47-A	0	10
1	48-A	0	8
1	49-A	0	10
1	50-A	0	7
1	51-A	0	5
1	52-A	0	8
1	53-A	0	10
1	54-A	0	9
1	55-A	0	7
1	56-A	0	14
1	57-A	0	7
1	58-A	0	9
1	59-A	0	7
1	60-A	0	7
1	61-A	0	8
1	62-A	0	9
1	63-A	0	6
1	64-A	0	11
1	65-A	0	3
1	66-A	0	12
1	67-A	0	11
1	68-A	0	5
1	69-A	0	4
1	70-A	0	9
1	71-A	0	10
1	72-A	0	6
1	73-A	0	11
1	74-A	0	11
1	75-A	0	12
All	All	0	584

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	145	CYS	CB-SG	24.01	2.23	1.82
1	19-A	145	CYS	CB-SG	23.08	2.21	1.82
1	67-A	145	CYS	CB-SG	15.91	2.09	1.82
1	41-A	22	CYS	CB-SG	14.06	2.06	1.82
1	48-A	300	CYS	CB-SG	11.55	2.01	1.82

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	11-A	145	CYS	CA-CB-SG	12.00	135.60	114.00
1	5-A	98	THR	C-N-CD	-9.21	100.33	120.60
1	19-A	145	CYS	CA-CB-SG	9.19	130.54	114.00
1	54-A	87	LEU	CA-CB-CG	8.71	135.34	115.30
1	17-A	165	MET	CG-SD-CE	8.68	114.09	100.20

There are no chirality outliers.

5 of 584 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	188	ARG	Sidechain
1	1-A	195	GLY	Peptide
1	1-A	23	GLY	Peptide
1	1-A	278	GLY	Peptide
1	2-A	4	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2367	2313	2313	0	0
1	2-A	2367	2313	2314	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	2313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2314	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	2314	0	0
1	20-A	2367	2313	2313	0	0
1	21-A	2367	2313	2313	0	0
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	2313	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
1	46-A	2367	2313	2313	0	0
1	47-A	2367	2313	2313	0	0
1	48-A	2367	2313	2313	0	0
1	49-A	2367	2313	2313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	50-A	2367	2313	2314	0	0
1	51-A	2367	2313	2313	0	0
1	52-A	2367	2313	2313	0	0
1	53-A	2367	2313	2313	0	0
1	54-A	2367	2313	2313	0	0
1	55-A	2367	2313	2313	0	0
1	56-A	2367	2313	2313	0	0
1	57-A	2367	2313	2313	0	0
1	58-A	2367	2313	2313	0	0
1	59-A	2367	2313	2313	0	0
1	60-A	2367	2313	2313	0	0
1	61-A	2367	2313	2312	0	0
1	62-A	2367	2313	2313	0	0
1	63-A	2367	2313	2313	0	0
1	64-A	2367	2313	2313	0	0
1	65-A	2367	2313	2313	0	0
1	66-A	2367	2313	2313	0	0
1	67-A	2367	2313	2314	0	0
1	68-A	2367	2313	2313	0	0
1	69-A	2367	2313	2313	0	0
1	70-A	2367	2313	2313	0	0
1	71-A	2367	2313	2313	0	0
1	72-A	2367	2313	2313	0	0
1	73-A	2367	2313	2313	0	0
1	74-A	2367	2313	2313	0	0
1	75-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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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
2	46-A	8	12	12	0	0
2	47-A	8	12	12	0	0
2	48-A	8	12	12	0	0
2	49-A	8	12	12	0	0
2	50-A	8	12	12	0	0
2	51-A	8	12	12	0	0
2	52-A	8	12	12	0	0
2	53-A	8	12	12	0	0
2	54-A	8	12	12	0	0
2	55-A	8	12	12	0	0
2	56-A	8	12	12	0	0
2	57-A	8	12	12	0	0
2	58-A	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	59-A	8	12	12	0	0
2	60-A	8	12	12	0	0
2	61-A	8	12	12	0	0
2	62-A	8	12	12	0	0
2	63-A	8	12	12	0	0
2	64-A	8	12	12	0	0
2	65-A	8	12	12	0	0
2	66-A	8	12	12	0	0
2	67-A	8	12	12	0	0
2	68-A	8	12	12	0	0
2	69-A	8	12	12	0	0
2	70-A	8	12	12	0	0
2	71-A	8	12	12	0	0
2	72-A	8	12	12	0	0
2	73-A	8	12	12	0	0
2	74-A	8	12	12	0	0
2	75-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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	46-A	1	0	0	0	0
3	47-A	1	0	0	0	0
3	48-A	1	0	0	0	0
3	49-A	1	0	0	0	0
3	50-A	1	0	0	0	0
3	51-A	1	0	0	0	0
3	52-A	1	0	0	0	0
3	53-A	1	0	0	0	0
3	54-A	1	0	0	0	0
3	55-A	1	0	0	0	0
3	56-A	1	0	0	0	0
3	57-A	1	0	0	0	0
3	58-A	1	0	0	0	0
3	59-A	1	0	0	0	0
3	60-A	1	0	0	0	0
3	61-A	1	0	0	0	0
3	62-A	1	0	0	0	0
3	63-A	1	0	0	0	0
3	64-A	1	0	0	0	0
3	65-A	1	0	0	0	0
3	66-A	1	0	0	0	0
3	67-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	68-A	1	0	0	0	0
3	69-A	1	0	0	0	0
3	70-A	1	0	0	0	0
3	71-A	1	0	0	0	0
3	72-A	1	0	0	0	0
3	73-A	1	0	0	0	0
3	74-A	1	0	0	0	0
3	75-A	1	0	0	0	0
4	1-A	40	0	0	0	0
4	2-A	38	0	0	0	0
4	3-A	50	0	0	0	0
4	4-A	44	0	0	0	0
4	5-A	37	0	0	0	0
4	6-A	41	0	0	0	0
4	7-A	37	0	0	0	0
4	8-A	33	0	0	0	0
4	9-A	38	0	0	0	0
4	10-A	38	0	0	0	0
4	11-A	43	0	0	0	0
4	12-A	48	0	0	0	0
4	13-A	48	0	0	0	0
4	14-A	49	0	0	0	0
4	15-A	47	0	0	0	0
4	16-A	49	0	0	0	0
4	17-A	39	0	0	0	0
4	18-A	43	0	0	0	0
4	19-A	39	0	0	0	0
4	20-A	48	0	0	0	0
4	21-A	45	0	0	0	0
4	22-A	49	0	0	0	0
4	23-A	44	0	0	0	0
4	24-A	51	0	0	0	0
4	25-A	52	0	0	0	0
4	26-A	48	0	0	0	0
4	27-A	43	0	0	0	0
4	28-A	41	0	0	0	0
4	29-A	43	0	0	0	0
4	30-A	43	0	0	0	0
4	31-A	44	0	0	0	0
4	32-A	46	0	0	0	0
4	33-A	47	0	0	0	0
4	34-A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	35-A	41	0	0	0	0
4	36-A	41	0	0	0	0
4	37-A	43	0	0	0	0
4	38-A	44	0	0	0	0
4	39-A	45	0	0	0	0
4	40-A	41	0	0	0	0
4	41-A	43	0	0	0	0
4	42-A	39	0	0	0	0
4	43-A	49	0	0	0	0
4	44-A	47	0	0	0	0
4	45-A	51	0	0	0	0
4	46-A	54	0	0	0	0
4	47-A	47	0	0	0	0
4	48-A	44	0	0	0	0
4	49-A	39	0	0	0	0
4	50-A	46	0	0	0	0
4	51-A	41	0	0	0	0
4	52-A	43	0	0	0	0
4	53-A	42	0	0	0	0
4	54-A	56	0	0	0	0
4	55-A	52	0	0	0	0
4	56-A	46	0	0	0	0
4	57-A	46	0	0	0	0
