wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2023 – 02:37 PM EDT

PDB ID	:	7MHL
Title	:	Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 100 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	:	1.55 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:

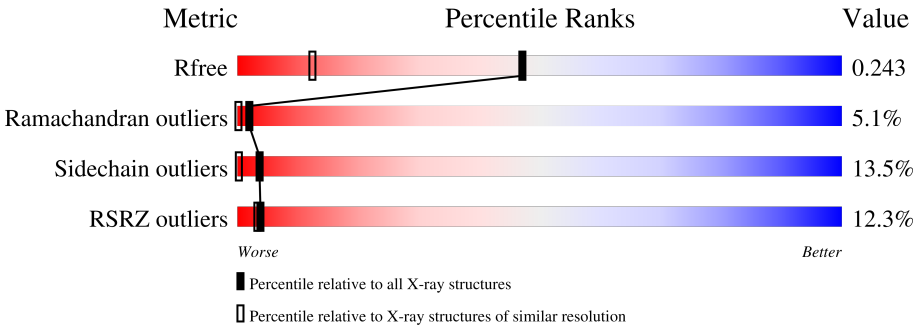
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.55 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	1483 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	12% 84% 11%
1	10-A	306	12% 82% 15%
1	11-A	306	12% 83% 12% 5%
1	12-A	306	12% 81% 16%
1	13-A	306	12% 82% 12% 5%
1	14-A	306	12% 84% 11% 5%
1	15-A	306	12% 84% 14%

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Mol	Chain	Length	Quality of chain
1	16-A	306	12% 83% 12% •
1	17-A	306	12% 79% 17% •
1	18-A	306	12% 81% 13% 6%
1	19-A	306	12% 80% 16% • •
1	2-A	306	12% 86% 10% •
1	20-A	306	12% 79% 16% 5%
1	21-A	306	12% 80% 14% 5% •
1	22-A	306	12% 81% 14% • •
1	23-A	306	12% 82% 14% •
1	24-A	306	12% 82% 14% •
1	25-A	306	12% 82% 13% • •
1	26-A	306	12% 81% 15% •
1	27-A	306	12% 77% 17% 5% •
1	28-A	306	12% 83% 14% • •
1	29-A	306	12% 84% 14% •
1	3-A	306	12% 88% 9% •
1	30-A	306	12% 85% 12% • •
1	31-A	306	12% 82% 14% •
1	32-A	306	12% 82% 16% •
1	33-A	306	12% 81% 13% 5% •
1	34-A	306	12% 83% 14% • •
1	35-A	306	12% 81% 14% • •
1	36-A	306	12% 81% 14% • •
1	37-A	306	12% 83% 14% • •
1	38-A	306	12% 84% 13% •

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Mol	Chain	Length	Quality of chain
1	39-A	306	12% 81% 15%
1	4-A	306	12% 86% 10%
1	40-A	306	12% 82% 16%
1	41-A	306	12% 82% 13%
1	42-A	306	12% 87% 9%
1	43-A	306	12% 85% 11%
1	44-A	306	12% 86% 11%
1	45-A	306	12% 84% 12%
1	46-A	306	12% 87% 11%
1	47-A	306	12% 81% 15%
1	48-A	306	12% 83% 13%
1	49-A	306	12% 84% 12%
1	5-A	306	12% 85% 12%
1	50-A	306	12% 82% 14%
1	51-A	306	12% 86% 11%
1	52-A	306	12% 83% 12% 5%
1	53-A	306	12% 82% 14%
1	54-A	306	12% 86% 10%
1	6-A	306	12% 83% 15%
1	7-A	306	12% 84% 13%
1	8-A	306	12% 85% 13%
1	9-A	306	12% 83% 15%

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	402	-	-	-	X
2	DMS	1-A	403	-	-	-	X
2	DMS	1-A	404	-	-	-	X
2	DMS	1-A	405	-	-	-	X
2	DMS	10-A	402	-	-	-	X
2	DMS	10-A	403	-	-	-	X
2	DMS	10-A	404	-	-	-	X
2	DMS	10-A	405	-	-	-	X
2	DMS	11-A	402	-	-	-	X
2	DMS	11-A	403	-	-	-	X
2	DMS	11-A	404	-	-	-	X
2	DMS	11-A	405	-	-	-	X
2	DMS	12-A	402	-	X	-	X
2	DMS	12-A	403	-	-	-	X
2	DMS	12-A	404	-	-	-	X
2	DMS	12-A	405	-	-	-	X
2	DMS	13-A	402	-	-	-	X
2	DMS	13-A	403	-	-	-	X
2	DMS	13-A	404	-	-	-	X
2	DMS	13-A	405	-	-	-	X
2	DMS	14-A	402	-	-	-	X
2	DMS	14-A	403	-	-	-	X
2	DMS	14-A	404	-	-	-	X
2	DMS	14-A	405	-	-	-	X
2	DMS	15-A	402	-	-	-	X
2	DMS	15-A	403	-	-	-	X
2	DMS	15-A	404	-	-	-	X
2	DMS	15-A	405	-	-	-	X
2	DMS	16-A	402	-	-	-	X
2	DMS	16-A	403	-	-	-	X
2	DMS	16-A	404	-	-	-	X
2	DMS	16-A	405	-	-	-	X
2	DMS	17-A	402	-	-	-	X
2	DMS	17-A	403	-	-	-	X
2	DMS	17-A	404	-	-	-	X
2	DMS	17-A	405	-	-	-	X
2	DMS	18-A	402	-	X	-	X
2	DMS	18-A	403	-	-	-	X
2	DMS	18-A	404	-	-	-	X
2	DMS	18-A	405	-	-	-	X
2	DMS	19-A	402	-	-	-	X
2	DMS	19-A	403	-	-	-	X
2	DMS	19-A	404	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	19-A	405	-	-	-	X
2	DMS	2-A	402	-	-	-	X
2	DMS	2-A	403	-	-	-	X
2	DMS	2-A	404	-	-	-	X
2	DMS	2-A	405	-	-	-	X
2	DMS	20-A	402	-	-	-	X
2	DMS	20-A	403	-	-	-	X
2	DMS	20-A	404	-	-	-	X
2	DMS	20-A	405	-	-	-	X
2	DMS	21-A	402	-	-	-	X
2	DMS	21-A	403	-	-	-	X
2	DMS	21-A	404	-	-	-	X
2	DMS	21-A	405	-	-	-	X
2	DMS	22-A	402	-	-	-	X
2	DMS	22-A	403	-	-	-	X
2	DMS	22-A	404	-	-	-	X
2	DMS	22-A	405	-	-	-	X
2	DMS	23-A	402	-	-	-	X
2	DMS	23-A	403	-	-	-	X
2	DMS	23-A	404	-	-	-	X
2	DMS	23-A	405	-	-	-	X
2	DMS	24-A	402	-	-	-	X
2	DMS	24-A	403	-	-	-	X
2	DMS	24-A	404	-	-	-	X
2	DMS	24-A	405	-	-	-	X
2	DMS	25-A	402	-	-	-	X
2	DMS	25-A	403	-	-	-	X
2	DMS	25-A	404	-	-	-	X
2	DMS	25-A	405	-	-	-	X
2	DMS	26-A	402	-	-	-	X
2	DMS	26-A	403	-	-	-	X
2	DMS	26-A	404	-	-	-	X
2	DMS	26-A	405	-	-	-	X
2	DMS	27-A	402	-	-	-	X
2	DMS	27-A	403	-	-	-	X
2	DMS	27-A	404	-	X	-	X
2	DMS	27-A	405	-	-	-	X
2	DMS	28-A	402	-	-	-	X
2	DMS	28-A	403	-	-	-	X
2	DMS	28-A	404	-	-	-	X
2	DMS	28-A	405	-	-	-	X
2	DMS	29-A	402	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	29-A	403	-	-	-	X
2	DMS	29-A	404	-	-	-	X
2	DMS	29-A	405	-	-	-	X
2	DMS	3-A	402	-	-	-	X
2	DMS	3-A	403	-	-	-	X
2	DMS	3-A	404	-	-	-	X
2	DMS	3-A	405	-	-	-	X
2	DMS	30-A	402	-	-	-	X
2	DMS	30-A	403	-	-	-	X
2	DMS	30-A	404	-	-	-	X
2	DMS	30-A	405	-	-	-	X
2	DMS	31-A	402	-	-	-	X
2	DMS	31-A	403	-	-	-	X
2	DMS	31-A	404	-	-	-	X
2	DMS	31-A	405	-	-	-	X
2	DMS	32-A	402	-	-	-	X
2	DMS	32-A	403	-	-	-	X
2	DMS	32-A	404	-	-	-	X
2	DMS	32-A	405	-	-	-	X
2	DMS	33-A	402	-	-	-	X
2	DMS	33-A	403	-	-	-	X
2	DMS	33-A	404	-	-	-	X
2	DMS	33-A	405	-	-	-	X
2	DMS	34-A	402	-	-	-	X
2	DMS	34-A	403	-	-	-	X
2	DMS	34-A	404	-	-	-	X
2	DMS	34-A	405	-	-	-	X
2	DMS	35-A	402	-	-	-	X
2	DMS	35-A	403	-	-	-	X
2	DMS	35-A	404	-	-	-	X
2	DMS	35-A	405	-	-	-	X
2	DMS	36-A	402	-	-	-	X
2	DMS	36-A	403	-	-	-	X
2	DMS	36-A	404	-	-	-	X
2	DMS	36-A	405	-	-	-	X
2	DMS	37-A	402	-	-	-	X
2	DMS	37-A	403	-	-	-	X
2	DMS	37-A	404	-	-	-	X
2	DMS	37-A	405	-	-	-	X
2	DMS	38-A	402	-	-	-	X
2	DMS	38-A	403	-	-	-	X
2	DMS	38-A	404	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	38-A	405	-	-	-	X
2	DMS	39-A	402	-	-	-	X
2	DMS	39-A	403	-	-	-	X
2	DMS	39-A	404	-	-	-	X
2	DMS	39-A	405	-	-	-	X
2	DMS	4-A	402	-	-	-	X
2	DMS	4-A	403	-	-	-	X
2	DMS	4-A	404	-	-	-	X
2	DMS	4-A	405	-	X	-	X
2	DMS	40-A	402	-	-	-	X
2	DMS	40-A	403	-	-	-	X
2	DMS	40-A	404	-	-	-	X
2	DMS	40-A	405	-	-	-	X
2	DMS	41-A	402	-	-	-	X
2	DMS	41-A	403	-	-	-	X
2	DMS	41-A	404	-	-	-	X
2	DMS	41-A	405	-	-	-	X
2	DMS	42-A	402	-	-	-	X
2	DMS	42-A	403	-	-	-	X
2	DMS	42-A	404	-	-	-	X
2	DMS	42-A	405	-	-	-	X
2	DMS	43-A	402	-	-	-	X
2	DMS	43-A	403	-	-	-	X
2	DMS	43-A	404	-	-	-	X
2	DMS	43-A	405	-	-	-	X
2	DMS	44-A	402	-	-	-	X
2	DMS	44-A	403	-	-	-	X
2	DMS	44-A	404	-	-	-	X
2	DMS	44-A	405	-	-	-	X
2	DMS	45-A	402	-	-	-	X
2	DMS	45-A	403	-	-	-	X
2	DMS	45-A	404	-	-	-	X
2	DMS	45-A	405	-	-	-	X
2	DMS	46-A	402	-	-	-	X
2	DMS	46-A	403	-	-	-	X
2	DMS	46-A	404	-	-	-	X
2	DMS	46-A	405	-	-	-	X
2	DMS	47-A	402	-	-	-	X
2	DMS	47-A	403	-	-	-	X
2	DMS	47-A	404	-	-	-	X
2	DMS	47-A	405	-	-	-	X
2	DMS	48-A	402	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	48-A	403	-	-	-	X
2	DMS	48-A	404	-	-	-	X
2	DMS	48-A	405	-	-	-	X
2	DMS	49-A	402	-	-	-	X
2	DMS	49-A	403	-	-	-	X
2	DMS	49-A	404	-	-	-	X
2	DMS	49-A	405	-	-	-	X
2	DMS	5-A	402	-	-	-	X
2	DMS	5-A	403	-	-	-	X
2	DMS	5-A	404	-	-	-	X
2	DMS	5-A	405	-	-	-	X
2	DMS	50-A	402	-	-	-	X
2	DMS	50-A	403	-	-	-	X
2	DMS	50-A	404	-	-	-	X
2	DMS	50-A	405	-	-	-	X
2	DMS	51-A	402	-	-	-	X
2	DMS	51-A	403	-	-	-	X
2	DMS	51-A	404	-	-	-	X
2	DMS	51-A	405	-	-	-	X
2	DMS	52-A	402	-	-	-	X
2	DMS	52-A	403	-	-	-	X
2	DMS	52-A	404	-	-	-	X
2	DMS	52-A	405	-	-	-	X
2	DMS	53-A	402	-	-	-	X
2	DMS	53-A	403	-	-	-	X
2	DMS	53-A	404	-	-	-	X
2	DMS	53-A	405	-	-	-	X
2	DMS	54-A	402	-	-	-	X
2	DMS	54-A	403	-	-	-	X
2	DMS	54-A	404	-	-	-	X
2	DMS	54-A	405	-	-	-	X
2	DMS	6-A	402	-	-	-	X
2	DMS	6-A	403	-	-	-	X
2	DMS	6-A	404	-	-	-	X
2	DMS	6-A	405	-	-	-	X
2	DMS	7-A	402	-	-	-	X
2	DMS	7-A	403	-	-	-	X
2	DMS	7-A	404	-	-	-	X
2	DMS	7-A	405	-	-	-	X
2	DMS	8-A	402	-	-	-	X
2	DMS	8-A	403	-	-	-	X
2	DMS	8-A	404	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	8-A	405	-	-	-	X
2	DMS	9-A	402	-	-	-	X
2	DMS	9-A	403	-	X	-	X
2	DMS	9-A	404	-	-	-	X
2	DMS	9-A	405	-	X	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 264643 atoms, of which 126576 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3C-like proteinase.