4	58-A	39	0	0	0	0
4	59-A	39	0	0	0	0
4	60-A	37	0	0	0	0
4	61-A	41	0	0	0	0
4	62-A	44	0	0	0	0
4	63-A	40	0	0	0	0
4	64-A	43	0	0	0	0
4	65-A	37	0	0	0	0
4	66-A	44	0	0	0	0
4	67-A	44	0	0	0	0
4	68-A	42	0	0	0	0
4	69-A	44	0	0	0	0
4	70-A	45	0	0	0	0
4	71-A	50	0	0	0	0
4	72-A	50	0	0	0	0
4	73-A	50	0	0	0	0
4	74-A	48	0	0	0	0
4	75-A	44	0	0	0	0
All	All	181505	174375	174378	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%)	261 (86%)	23 (8%)	20 (7%)	1	0
1	2-A	304/306 (99%)	268 (88%)	18 (6%)	18 (6%)	1	0
1	3-A	304/306 (99%)	260 (86%)	24 (8%)	20 (7%)	1	0
1	4-A	304/306 (99%)	260 (86%)	27 (9%)	17 (6%)	2	0
1	5-A	304/306 (99%)	260 (86%)	27 (9%)	17 (6%)	2	0
1	6-A	304/306 (99%)	258 (85%)	24 (8%)	22 (7%)	1	0
1	7-A	304/306 (99%)	258 (85%)	25 (8%)	21 (7%)	1	0
1	8-A	304/306 (99%)	261 (86%)	28 (9%)	15 (5%)	2	0
1	9-A	304/306 (99%)	257 (84%)	31 (10%)	16 (5%)	2	0
1	10-A	304/306 (99%)	262 (86%)	24 (8%)	18 (6%)	1	0
1	11-A	304/306 (99%)	258 (85%)	32 (10%)	14 (5%)	2	0
1	12-A	304/306 (99%)	263 (86%)	26 (9%)	15 (5%)	2	0
1	13-A	304/306 (99%)	264 (87%)	26 (9%)	14 (5%)	2	0
1	14-A	304/306 (99%)	266 (88%)	20 (7%)	18 (6%)	1	0
1	15-A	304/306 (99%)	263 (86%)	29 (10%)	12 (4%)	3	0
1	16-A	304/306 (99%)	271 (89%)	20 (7%)	13 (4%)	2	0
1	17-A	304/306 (99%)	265 (87%)	25 (8%)	14 (5%)	2	0
1	18-A	304/306 (99%)	261 (86%)	34 (11%)	9 (3%)	4	0
1	19-A	304/306 (99%)	266 (88%)	27 (9%)	11 (4%)	3	0
1	20-A	304/306 (99%)	266 (88%)	25 (8%)	13 (4%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	21-A	304/306 (99%)	267 (88%)	23 (8%)	14 (5%)	2	0
1	22-A	304/306 (99%)	269 (88%)	19 (6%)	16 (5%)	2	0
1	23-A	304/306 (99%)	261 (86%)	30 (10%)	13 (4%)	2	0
1	24-A	304/306 (99%)	259 (85%)	32 (10%)	13 (4%)	2	0
1	25-A	304/306 (99%)	267 (88%)	22 (7%)	15 (5%)	2	0
1	26-A	304/306 (99%)	264 (87%)	26 (9%)	14 (5%)	2	0
1	27-A	304/306 (99%)	266 (88%)	27 (9%)	11 (4%)	3	0
1	28-A	304/306 (99%)	267 (88%)	27 (9%)	10 (3%)	4	0
1	29-A	304/306 (99%)	265 (87%)	27 (9%)	12 (4%)	3	0
1	30-A	304/306 (99%)	269 (88%)	25 (8%)	10 (3%)	4	0
1	31-A	304/306 (99%)	268 (88%)	18 (6%)	18 (6%)	1	0
1	32-A	304/306 (99%)	274 (90%)	19 (6%)	11 (4%)	3	0
1	33-A	304/306 (99%)	263 (86%)	24 (8%)	17 (6%)	2	0
1	34-A	304/306 (99%)	270 (89%)	16 (5%)	18 (6%)	1	0
1	35-A	304/306 (99%)	253 (83%)	34 (11%)	17 (6%)	2	0
1	36-A	304/306 (99%)	258 (85%)	26 (9%)	20 (7%)	1	0
1	37-A	304/306 (99%)	262 (86%)	24 (8%)	18 (6%)	1	0
1	38-A	304/306 (99%)	264 (87%)	20 (7%)	20 (7%)	1	0
1	39-A	304/306 (99%)	251 (83%)	33 (11%)	20 (7%)	1	0
1	40-A	304/306 (99%)	260 (86%)	28 (9%)	16 (5%)	2	0
1	41-A	304/306 (99%)	256 (84%)	31 (10%)	17 (6%)	2	0
1	42-A	304/306 (99%)	248 (82%)	41 (14%)	15 (5%)	2	0
1	43-A	304/306 (99%)	255 (84%)	32 (10%)	17 (6%)	2	0
1	44-A	304/306 (99%)	256 (84%)	24 (8%)	24 (8%)	1	0
1	45-A	304/306 (99%)	256 (84%)	27 (9%)	21 (7%)	1	0
1	46-A	304/306 (99%)	257 (84%)	25 (8%)	22 (7%)	1	0
1	47-A	304/306 (99%)	252 (83%)	31 (10%)	21 (7%)	1	0
1	48-A	304/306 (99%)	256 (84%)	31 (10%)	17 (6%)	2	0
1	49-A	304/306 (99%)	261 (86%)	29 (10%)	14 (5%)	2	0
1	50-A	304/306 (99%)	268 (88%)	21 (7%)	15 (5%)	2	0
1	51-A	304/306 (99%)	263 (86%)	25 (8%)	16 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	52-A	304/306 (99%)	260 (86%)	31 (10%)	13 (4%)	2	0
1	53-A	304/306 (99%)	261 (86%)	23 (8%)	20 (7%)	1	0
1	54-A	304/306 (99%)	263 (86%)	23 (8%)	18 (6%)	1	0
1	55-A	304/306 (99%)	271 (89%)	25 (8%)	8 (3%)	5	1
1	56-A	304/306 (99%)	264 (87%)	24 (8%)	16 (5%)	2	0
1	57-A	304/306 (99%)	260 (86%)	30 (10%)	14 (5%)	2	0
1	58-A	304/306 (99%)	266 (88%)	25 (8%)	13 (4%)	2	0
1	59-A	304/306 (99%)	264 (87%)	26 (9%)	14 (5%)	2	0
1	60-A	304/306 (99%)	265 (87%)	18 (6%)	21 (7%)	1	0
1	61-A	304/306 (99%)	266 (88%)	25 (8%)	13 (4%)	2	0
1	62-A	304/306 (99%)	264 (87%)	26 (9%)	14 (5%)	2	0
1	63-A	304/306 (99%)	261 (86%)	25 (8%)	18 (6%)	1	0
1	64-A	304/306 (99%)	262 (86%)	28 (9%)	14 (5%)	2	0
1	65-A	304/306 (99%)	264 (87%)	26 (9%)	14 (5%)	2	0
1	66-A	304/306 (99%)	259 (85%)	31 (10%)	14 (5%)	2	0
1	67-A	304/306 (99%)	262 (86%)	28 (9%)	14 (5%)	2	0
1	68-A	304/306 (99%)	267 (88%)	20 (7%)	17 (6%)	2	0
1	69-A	304/306 (99%)	270 (89%)	19 (6%)	15 (5%)	2	0
1	70-A	304/306 (99%)	258 (85%)	27 (9%)	19 (6%)	1	0
1	71-A	304/306 (99%)	259 (85%)	25 (8%)	20 (7%)	1	0
1	72-A	304/306 (99%)	257 (84%)	31 (10%)	16 (5%)	2	0
1	73-A	304/306 (99%)	255 (84%)	30 (10%)	19 (6%)	1	0
1	74-A	304/306 (99%)	263 (86%)	21 (7%)	20 (7%)	1	0
1	75-A	304/306 (99%)	254 (84%)	30 (10%)	20 (7%)	1	0
All	All	22800/22950 (99%)	19648 (86%)	1949 (8%)	1203 (5%)	2	0

5 of 1203 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	24	THR
1	1-A	72	ASN
1	1-A	74	GLN
1	1-A	97	LYS
1	1-A	154	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	2-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	3-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	4-A	263/263 (100%)	229 (87%)	34 (13%)	4	1