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

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

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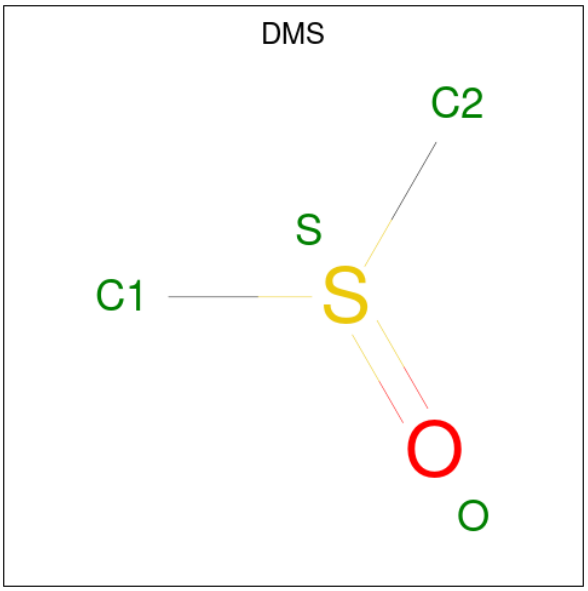
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	39-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	40-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	41-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	42-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	43-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	44-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	45-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	46-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	47-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	48-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	49-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	50-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	51-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	52-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	53-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			
1	54-A	306	Total	C	H	N	O	S	0	0	0
			4681	1499	2314	402	444	22			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	44-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	45-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	54-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	1-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	2-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	3-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	4-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	5-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	6-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	7-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	8-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	9-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	10-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	11-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	12-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	13-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	14-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	15-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	16-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	17-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	18-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	19-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	20-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	30-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	31-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	32-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	33-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	34-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	35-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	36-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	37-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	38-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	39-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	40-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	41-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	42-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	43-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	44-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	45-A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	190	Total O 190 190	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	2-A	172	Total O 172 172	0	0
4	3-A	162	Total O 162 162	0	0
4	4-A	157	Total O 157 157	0	0
4	5-A	164	Total O 164 164	0	0
4	6-A	181	Total O 181 181	0	0
4	7-A	173	Total O 173 173	0	0
4	8-A	177	Total O 177 177	0	0
4	9-A	174	Total O 174 174	0	0
4	10-A	168	Total O 168 168	0	0
4	11-A	164	Total O 164 164	0	0
4	12-A	195	Total O 195 195	0	0
4	13-A	196	Total O 196 196	0	0
4	14-A	152	Total O 152 152	0	0
4	15-A	164	Total O 164 164	0	0
4	16-A	166	Total O 166 166	0	0
4	17-A	176	Total O 176 176	0	0
4	18-A	177	Total O 177 177	0	0
4	19-A	160	Total O 160 160	0	0
4	20-A	161	Total O 161 161	0	0
4	21-A	179	Total O 179 179	0	0
4	22-A	175	Total O 175 175	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	23-A	170	Total O 170 170	0	0
4	24-A	164	Total O 164 164	0	0
4	25-A	166	Total O 166 166	0	0
4	26-A	178	Total O 178 178	0	0
4	27-A	181	Total O 181 181	0	0
4	28-A	167	Total O 167 167	0	0
4	29-A	158	Total O 158 158	0	0
4	30-A	170	Total O 170 170	0	0
4	31-A	183	Total O 183 183	0	0
4	32-A	169	Total O 169 169	0	0
4	33-A	181	Total O 181 181	0	0
4	34-A	182	Total O 182 182	0	0
4	35-A	165	Total O 165 165	0	0
4	36-A	165	Total O 165 165	0	0
4	37-A	169	Total O 169 169	0	0
4	38-A	170	Total O 170 170	0	0
4	39-A	182	Total O 182 182	0	0
4	40-A	172	Total O 172 172	0	0
4	41-A	158	Total O 158 158	0	0
4	42-A	163	Total O 163 163	0	0
4	43-A	164	Total O 164 164	0	0

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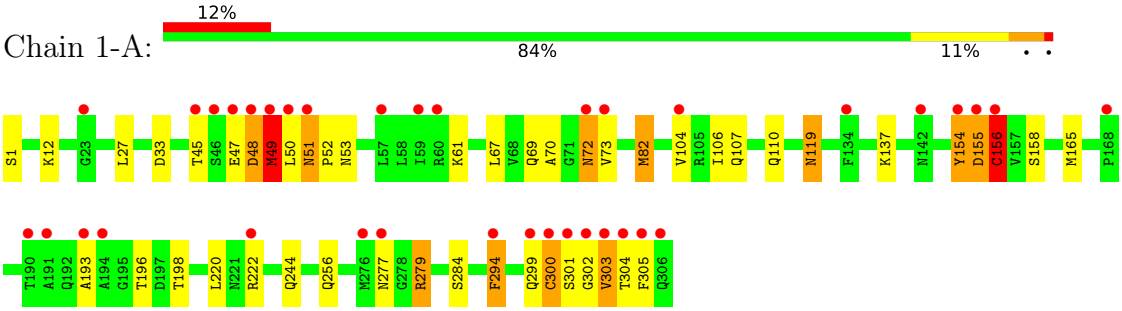
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	44-A	172	Total O 172 172	0	0
4	45-A	150	Total O 150 150	0	0
4	46-A	162	Total O 162 162	0	0
4	47-A	152	Total O 152 152	0	0
4	48-A	151	Total O 151 151	0	0
4	49-A	145	Total O 145 145	0	0
4	50-A	185	Total O 185 185	0	0
4	51-A	168	Total O 168 168	0	0
4	52-A	151	Total O 151 151	0	0
4	53-A	145	Total O 145 145	0	0
4	54-A	174	Total O 174 174	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.

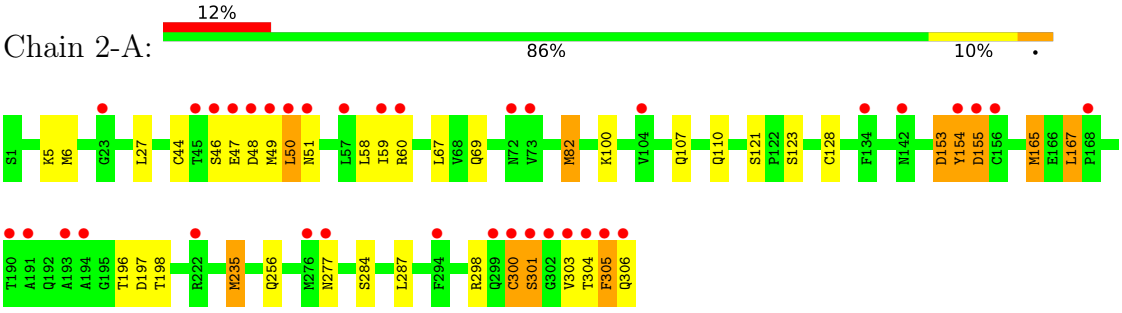
- Molecule 1: 3C-like proteinase

Chain 1-A:



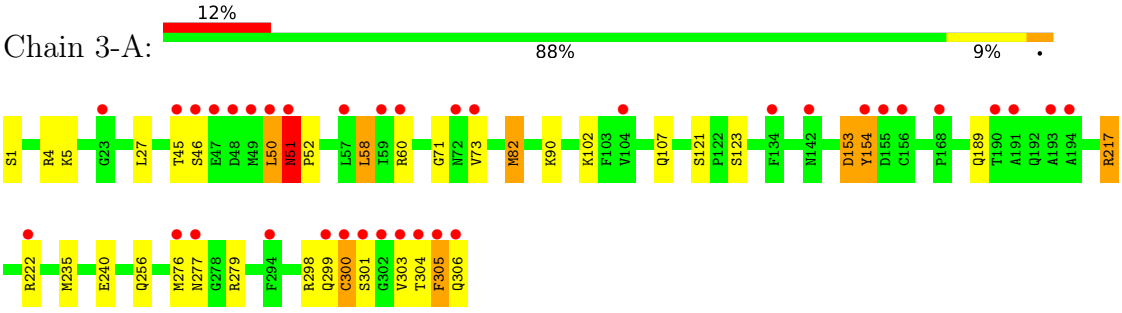
- Molecule 1: 3C-like proteinase

Chain 2-A:



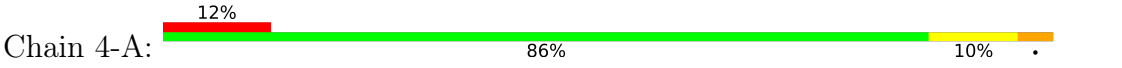
- Molecule 1: 3C-like proteinase

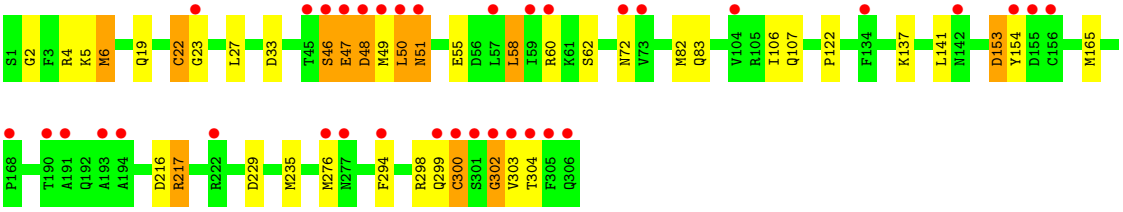
Chain 3-A:



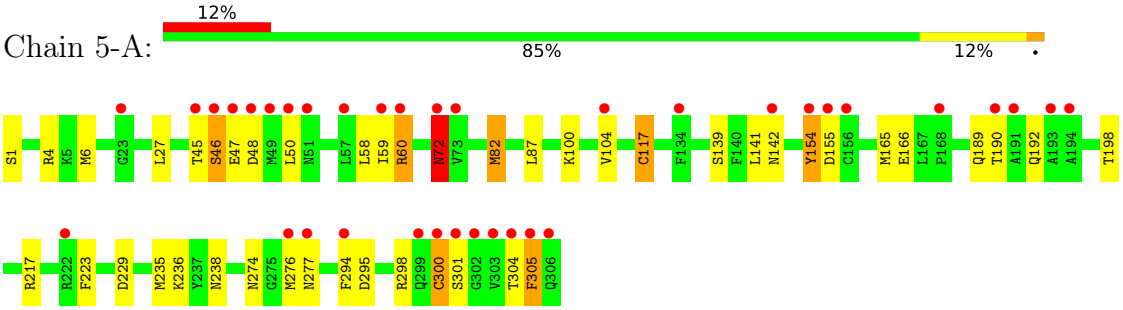
- Molecule 1: 3C-like proteinase

Chain 4-A:

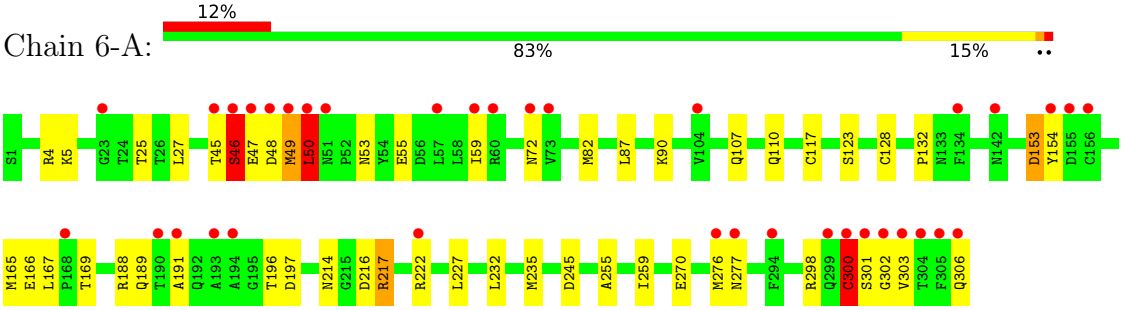




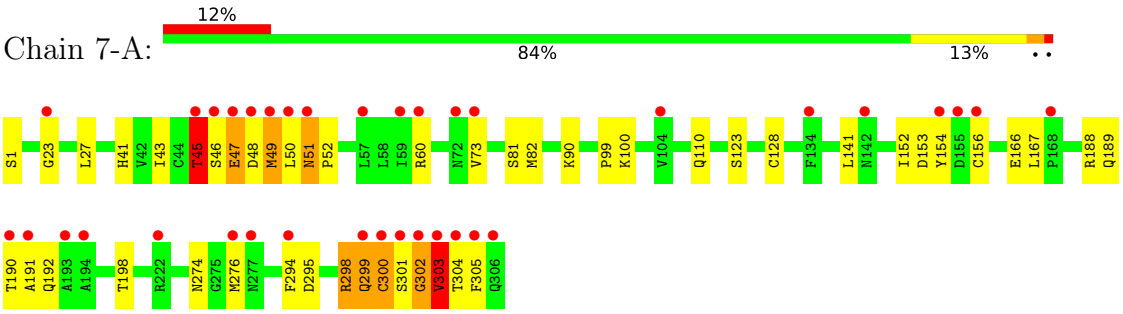
• Molecule 1: 3C-like proteinase



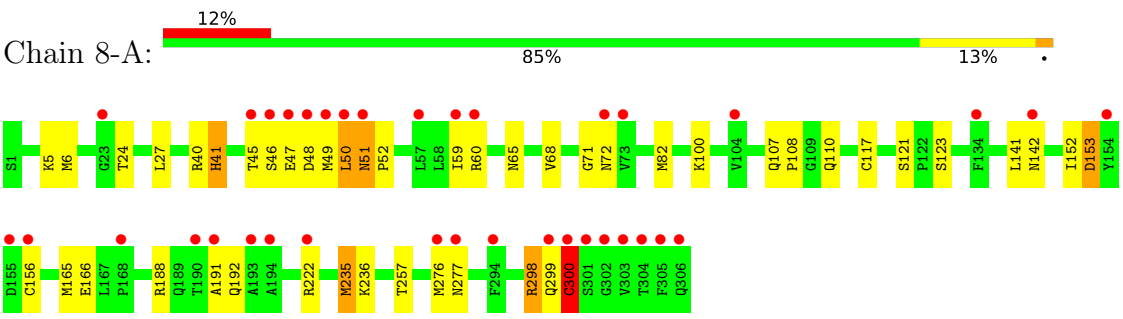
• Molecule 1: 3C-like proteinase



• Molecule 1: 3C-like proteinase

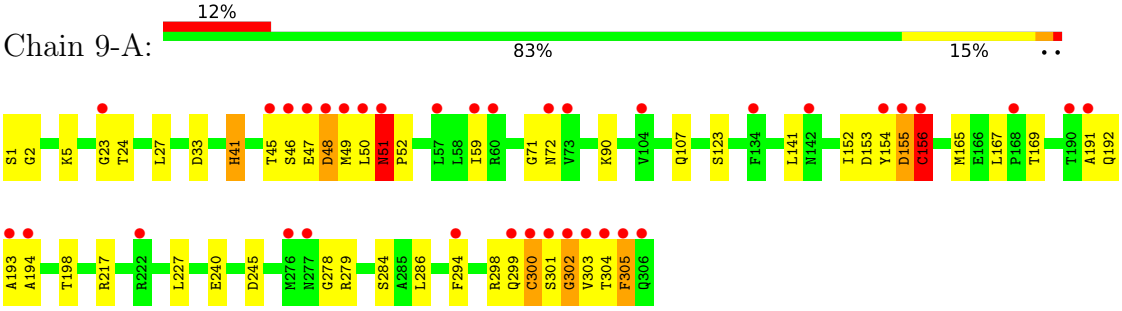


• Molecule 1: 3C-like proteinase



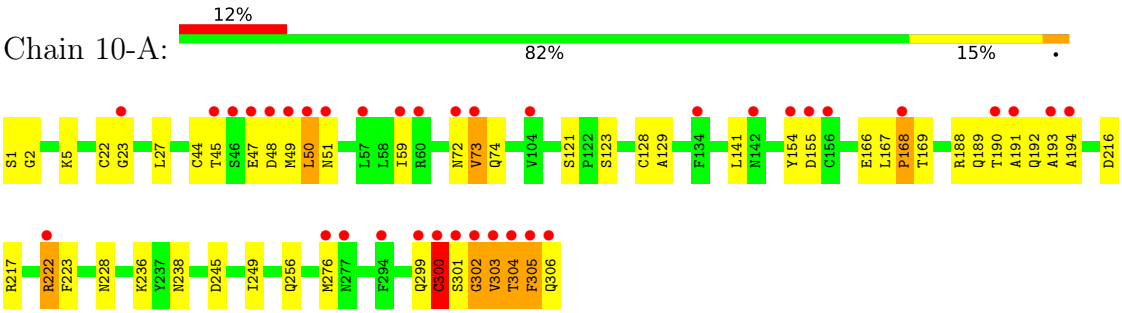
• Molecule 1: 3C-like proteinase

Chain 9-A:



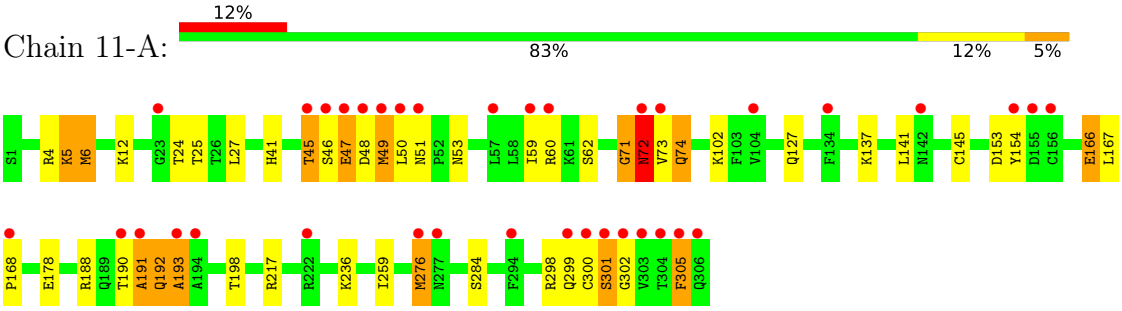
• Molecule 1: 3C-like proteinase

Chain 10-A:



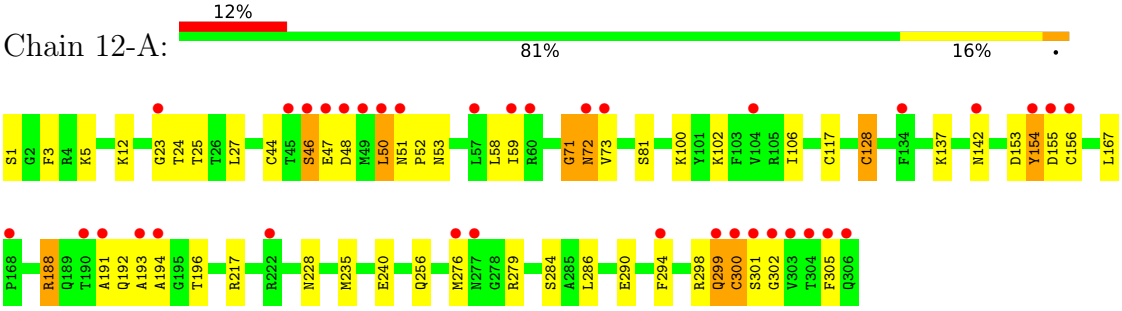
• Molecule 1: 3C-like proteinase

Chain 11-A:



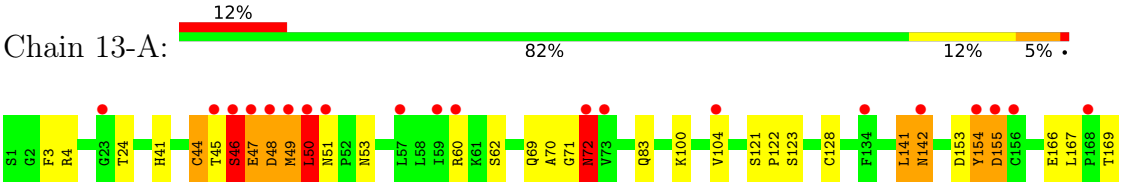
• Molecule 1: 3C-like proteinase

Chain 12-A:



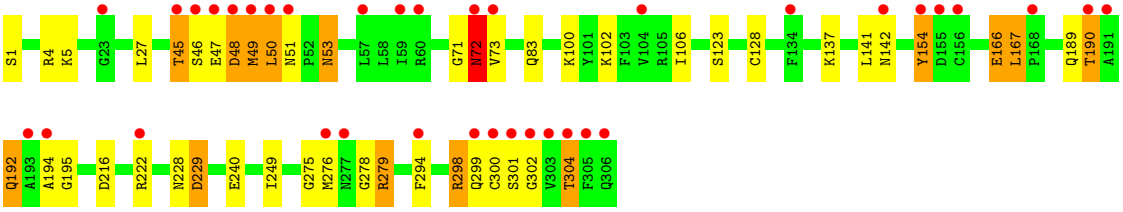
• Molecule 1: 3C-like proteinase

Chain 13-A:



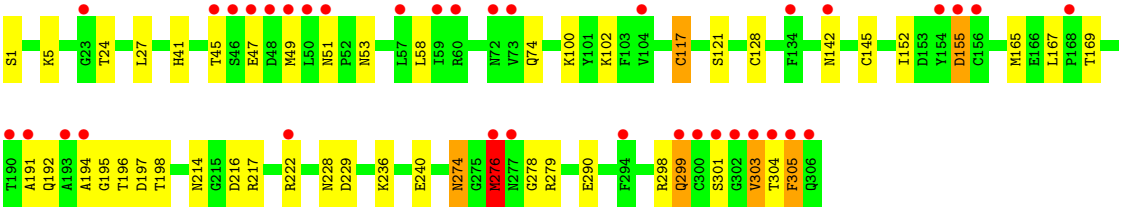
• Molecule 1: 3C-like proteinase

Chain 14-A:



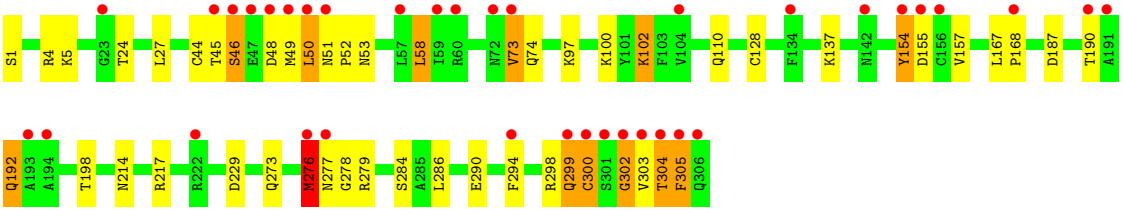
• Molecule 1: 3C-like proteinase

Chain 15-A:



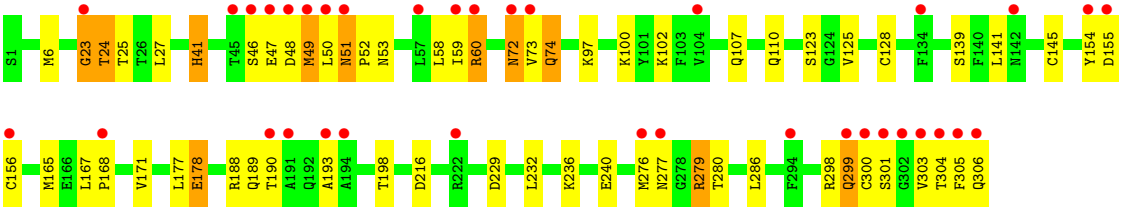
• Molecule 1: 3C-like proteinase

Chain 16-A:



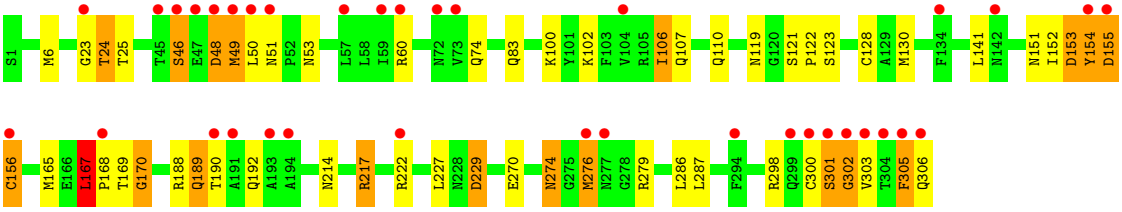
• Molecule 1: 3C-like proteinase

Chain 17-A:

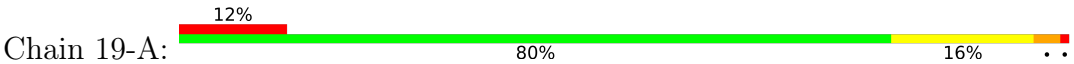


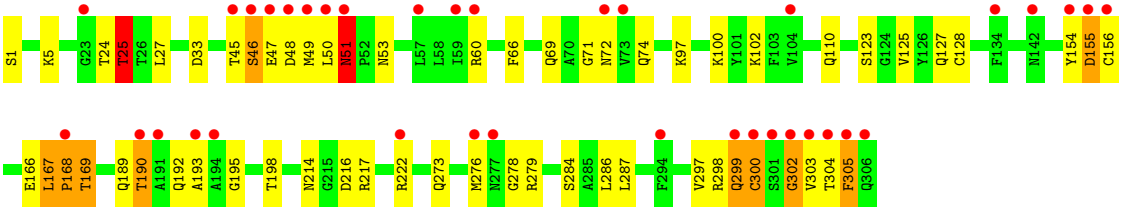
• Molecule 1: 3C-like proteinase

Chain 18-A:

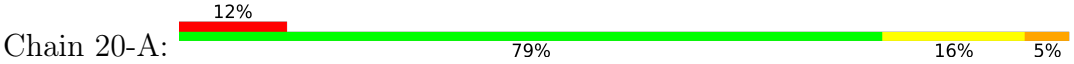


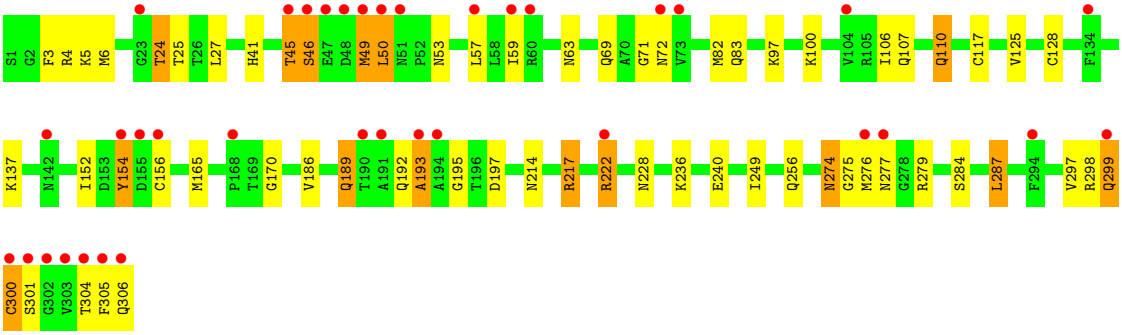
• Molecule 1: 3C-like proteinase



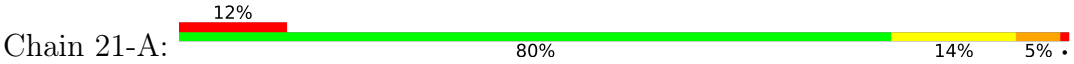


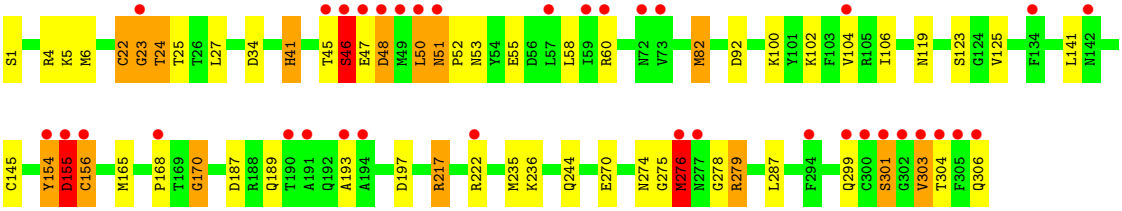
• Molecule 1: 3C-like proteinase



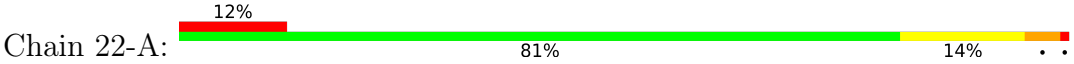


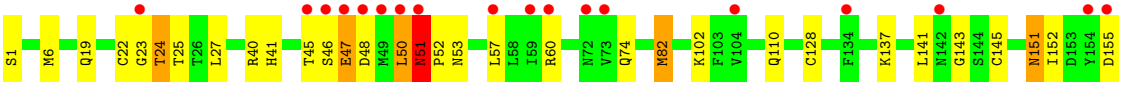
• Molecule 1: 3C-like proteinase

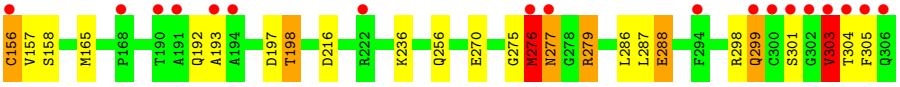




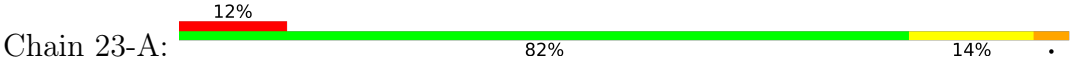
• Molecule 1: 3C-like proteinase

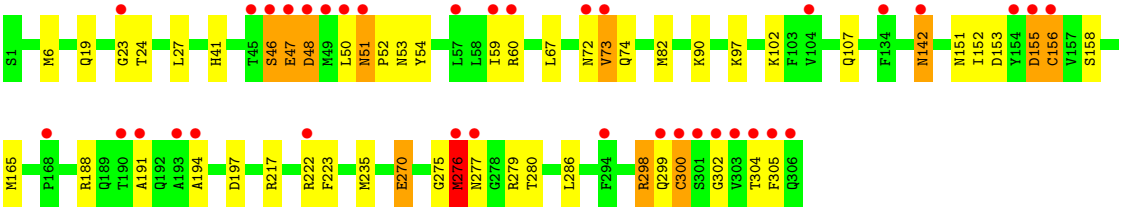




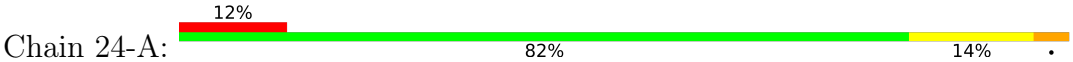


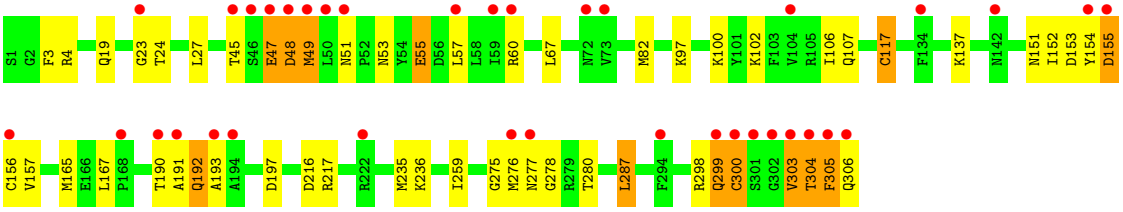
• Molecule 1: 3C-like proteinase



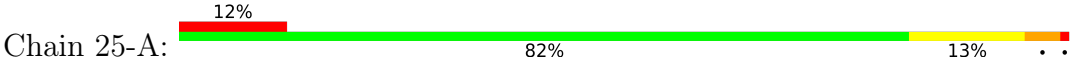


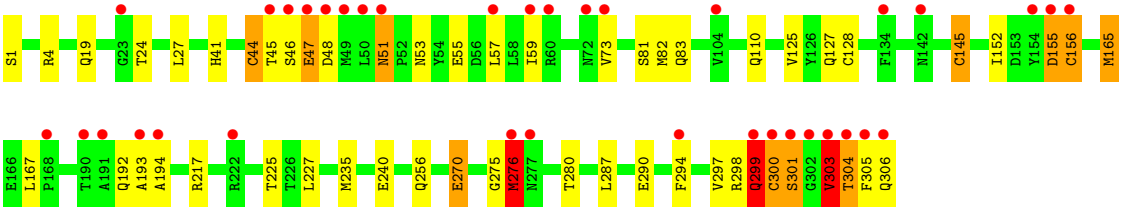
• Molecule 1: 3C-like proteinase



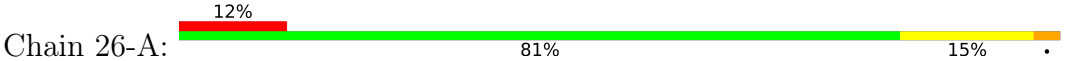


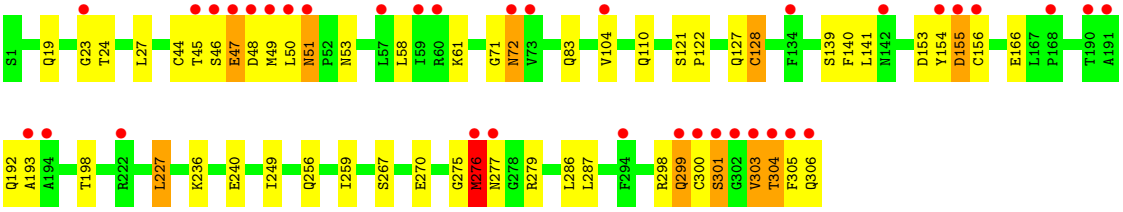
• Molecule 1: 3C-like proteinase



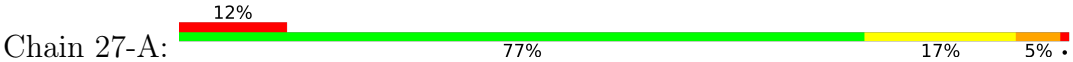


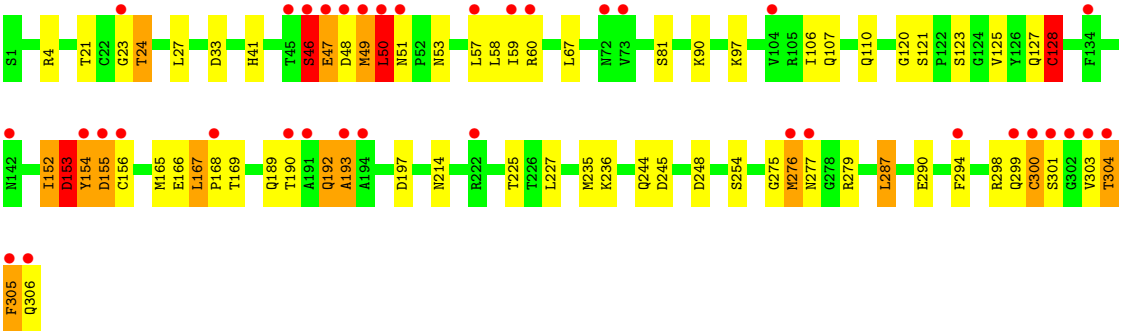
• Molecule 1: 3C-like proteinase





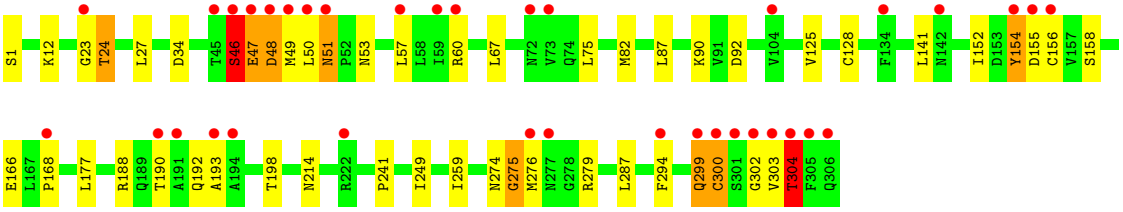
• Molecule 1: 3C-like proteinase





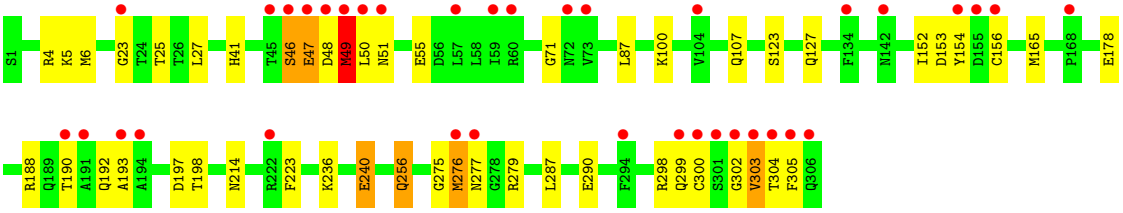
• Molecule 1: 3C-like proteinase

Chain 28-A:



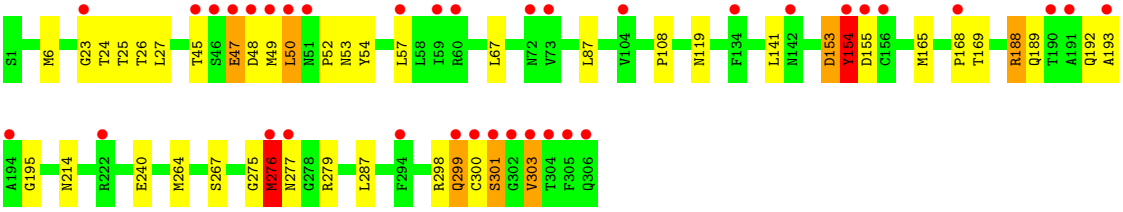
• Molecule 1: 3C-like proteinase

Chain 29-A:



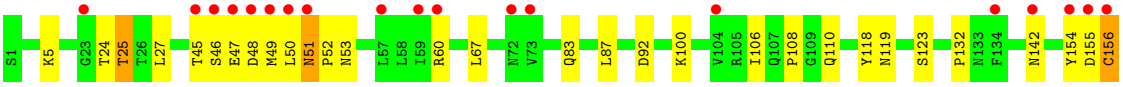
• Molecule 1: 3C-like proteinase

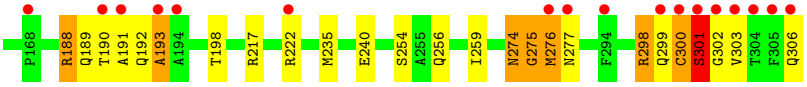
Chain 30-A:



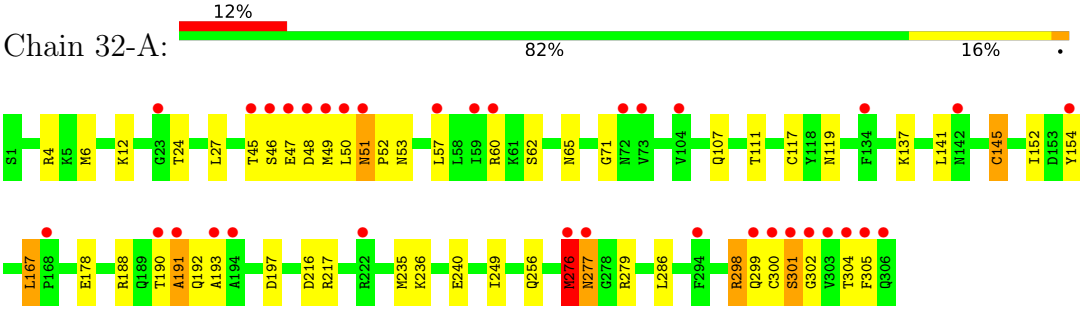
• Molecule 1: 3C-like proteinase

Chain 31-A:

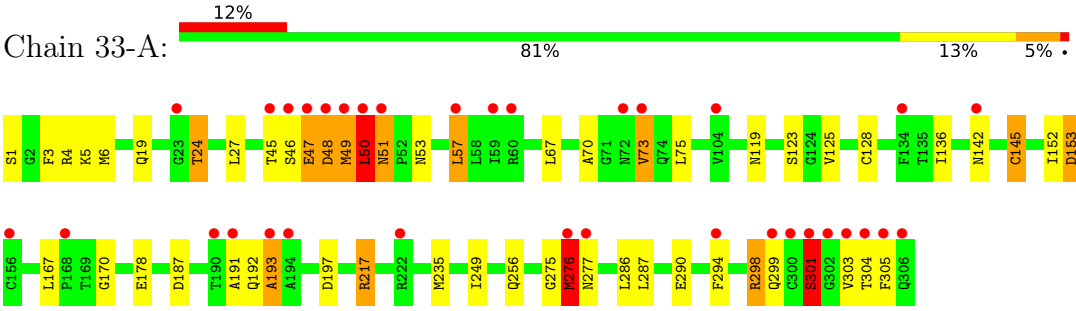




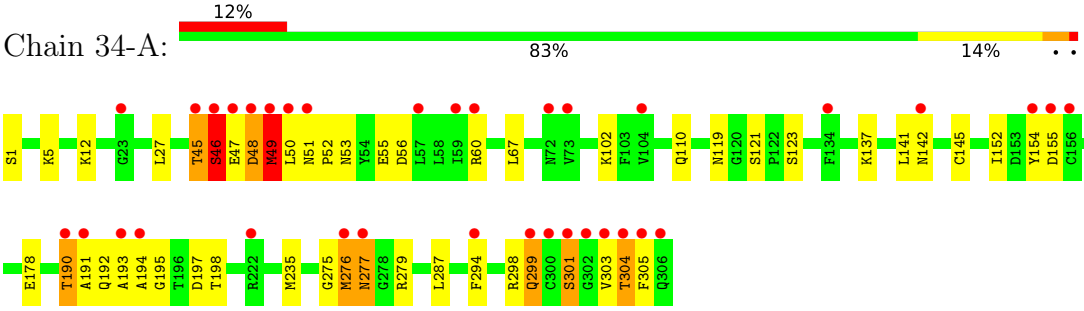
• Molecule 1: 3C-like proteinase



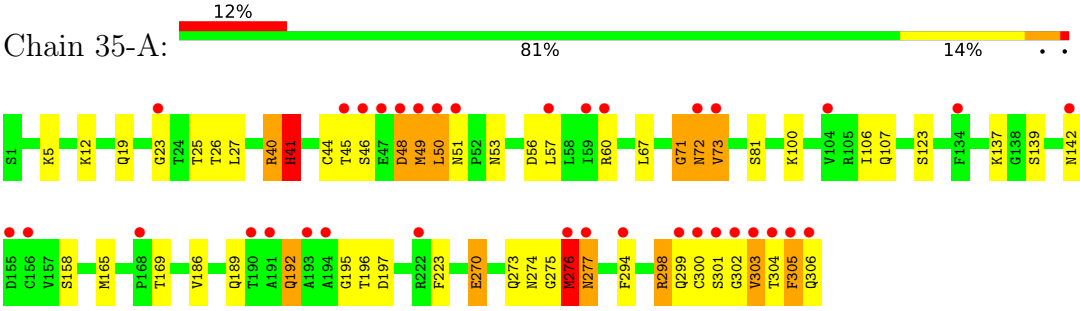
• Molecule 1: 3C-like proteinase



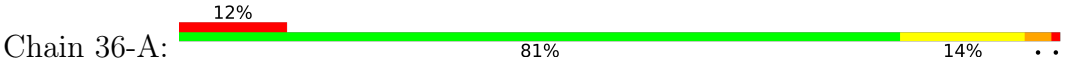
• Molecule 1: 3C-like proteinase

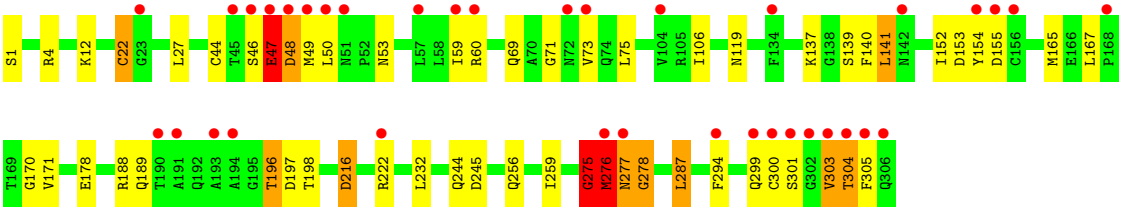


• Molecule 1: 3C-like proteinase



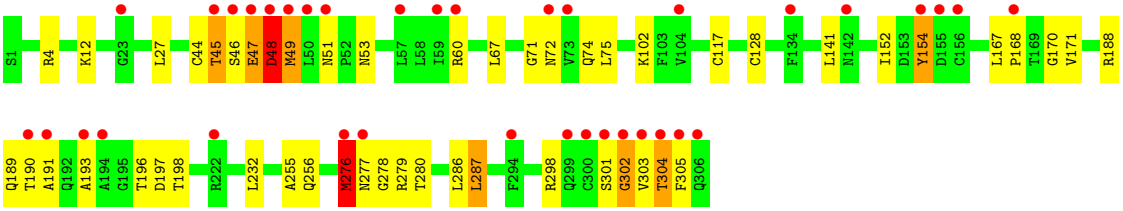
• Molecule 1: 3C-like proteinase





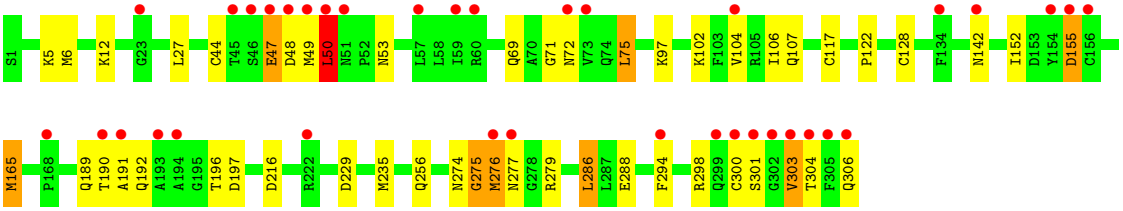
• Molecule 1: 3C-like proteinase

Chain 37-A:



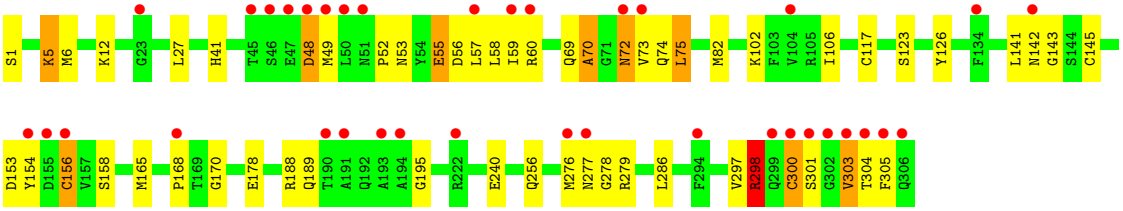
• Molecule 1: 3C-like proteinase

Chain 38-A:



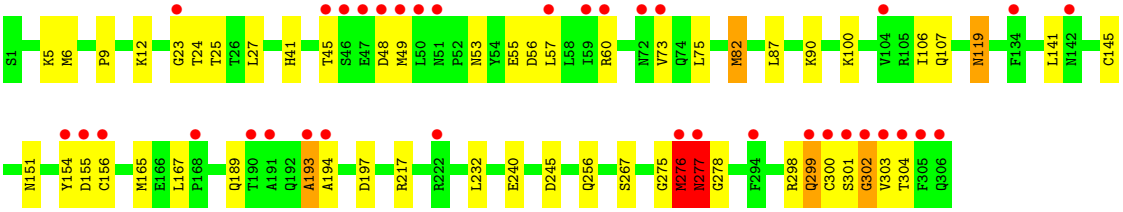
• Molecule 1: 3C-like proteinase

Chain 39-A:



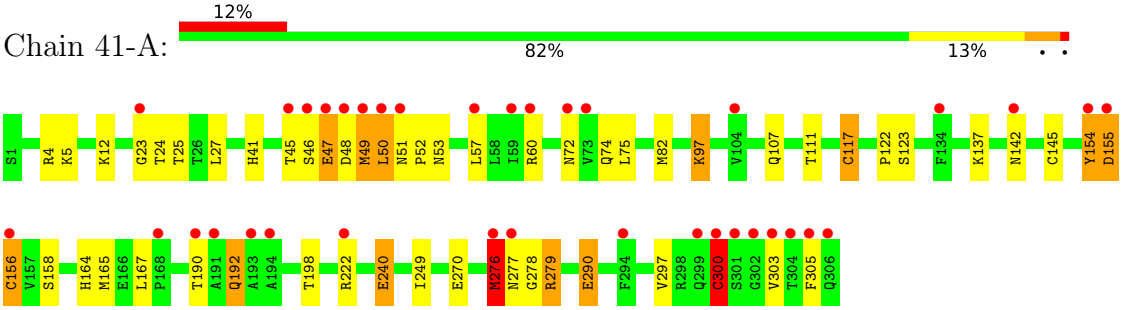
• Molecule 1: 3C-like proteinase

Chain 40-A:



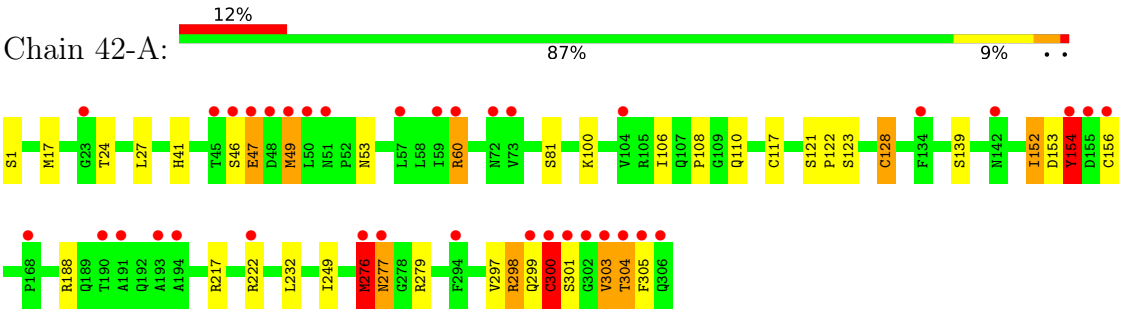
• Molecule 1: 3C-like proteinase

Chain 41-A:



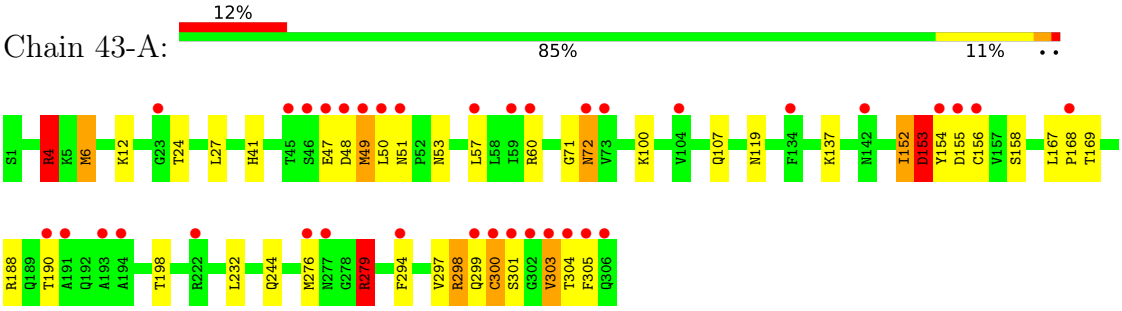
• Molecule 1: 3C-like proteinase

Chain 42-A:



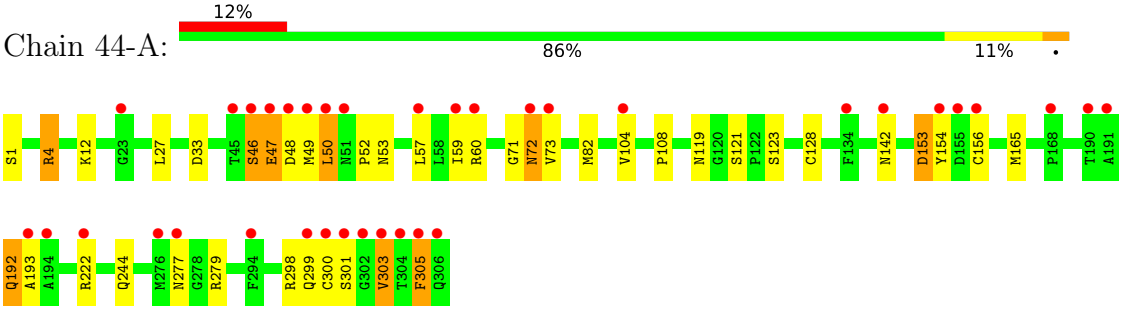
• Molecule 1: 3C-like proteinase

Chain 43-A:



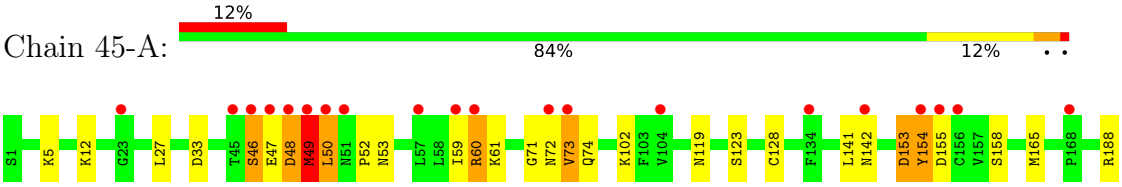
• Molecule 1: 3C-like proteinase

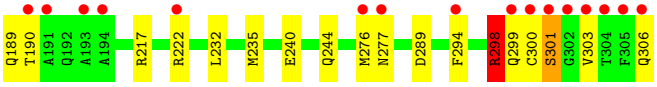
Chain 44-A:



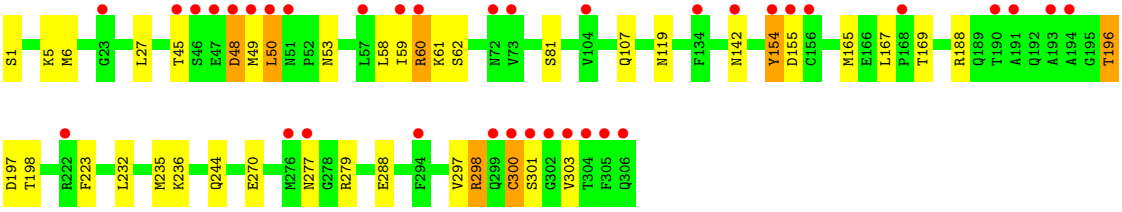
• Molecule 1: 3C-like proteinase

Chain 45-A:

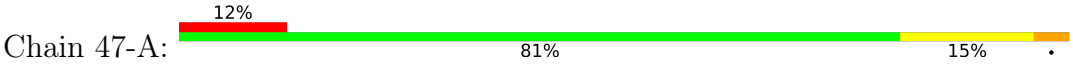


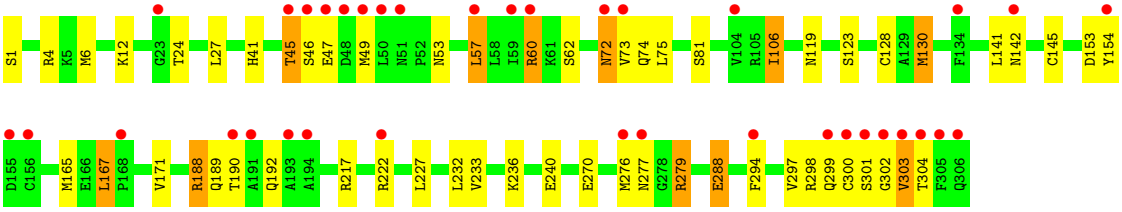


• Molecule 1: 3C-like proteinase

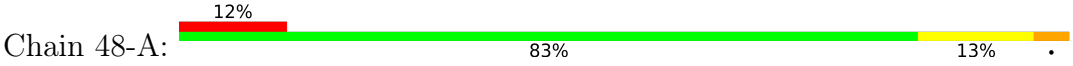


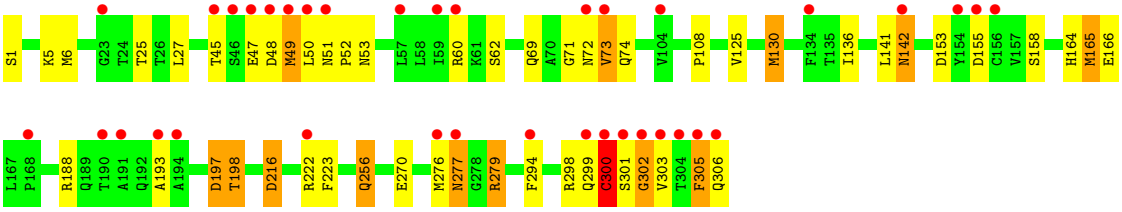
• Molecule 1: 3C-like proteinase



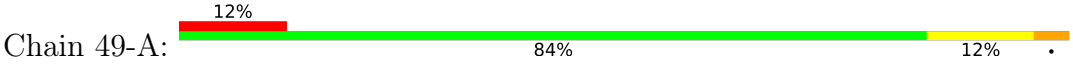


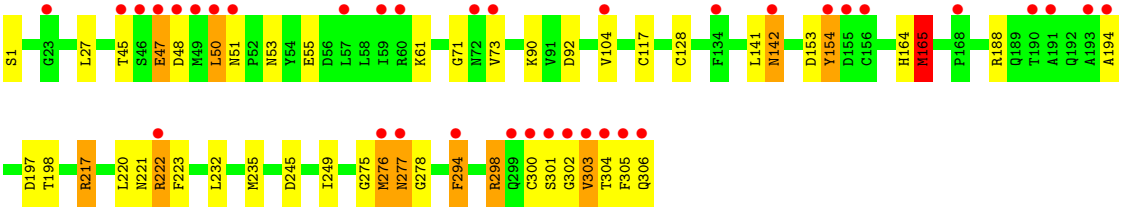
• Molecule 1: 3C-like proteinase



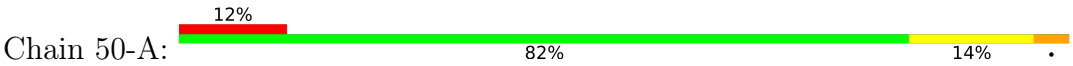


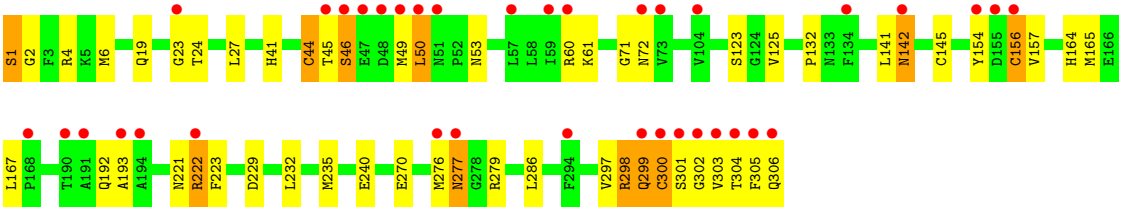
• Molecule 1: 3C-like proteinase





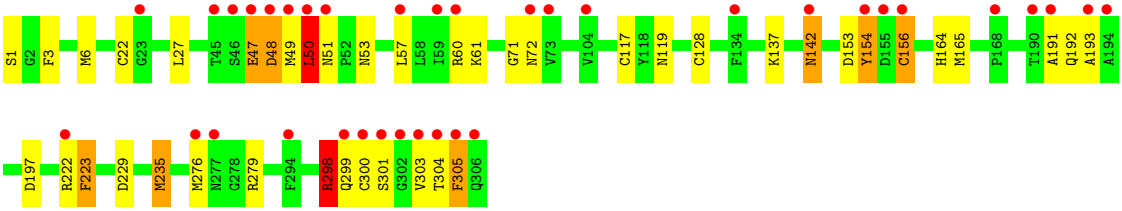
• Molecule 1: 3C-like proteinase





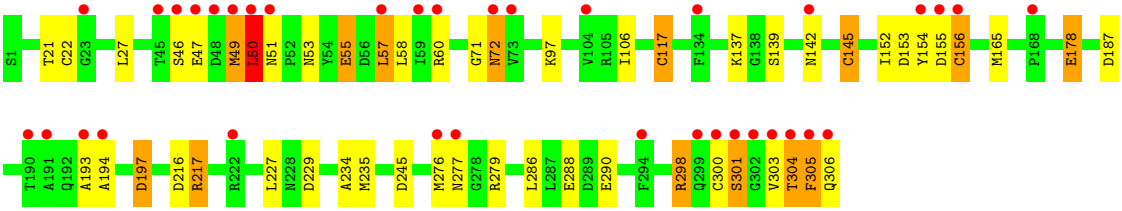
• Molecule 1: 3C-like proteinase

Chain 51-A:



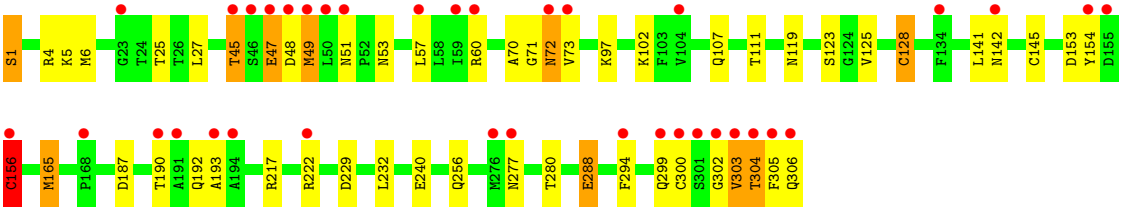
• Molecule 1: 3C-like proteinase

Chain 52-A:



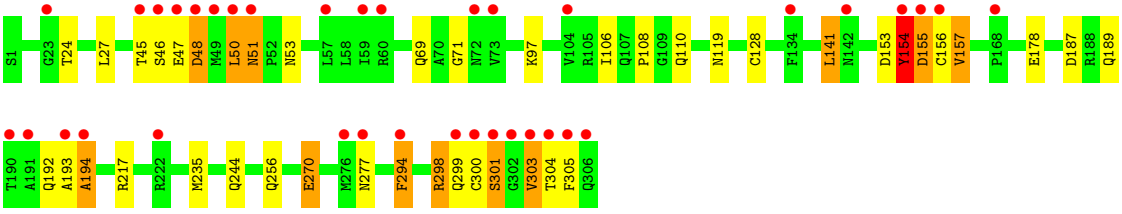
• Molecule 1: 3C-like proteinase

Chain 53-A:



• Molecule 1: 3C-like proteinase

Chain 54-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	113.71Å 53.32Å 44.57Å 90.00° 102.96° 90.00°	Depositor
Resolution (Å)	48.05 – 1.55 48.05 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.05-1.55) 97.7 (48.05-1.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.166 , 0.227 0.177 , 0.243	Depositor DCC
R_{free} test set	1906 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 578.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	264643	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1-A	0.82	6/2420 (0.2%)	0.94	6/3289 (0.2%)
1	2-A	0.73	2/2420 (0.1%)	0.92	9/3289 (0.3%)
1	3-A	0.70	1/2420 (0.0%)	0.91	6/3289 (0.2%)
1	4-A	0.78	2/2420 (0.1%)	0.92	6/3289 (0.2%)
1	5-A	0.76	2/2420 (0.1%)	0.91	3/3289 (0.1%)
1	6-A	0.75	2/2420 (0.1%)	0.91	4/3289 (0.1%)
1	7-A	0.78	3/2420 (0.1%)	0.89	3/3289 (0.1%)
1	8-A	0.78	2/2420 (0.1%)	0.91	3/3289 (0.1%)
1	9-A	0.78	1/2420 (0.0%)	0.96	6/3289 (0.2%)
1	10-A	0.70	0/2420	0.90	2/3289 (0.1%)
1	11-A	0.79	5/2420 (0.2%)	0.93	6/3289 (0.2%)
1	12-A	0.70	1/2420 (0.0%)	0.91	3/3289 (0.1%)
1	13-A	0.76	1/2420 (0.0%)	0.94	4/3289 (0.1%)
1	14-A	0.72	1/2420 (0.0%)	0.90	6/3289 (0.2%)
1	15-A	0.85	4/2420 (0.2%)	0.96	4/3289 (0.1%)
1	16-A	0.74	3/2420 (0.1%)	0.93	6/3289 (0.2%)
1	17-A	0.81	7/2420 (0.3%)	0.96	2/3289 (0.1%)
1	18-A	0.80	4/2420 (0.2%)	0.99	11/3289 (0.3%)
1	19-A	0.73	1/2420 (0.0%)	0.92	2/3289 (0.1%)
1	20-A	0.81	4/2420 (0.2%)	0.93	4/3289 (0.1%)
1	21-A	0.82	2/2420 (0.1%)	0.97	8/3289 (0.2%)
1	22-A	0.79	5/2420 (0.2%)	0.95	4/3289 (0.1%)
1	23-A	0.84	4/2420 (0.2%)	0.94	3/3289 (0.1%)
1	24-A	0.78	4/2420 (0.2%)	0.92	2/3289 (0.1%)
1	25-A	0.81	7/2420 (0.3%)	0.92	4/3289 (0.1%)
1	26-A	0.80	2/2420 (0.1%)	0.92	3/3289 (0.1%)
1	27-A	0.78	2/2420 (0.1%)	0.95	8/3289 (0.2%)
1	28-A	0.75	1/2420 (0.0%)	0.88	0/3289
1	29-A	0.78	4/2420 (0.2%)	0.94	2/3289 (0.1%)
1	30-A	0.72	0/2420	0.93	4/3289 (0.1%)
1	31-A	0.73	3/2420 (0.1%)	0.89	4/3289 (0.1%)
1	32-A	0.72	3/2420 (0.1%)	0.89	0/3289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	33-A	0.78	3/2420 (0.1%)	0.93	8/3289 (0.2%)
1	34-A	0.76	2/2420 (0.1%)	0.92	3/3289 (0.1%)
1	35-A	0.75	3/2420 (0.1%)	0.97	7/3289 (0.2%)
1	36-A	0.77	4/2420 (0.2%)	0.95	5/3289 (0.2%)
1	37-A	0.75	1/2420 (0.0%)	0.92	4/3289 (0.1%)
1	38-A	0.78	4/2420 (0.2%)	0.90	5/3289 (0.2%)
1	39-A	0.89	8/2420 (0.3%)	0.91	3/3289 (0.1%)
1	40-A	0.96	4/2420 (0.2%)	0.94	3/3289 (0.1%)
1	41-A	0.76	6/2420 (0.2%)	0.93	6/3289 (0.2%)
1	42-A	0.76	5/2420 (0.2%)	0.91	7/3289 (0.2%)
1	43-A	0.74	3/2420 (0.1%)	0.90	4/3289 (0.1%)
1	44-A	0.70	0/2420	0.87	0/3289
1	45-A	0.71	1/2420 (0.0%)	0.90	5/3289 (0.2%)
1	46-A	0.74	2/2420 (0.1%)	0.91	3/3289 (0.1%)
1	47-A	0.84	6/2420 (0.2%)	0.95	7/3289 (0.2%)
1	48-A	0.73	1/2420 (0.0%)	0.89	5/3289 (0.2%)
1	49-A	0.72	1/2420 (0.0%)	0.90	4/3289 (0.1%)
1	50-A	0.79	4/2420 (0.2%)	0.90	1/3289 (0.0%)
1	51-A	0.77	6/2420 (0.2%)	0.93	6/3289 (0.2%)
1	52-A	0.78	6/2420 (0.2%)	0.95	11/3289 (0.3%)
1	53-A	0.86	5/2420 (0.2%)	0.90	2/3289 (0.1%)
1	54-A	0.78	5/2420 (0.2%)	0.93	4/3289 (0.1%)
All	All	0.77	169/130680 (0.1%)	0.92	241/177606 (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	9
1	2-A	0	4
1	3-A	0	6
1	4-A	0	4
1	5-A	0	2
1	6-A	0	5
1	7-A	0	6
1	8-A	0	9
1	9-A	0	7
1	10-A	0	7
1	11-A	0	6
1	12-A	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	13-A	0	13
1	14-A	0	12
1	15-A	0	6
1	16-A	0	10
1	17-A	0	9
1	18-A	0	12
1	19-A	0	13
1	20-A	0	9
1	21-A	0	10
1	22-A	0	7
1	23-A	0	8
1	24-A	0	8
1	25-A	0	10
1	26-A	0	12
1	27-A	0	8
1	28-A	0	6
1	29-A	0	6
1	30-A	0	8
1	31-A	0	10
1	32-A	0	5
1	33-A	0	13
1	34-A	0	11
1	35-A	0	14
1	36-A	0	8
1	37-A	0	7
1	38-A	0	5
1	39-A	0	10
1	40-A	0	7
1	41-A	0	6
1	42-A	0	7
1	43-A	0	7
1	44-A	0	4
1	45-A	0	7
1	46-A	0	8
1	47-A	0	6
1	48-A	0	8
1	49-A	0	10
1	50-A	0	9
1	51-A	0	7
1	52-A	0	6
1	53-A	0	8
1	54-A	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	434

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	40-A	145	CYS	CB-SG	27.83	2.29	1.82
1	53-A	128	CYS	CB-SG	-19.86	1.48	1.82
1	39-A	145	CYS	CB-SG	18.45	2.13	1.82
1	15-A	145	CYS	CB-SG	17.86	2.12	1.82
1	18-A	128	CYS	CB-SG	16.59	2.10	1.82

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	19-A	156	CYS	CA-CB-SG	-15.62	85.88	114.00
1	40-A	145	CYS	CA-CB-SG	14.02	139.24	114.00
1	23-A	156	CYS	CA-CB-SG	-13.82	89.12	114.00
1	35-A	41	HIS	N-CA-CB	13.06	134.12	110.60
1	15-A	145	CYS	CA-CB-SG	10.60	133.07	114.00

There are no chirality outliers.