1	5-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	6-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	7-A	263/263 (100%)	212 (81%)	51 (19%)	1	0
1	8-A	263/263 (100%)	216 (82%)	47 (18%)	2	0
1	9-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	10-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	11-A	263/263 (100%)	215 (82%)	48 (18%)	1	0
1	12-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	13-A	263/263 (100%)	228 (87%)	35 (13%)	4	1
1	14-A	263/263 (100%)	217 (82%)	46 (18%)	2	0
1	15-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	16-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	17-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	18-A	263/263 (100%)	207 (79%)	56 (21%)	1	0
1	19-A	263/263 (100%)	217 (82%)	46 (18%)	2	0
1	20-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	21-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
1	22-A	263/263 (100%)	226 (86%)	37 (14%)	3	1
1	23-A	263/263 (100%)	233 (89%)	30 (11%)	5	1
1	24-A	263/263 (100%)	231 (88%)	32 (12%)	5	1
1	25-A	263/263 (100%)	225 (86%)	38 (14%)	3	1
1	26-A	263/263 (100%)	222 (84%)	41 (16%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	27-A	263/263 (100%)	214 (81%)	49 (19%)	1 0
1	28-A	263/263 (100%)	229 (87%)	34 (13%)	4 1
1	29-A	263/263 (100%)	224 (85%)	39 (15%)	3 0
1	30-A	263/263 (100%)	225 (86%)	38 (14%)	3 1
1	31-A	263/263 (100%)	221 (84%)	42 (16%)	2 0
1	32-A	263/263 (100%)	219 (83%)	44 (17%)	2 0
1	33-A	263/263 (100%)	230 (88%)	33 (12%)	4 1
1	34-A	263/263 (100%)	221 (84%)	42 (16%)	2 0
1	35-A	263/263 (100%)	221 (84%)	42 (16%)	2 0
1	36-A	263/263 (100%)	227 (86%)	36 (14%)	3 1
1	37-A	263/263 (100%)	215 (82%)	48 (18%)	1 0
1	38-A	263/263 (100%)	216 (82%)	47 (18%)	2 0
1	39-A	263/263 (100%)	213 (81%)	50 (19%)	1 0
1	40-A	263/263 (100%)	221 (84%)	42 (16%)	2 0
1	41-A	263/263 (100%)	216 (82%)	47 (18%)	2 0
1	42-A	263/263 (100%)	215 (82%)	48 (18%)	1 0
1	43-A	263/263 (100%)	216 (82%)	47 (18%)	2 0
1	44-A	263/263 (100%)	222 (84%)	41 (16%)	2 0
1	45-A	263/263 (100%)	222 (84%)	41 (16%)	2 0
1	46-A	263/263 (100%)	219 (83%)	44 (17%)	2 0
1	47-A	263/263 (100%)	224 (85%)	39 (15%)	3 0
1	48-A	263/263 (100%)	221 (84%)	42 (16%)	2 0
1	49-A	263/263 (100%)	222 (84%)	41 (16%)	2 0
1	50-A	263/263 (100%)	220 (84%)	43 (16%)	2 0
1	51-A	263/263 (100%)	225 (86%)	38 (14%)	3 1
1	52-A	263/263 (100%)	229 (87%)	34 (13%)	4 1
1	53-A	263/263 (100%)	218 (83%)	45 (17%)	2 0
1	54-A	263/263 (100%)	224 (85%)	39 (15%)	3 0
1	55-A	263/263 (100%)	212 (81%)	51 (19%)	1 0
1	56-A	263/263 (100%)	221 (84%)	42 (16%)	2 0
1	57-A	263/263 (100%)	214 (81%)	49 (19%)	1 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	58-A	263/263 (100%)	230 (88%)	33 (12%)	4	1
1	59-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	60-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
1	61-A	263/263 (100%)	216 (82%)	47 (18%)	2	0
1	62-A	263/263 (100%)	214 (81%)	49 (19%)	1	0
1	63-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	64-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	65-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	66-A	263/263 (100%)	225 (86%)	38 (14%)	3	1
1	67-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	68-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	69-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	70-A	263/263 (100%)	211 (80%)	52 (20%)	1	0
1	71-A	263/263 (100%)	209 (80%)	54 (20%)	1	0
1	72-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	73-A	263/263 (100%)	218 (83%)	45 (17%)	2	0
1	74-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
1	75-A	263/263 (100%)	214 (81%)	49 (19%)	1	0
All	All	19725/19725 (100%)	16533 (84%)	3192 (16%)	2	0

5 of 3192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	44-A	286	LEU
1	55-A	222	ARG
1	46-A	80	HIS
1	44-A	262	LEU
1	50-A	102	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 225 ligands modelled in this entry, 75 are monoatomic - leaving 150 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	66-A	401	-	3,3,3	0.75	0	3,3,3	0.84	0
2	DMS	22-A	401	-	3,3,3	0.76	0	3,3,3	1.87	2 (66%)
2	DMS	71-A	402	-	3,3,3	0.71	0	3,3,3	0.70	0
2	DMS	34-A	402	-	3,3,3	0.91	0	3,3,3	1.73	1 (33%)
2	DMS	16-A	401	-	3,3,3	0.91	0	3,3,3	1.72	1 (33%)
2	DMS	4-A	401	-	3,3,3	0.98	0	3,3,3	0.48	0
2	DMS	74-A	401	-	3,3,3	0.84	0	3,3,3	0.76	0
2	DMS	75-A	402	-	3,3,3	0.59	0	3,3,3	0.26	0
2	DMS	17-A	402	-	3,3,3	1.14	0	3,3,3	1.60	0
2	DMS	7-A	402	-	3,3,3	0.91	0	3,3,3	1.23	0
2	DMS	49-A	402	-	3,3,3	0.73	0	3,3,3	1.31	0
2	DMS	9-A	402	-	3,3,3	0.80	0	3,3,3	2.07	1 (33%)
2	DMS	14-A	401	-	3,3,3	0.94	0	3,3,3	0.74	0
2	DMS	56-A	401	-	3,3,3	0.96	0	3,3,3	0.62	0
2	DMS	26-A	401	-	3,3,3	0.81	0	3,3,3	0.72	0
2	DMS	64-A	402	-	3,3,3	0.83	0	3,3,3	2.06	1 (33%)
2	DMS	30-A	401	-	3,3,3	0.58	0	3,3,3	1.93	1 (33%)
2	DMS	60-A	402	-	3,3,3	0.89	0	3,3,3	1.65	0
2	DMS	47-A	402	-	3,3,3	0.93	0	3,3,3	1.45	1 (33%)
2	DMS	51-A	402	-	3,3,3	0.86	0	3,3,3	0.98	0
2	DMS	21-A	401	-	3,3,3	0.77	0	3,3,3	1.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	72-A	401	-	3,3,3	0.77	0	3,3,3	0.55	0
2	DMS	61-A	401	-	3,3,3	0.73	0	3,3,3	1.19	0
2	DMS	70-A	402	-	3,3,3	0.75	0	3,3,3	2.77	3 (100%)
2	DMS	30-A	402	-	3,3,3	0.77	0	3,3,3	1.19	0
2	DMS	34-A	401	-	3,3,3	0.76	0	3,3,3	3.16	3 (100%)
2	DMS	59-A	402	-	3,3,3	0.78	0	3,3,3	1.06	0
2	DMS	17-A	401	-	3,3,3	0.85	0	3,3,3	0.57	0
2	DMS	3-A	401	-	3,3,3	0.57	0	3,3,3	1.92	1 (33%)
2	DMS	41-A	402	-	3,3,3	0.77	0	3,3,3	1.48	1 (33%)
2	DMS	61-A	402	-	3,3,3	0.67	0	3,3,3	1.58	1 (33%)
2	DMS	18-A	401	-	3,3,3	0.90	0	3,3,3	1.41	0
2	DMS	7-A	401	-	3,3,3	0.68	0	3,3,3	1.86	1 (33%)
2	DMS	69-A	402	-	3,3,3	0.78	0	3,3,3	1.55	1 (33%)
2	DMS	10-A	401	-	3,3,3	0.91	0	3,3,3	0.59	0
2	DMS	13-A	402	-	3,3,3	0.87	0	3,3,3	0.65	0
2	DMS	5-A	401	-	3,3,3	0.95	0	3,3,3	0.40	0
2	DMS	58-A	401	-	3,3,3	0.85	0	3,3,3	3.06	3 (100%)
2	DMS	62-A	401	-	3,3,3	0.72	0	3,3,3	0.78	0
2	DMS	11-A	401	-	3,3,3	0.79	0	3,3,3	1.04	0
2	DMS	45-A	401	-	3,3,3	0.99	0	3,3,3	0.52	0
2	DMS	33-A	401	-	3,3,3	0.71	0	3,3,3	1.30	0
2	DMS	71-A	401	-	3,3,3	0.84	0	3,3,3	0.93	0
2	DMS	28-A	402	-	3,3,3	0.74	0	3,3,3	0.37	0
2	DMS	55-A	401	-	3,3,3	0.84	0	3,3,3	1.68	1 (33%)
2	DMS	40-A	402	-	3,3,3	0.74	0	3,3,3	0.97	0
2	DMS	39-A	402	-	3,3,3	0.82	0	3,3,3	0.91	0
2	DMS	73-A	401	-	3,3,3	0.72	0	3,3,3	0.98	0
2	DMS	67-A	402	-	3,3,3	0.69	0	3,3,3	0.47	0
2	DMS	69-A	401	-	3,3,3	0.88	0	3,3,3	1.14	0
2	DMS	27-A	401	-	3,3,3	0.73	0	3,3,3	1.07	0
2	DMS	6-A	402	-	3,3,3	0.63	0	3,3,3	1.28	0
2	DMS	19-A	401	-	3,3,3	0.83	0	3,3,3	0.68	0
2	DMS	60-A	401	-	3,3,3	0.77	0	3,3,3	0.81	0
2	DMS	64-A	401	-	3,3,3	0.79	0	3,3,3	1.81	1 (33%)
2	DMS	50-A	402	-	3,3,3	0.89	0	3,3,3	1.51	0
2	DMS	25-A	401	-	3,3,3	0.84	0	3,3,3	0.74	0
2	DMS	63-A	402	-	3,3,3	0.74	0	3,3,3	0.80	0
2	DMS	46-A	402	-	3,3,3	0.98	0	3,3,3	1.98	1 (33%)
2	DMS	48-A	402	-	3,3,3	0.81	0	3,3,3	1.36	0
2	DMS	15-A	401	-	3,3,3	1.02	0	3,3,3	2.11	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	8-A	401	-	3,3,3	0.97	0	3,3,3	0.82	0
2	DMS	68-A	401	-	3,3,3	0.77	0	3,3,3	1.35	1 (33%)
2	DMS	52-A	401	-	3,3,3	0.91	0	3,3,3	1.58	1 (33%)
2	DMS	27-A	402	-	3,3,3	0.73	0	3,3,3	0.82	0
2	DMS	25-A	402	-	3,3,3	1.03	0	3,3,3	1.05	0
2	DMS	2-A	402	-	3,3,3	0.74	0	3,3,3	1.51	1 (33%)
2	DMS	41-A	401	-	3,3,3	0.77	0	3,3,3	1.39	0
2	DMS	40-A	401	-	3,3,3	0.95	0	3,3,3	0.60	0
2	DMS	56-A	402	-	3,3,3	0.70	0	3,3,3	0.53	0
2	DMS	49-A	401	-	3,3,3	0.62	0	3,3,3	1.00	0
2	DMS	37-A	401	-	3,3,3	0.71	0	3,3,3	1.36	0
2	DMS	44-A	402	-	3,3,3	0.70	0	3,3,3	1.22	0
2	DMS	42-A	401	-	3,3,3	0.79	0	3,3,3	0.61	0
2	DMS	67-A	401	-	3,3,3	0.84	0	3,3,3	1.12	0
2	DMS	24-A	402	-	3,3,3	0.78	0	3,3,3	0.75	0
2	DMS	59-A	401	-	3,3,3	0.78	0	3,3,3	0.55	0
2	DMS	20-A	402	-	3,3,3	0.86	0	3,3,3	1.02	0
2	DMS	23-A	401	-	3,3,3	0.89	0	3,3,3	0.45	0
2	DMS	22-A	402	-	3,3,3	0.79	0	3,3,3	2.53	2 (66%)
2	DMS	72-A	402	-	3,3,3	0.62	0	3,3,3	1.00	0
2	DMS	38-A	402	-	3,3,3	0.88	0	3,3,3	1.02	0
2	DMS	29-A	402	-	3,3,3	0.87	0	3,3,3	2.87	2 (66%)
2	DMS	31-A	402	-	3,3,3	0.70	0	3,3,3	1.12	0
2	DMS	35-A	401	-	3,3,3	0.71	0	3,3,3	1.17	0
2	DMS	6-A	401	-	3,3,3	0.55	0	3,3,3	0.94	0
2	DMS	28-A	401	-	3,3,3	0.73	0	3,3,3	0.85	0
2	DMS	46-A	401	-	3,3,3	0.93	0	3,3,3	1.30	1 (33%)
2	DMS	48-A	401	-	3,3,3	0.76	0	3,3,3	1.17	0
2	DMS	20-A	401	-	3,3,3	0.64	0	3,3,3	1.14	0
2	DMS	10-A	402	-	3,3,3	0.77	0	3,3,3	1.17	0
2	DMS	35-A	402	-	3,3,3	0.74	0	3,3,3	0.94	0
2	DMS	36-A	402	-	3,3,3	0.91	0	3,3,3	2.06	1 (33%)
2	DMS	47-A	401	-	3,3,3	0.78	0	3,3,3	0.48	0
2	DMS	12-A	402	-	3,3,3	0.83	0	3,3,3	1.06	0
2	DMS	55-A	402	-	3,3,3	0.54	0	3,3,3	1.29	0
2	DMS	43-A	402	-	3,3,3	0.66	0	3,3,3	1.33	0
2	DMS	5-A	402	-	3,3,3	0.69	0	3,3,3	1.97	1 (33%)
2	DMS	75-A	401	-	3,3,3	0.78	0	3,3,3	1.12	0
2	DMS	58-A	402	-	3,3,3	0.76	0	3,3,3	1.89	2 (66%)
2	DMS	42-A	402	-	3,3,3	0.68	0	3,3,3	0.52	0
2	DMS	53-A	401	-	3,3,3	0.85	0	3,3,3	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	51-A	401	-	3,3,3	0.79	0	3,3,3	3.08	2 (66%)
2	DMS	11-A	402	-	3,3,3	0.84	0	3,3,3	0.87	0
2	DMS	45-A	402	-	3,3,3	0.82	0	3,3,3	1.25	1 (33%)
2	DMS	62-A	402	-	3,3,3	0.79	0	3,3,3	1.05	0
2	DMS	33-A	402	-	3,3,3	0.74	0	3,3,3	1.29	1 (33%)
2	DMS	66-A	402	-	3,3,3	0.61	0	3,3,3	1.55	1 (33%)
2	DMS	1-A	401	-	3,3,3	0.82	0	3,3,3	1.86	1 (33%)
2	DMS	50-A	401	-	3,3,3	0.83	0	3,3,3	1.20	0
2	DMS	70-A	401	-	3,3,3	0.62	0	3,3,3	0.11	0
2	DMS	74-A	402	-	3,3,3	0.79	0	3,3,3	1.12	0
2	DMS	23-A	402	-	3,3,3	0.74	0	3,3,3	0.42	0
2	DMS	32-A	402	-	3,3,3	0.66	0	3,3,3	0.54	0
2	DMS	63-A	401	-	3,3,3	0.67	0	3,3,3	0.87	0
2	DMS	73-A	402	-	3,3,3	0.88	0	3,3,3	0.34	0
2	DMS	44-A	401	-	3,3,3	0.93	0	3,3,3	0.66	0
2	DMS	32-A	401	-	3,3,3	0.73	0	3,3,3	2.56	2 (66%)
2	DMS	24-A	401	-	3,3,3	0.79	0	3,3,3	0.92	0
2	DMS	13-A	401	-	3,3,3	0.93	0	3,3,3	2.23	2 (66%)
2	DMS	1-A	402	-	3,3,3	0.74	0	3,3,3	1.82	1 (33%)
2	DMS	43-A	401	-	3,3,3	0.67	0	3,3,3	1.69	1 (33%)
2	DMS	26-A	402	-	3,3,3	0.83	0	3,3,3	0.37	0
2	DMS	53-A	402	-	3,3,3	0.85	0	3,3,3	0.68	0
2	DMS	54-A	402	-	3,3,3	0.85	0	3,3,3	0.67	0
2	DMS	54-A	401	-	3,3,3	0.89	0	3,3,3	0.50	0
2	DMS	36-A	401	-	3,3,3	0.76	0	3,3,3	0.59	0
2	DMS	16-A	402	-	3,3,3	0.69	0	3,3,3	0.75	0
2	DMS	19-A	402	-	3,3,3	0.81	0	3,3,3	1.08	0
2	DMS	57-A	401	-	3,3,3	0.70	0	3,3,3	1.18	0
2	DMS	38-A	401	-	3,3,3	0.82	0	3,3,3	0.96	0
2	DMS	4-A	402	-	3,3,3	0.75	0	3,3,3	1.15	0
2	DMS	29-A	401	-	3,3,3	0.87	0	3,3,3	1.04	0
2	DMS	31-A	401	-	3,3,3	0.80	0	3,3,3	0.60	0
2	DMS	14-A	402	-	3,3,3	0.67	0	3,3,3	0.90	0
2	DMS	3-A	402	-	3,3,3	0.76	0	3,3,3	0.79	0
2	DMS	52-A	402	-	3,3,3	0.65	0	3,3,3	2.02	1 (33%)
2	DMS	68-A	402	-	3,3,3	0.76	0	3,3,3	1.28	0
2	DMS	18-A	402	-	3,3,3	0.61	0	3,3,3	1.91	1 (33%)
2	DMS	21-A	402	-	3,3,3	0.91	0	3,3,3	1.24	0
2	DMS	39-A	401	-	3,3,3	0.84	0	3,3,3	1.56	0
2	DMS	65-A	401	-	3,3,3	0.81	0	3,3,3	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	2-A	401	-	3,3,3	0.83	0	3,3,3	0.88	0
2	DMS	15-A	402	-	3,3,3	0.66	0	3,3,3	1.28	0
2	DMS	8-A	402	-	3,3,3	0.73	0	3,3,3	1.66	1 (33%)
2	DMS	37-A	402	-	3,3,3	0.87	0	3,3,3	1.48	1 (33%)
2	DMS	12-A	401	-	3,3,3	0.59	0	3,3,3	1.42	0
2	DMS	9-A	401	-	3,3,3	0.96	0	3,3,3	0.92	0
2	DMS	65-A	402	-	3,3,3	0.60	0	3,3,3	0.45	0
2	DMS	57-A	402	-	3,3,3	0.86	0	3,3,3	1.06	0

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	29-A	402	DMS	O-S-C2	3.69	125.38	106.54
2	34-A	401	DMS	O-S-C2	3.64	125.09	106.54
2	32-A	401	DMS	O-S-C1	3.61	124.95	106.54
2	51-A	401	DMS	O-S-C2	3.60	124.91	106.54
2	51-A	401	DMS	C2-S-C1	3.46	116.25	98.44

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	2-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	3-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	4-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	5-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	6-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	7-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	8-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	9-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	10-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	11-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	12-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	13-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	14-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	15-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	16-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	17-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	18-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	19-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	20-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	21-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	22-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	23-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	24-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	25-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	26-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	27-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	28-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	29-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	30-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	31-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	32-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	33-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	34-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	35-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	36-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	37-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	38-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	39-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	40-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	41-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	42-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	43-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	44-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	45-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	46-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	47-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	48-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	49-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	50-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	51-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	52-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	53-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	54-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	55-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	56-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	57-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	58-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	59-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	60-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	61-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	62-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	63-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	64-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	65-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	66-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	67-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	68-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	69-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	70-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	71-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	72-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	73-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	74-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
1	75-A	306/306 (100%)	0.62	30 (9%)	7	8	32, 37, 45, 48	306 (100%)
All	All	22950/22950 (100%)	0.62	2250 (9%)	9	8	32, 37, 45, 48	22950 (100%)

The worst 5 of 2250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	302	GLY	24.8
1	2-A	302	GLY	24.8
1	3-A	302	GLY	24.8
1	4-A	302	GLY	24.8
1	5-A	302	GLY	24.8

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	1-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	2-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	3-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	4-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	5-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	6-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	7-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	8-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	9-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	10-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	11-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	12-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	13-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	14-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	15-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	16-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	17-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	18-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	19-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	20-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	21-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	22-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	23-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	24-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	25-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	26-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	27-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	28-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	29-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	30-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	31-A	401	4/4	0.12	1.42	32,33,33,34	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	32-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	33-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	34-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	35-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	36-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	37-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	38-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	39-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	40-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	41-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	42-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	43-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	44-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	45-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	46-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	47-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	48-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	49-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	50-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	51-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	52-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	53-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	54-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	55-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	56-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	57-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	58-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	59-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	60-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	61-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	62-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	63-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	64-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	65-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	66-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	67-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	68-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	69-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	70-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	71-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	72-A	401	4/4	0.12	1.42	32,33,33,34	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	73-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	74-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	75-A	401	4/4	0.12	1.42	32,33,33,34	10
2	DMS	1-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	2-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	3-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	4-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	5-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	6-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	7-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	8-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	9-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	10-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	11-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	12-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	13-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	14-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	15-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	16-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	17-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	18-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	19-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	20-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	21-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	22-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	23-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	24-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	25-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	26-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	27-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	28-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	29-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	30-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	31-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	32-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	33-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	34-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	35-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	36-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	37-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	38-A	402	4/4	0.60	0.64	34,35,35,35	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	39-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	40-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	41-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	42-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	43-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	44-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	45-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	46-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	47-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	48-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	49-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	50-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	51-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	52-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	53-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	54-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	55-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	56-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	57-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	58-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	59-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	60-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	61-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	62-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	63-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	64-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	65-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	66-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	67-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	68-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	69-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	70-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	71-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	72-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	73-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	74-A	402	4/4	0.60	0.64	34,35,35,35	10
2	DMS	75-A	402	4/4	0.60	0.64	34,35,35,35	10
3	ZN	1-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	2-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	3-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	4-A	403	1/1	0.93	0.38	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	5-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	6-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	7-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	8-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	9-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	10-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	11-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	12-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	13-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	14-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	15-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	16-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	17-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	18-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	19-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	20-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	21-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	22-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	23-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	24-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	25-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	26-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	27-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	28-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	29-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	30-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	31-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	32-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	33-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	34-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	35-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	36-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	37-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	38-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	39-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	40-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	41-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	42-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	43-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	44-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	45-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	46-A	403	1/1	0.93	0.38	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	47-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	48-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	49-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	50-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	51-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	52-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	53-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	54-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	55-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	56-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	57-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	58-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	59-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	60-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	61-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	62-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	63-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	64-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	65-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	66-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	67-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	68-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	69-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	70-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	71-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	72-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	73-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	74-A	403	1/1	0.93	0.38	35,35,35,35	1
3	ZN	75-A	403	1/1	0.93	0.38	35,35,35,35	1

6.5 Other polymers (i)

There are no such residues in this entry.