5 of 434 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	48	ASP	Peptide
1	1-A	49	MET	Peptide
1	1-A	69	GLN	Peptide
1	1-A	70	ALA	Peptide
1	1-A	72	ASN	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	2314	2313	0	0
1	2-A	2367	2314	2313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-A	2367	2314	2313	0	0
1	4-A	2367	2314	2313	0	0
1	5-A	2367	2314	2313	0	0
1	6-A	2367	2314	2313	0	0
1	7-A	2367	2314	2313	0	0
1	8-A	2367	2314	2313	0	0
1	9-A	2367	2314	2313	0	0
1	10-A	2367	2314	2313	0	0
1	11-A	2367	2314	2313	0	0
1	12-A	2367	2314	2313	0	0
1	13-A	2367	2314	2313	0	0
1	14-A	2367	2314	2312	0	0
1	15-A	2367	2314	2314	0	0
1	16-A	2367	2314	2313	0	0
1	17-A	2367	2314	2313	0	0
1	18-A	2367	2314	2312	0	0
1	19-A	2367	2314	2313	0	0
1	20-A	2367	2314	2312	0	0
1	21-A	2367	2314	2314	0	0
1	22-A	2367	2314	2313	0	0
1	23-A	2367	2314	2313	0	0
1	24-A	2367	2314	2313	0	0
1	25-A	2367	2314	2313	0	0
1	26-A	2367	2314	2313	0	0
1	27-A	2367	2314	2313	0	0
1	28-A	2367	2314	2313	0	0
1	29-A	2367	2314	2313	0	0
1	30-A	2367	2314	2313	0	0
1	31-A	2367	2314	2313	0	0
1	32-A	2367	2314	2313	0	0
1	33-A	2367	2314	2313	0	0
1	34-A	2367	2314	2313	0	0
1	35-A	2367	2314	2311	0	0
1	36-A	2367	2314	2313	0	0
1	37-A	2367	2314	2313	0	0
1	38-A	2367	2314	2312	0	0
1	39-A	2367	2314	2313	0	0
1	40-A	2367	2314	2313	0	0
1	41-A	2367	2314	2313	0	0
1	42-A	2367	2314	2313	0	0
1	43-A	2367	2314	2313	0	0
1	44-A	2367	2314	2313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	45-A	2367	2314	2313	0	0
1	46-A	2367	2314	2313	0	0
1	47-A	2367	2314	2312	0	0
1	48-A	2367	2314	2313	0	0
1	49-A	2367	2314	2313	0	0
1	50-A	2367	2314	2313	0	0
1	51-A	2367	2314	2313	0	0
1	52-A	2367	2314	2313	0	0
1	53-A	2367	2314	2313	0	0
1	54-A	2367	2314	2313	0	0
2	1-A	20	30	30	0	0
2	2-A	20	30	30	0	0
2	3-A	20	30	30	0	0
2	4-A	20	30	30	0	0
2	5-A	20	30	30	0	0
2	6-A	20	30	30	0	0
2	7-A	20	30	30	0	0
2	8-A	20	30	30	0	0
2	9-A	20	30	30	0	0
2	10-A	20	30	30	0	0
2	11-A	20	30	30	0	0
2	12-A	20	30	30	0	0
2	13-A	20	30	30	0	0
2	14-A	20	30	30	0	0
2	15-A	20	30	30	0	0
2	16-A	20	30	30	0	0
2	17-A	20	30	30	0	0
2	18-A	20	30	30	0	0
2	19-A	20	30	30	0	0
2	20-A	20	30	30	0	0
2	21-A	20	30	30	0	0
2	22-A	20	30	30	0	0
2	23-A	20	30	30	0	0
2	24-A	20	30	30	0	0
2	25-A	20	30	30	0	0
2	26-A	20	30	30	0	0
2	27-A	20	30	30	0	0
2	28-A	20	30	30	0	0
2	29-A	20	30	30	0	0
2	30-A	20	30	30	0	0
2	31-A	20	30	30	0	0
2	32-A	20	30	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	33-A	20	30	30	0	0
2	34-A	20	30	30	0	0
2	35-A	20	30	30	0	0
2	36-A	20	30	30	0	0
2	37-A	20	30	30	0	0
2	38-A	20	30	30	0	0
2	39-A	20	30	30	0	0
2	40-A	20	30	30	0	0
2	41-A	20	30	30	0	0
2	42-A	20	30	30	0	0
2	43-A	20	30	30	0	0
2	44-A	20	30	30	0	0
2	45-A	20	30	30	0	0
2	46-A	20	30	30	0	0
2	47-A	20	30	30	0	0
2	48-A	20	30	30	0	0
2	49-A	20	30	30	0	0
2	50-A	20	30	30	0	0
2	51-A	20	30	30	0	0
2	52-A	20	30	30	0	0
2	53-A	20	30	30	0	0
2	54-A	20	30	30	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	21-A	1	0	0	0	0
3	22-A	1	0	0	0	0
3	23-A	1	0	0	0	0
3	24-A	1	0	0	0	0
3	25-A	1	0	0	0	0
3	26-A	1	0	0	0	0
3	27-A	1	0	0	0	0
3	28-A	1	0	0	0	0
3	29-A	1	0	0	0	0
3	30-A	1	0	0	0	0
3	31-A	1	0	0	0	0
3	32-A	1	0	0	0	0
3	33-A	1	0	0	0	0
3	34-A	1	0	0	0	0
3	35-A	1	0	0	0	0
3	36-A	1	0	0	0	0
3	37-A	1	0	0	0	0
3	38-A	1	0	0	0	0
3	39-A	1	0	0	0	0
3	40-A	1	0	0	0	0
3	41-A	1	0	0	0	0
3	42-A	1	0	0	0	0
3	43-A	1	0	0	0	0
3	44-A	1	0	0	0	0
3	45-A	1	0	0	0	0
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
4	1-A	190	0	0	0	0
4	2-A	172	0	0	0	0
4	3-A	162	0	0	0	0
4	4-A	157	0	0	0	0
4	5-A	164	0	0	0	0
4	6-A	181	0	0	0	0
4	7-A	173	0	0	0	0
4	8-A	177	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	9-A	174	0	0	0	0
4	10-A	168	0	0	0	0
4	11-A	164	0	0	0	0
4	12-A	195	0	0	0	0
4	13-A	196	0	0	0	0
4	14-A	152	0	0	0	0
4	15-A	164	0	0	0	0
4	16-A	166	0	0	0	0
4	17-A	176	0	0	0	0
4	18-A	177	0	0	0	0
4	19-A	160	0	0	0	0
4	20-A	161	0	0	0	0
4	21-A	179	0	0	0	0
4	22-A	175	0	0	0	0
4	23-A	170	0	0	0	0
4	24-A	164	0	0	0	0
4	25-A	166	0	0	0	0
4	26-A	178	0	0	0	0
4	27-A	181	0	0	0	0
4	28-A	167	0	0	0	0
4	29-A	158	0	0	0	0
4	30-A	170	0	0	0	0
4	31-A	183	0	0	0	0
4	32-A	169	0	0	0	0
4	33-A	181	0	0	0	0
4	34-A	182	0	0	0	0
4	35-A	165	0	0	0	0
4	36-A	165	0	0	0	0
4	37-A	169	0	0	0	0
4	38-A	170	0	0	0	0
4	39-A	182	0	0	0	0
4	40-A	172	0	0	0	0
4	41-A	158	0	0	0	0
4	42-A	163	0	0	0	0
4	43-A	164	0	0	0	0
4	44-A	172	0	0	0	0
4	45-A	150	0	0	0	0
4	46-A	162	0	0	0	0
4	47-A	152	0	0	0	0
4	48-A	151	0	0	0	0
4	49-A	145	0	0	0	0
4	50-A	185	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	51-A	168	0	0	0	0
4	52-A	151	0	0	0	0
4	53-A	145	0	0	0	0
4	54-A	174	0	0	0	0
All	All	138067	126576	126517	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%)	277 (91%)	17 (6%)	10 (3%)	4 0
1	2-A	304/306 (99%)	277 (91%)	18 (6%)	9 (3%)	4 0
1	3-A	304/306 (99%)	280 (92%)	16 (5%)	8 (3%)	5 0
1	4-A	304/306 (99%)	281 (92%)	12 (4%)	11 (4%)	3 0
1	5-A	304/306 (99%)	271 (89%)	22 (7%)	11 (4%)	3 0
1	6-A	304/306 (99%)	274 (90%)	16 (5%)	14 (5%)	2 0
1	7-A	304/306 (99%)	273 (90%)	15 (5%)	16 (5%)	2 0
1	8-A	304/306 (99%)	273 (90%)	20 (7%)	11 (4%)	3 0
1	9-A	304/306 (99%)	265 (87%)	16 (5%)	23 (8%)	1 0
1	10-A	304/306 (99%)	273 (90%)	13 (4%)	18 (6%)	1 0
1	11-A	304/306 (99%)	266 (88%)	24 (8%)	14 (5%)	2 0
1	12-A	304/306 (99%)	270 (89%)	15 (5%)	19 (6%)	1 0
1	13-A	304/306 (99%)	271 (89%)	18 (6%)	15 (5%)	2 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	14-A	304/306 (99%)	266 (88%)	25 (8%)	13 (4%)	2	0
1	15-A	304/306 (99%)	265 (87%)	26 (9%)	13 (4%)	2	0
1	16-A	304/306 (99%)	269 (88%)	16 (5%)	19 (6%)	1	0
1	17-A	304/306 (99%)	262 (86%)	24 (8%)	18 (6%)	1	0
1	18-A	304/306 (99%)	257 (84%)	28 (9%)	19 (6%)	1	0
1	19-A	304/306 (99%)	258 (85%)	25 (8%)	21 (7%)	1	0
1	20-A	304/306 (99%)	263 (86%)	22 (7%)	19 (6%)	1	0
1	21-A	304/306 (99%)	260 (86%)	24 (8%)	20 (7%)	1	0
1	22-A	304/306 (99%)	261 (86%)	23 (8%)	20 (7%)	1	0
1	23-A	304/306 (99%)	265 (87%)	21 (7%)	18 (6%)	1	0
1	24-A	304/306 (99%)	264 (87%)	25 (8%)	15 (5%)	2	0
1	25-A	304/306 (99%)	264 (87%)	22 (7%)	18 (6%)	1	0
1	26-A	304/306 (99%)	269 (88%)	22 (7%)	13 (4%)	2	0
1	27-A	304/306 (99%)	266 (88%)	15 (5%)	23 (8%)	1	0
1	28-A	304/306 (99%)	269 (88%)	21 (7%)	14 (5%)	2	0
1	29-A	304/306 (99%)	272 (90%)	18 (6%)	14 (5%)	2	0
1	30-A	304/306 (99%)	271 (89%)	14 (5%)	19 (6%)	1	0
1	31-A	304/306 (99%)	264 (87%)	24 (8%)	16 (5%)	2	0
1	32-A	304/306 (99%)	262 (86%)	25 (8%)	17 (6%)	2	0
1	33-A	304/306 (99%)	266 (88%)	19 (6%)	19 (6%)	1	0
1	34-A	304/306 (99%)	269 (88%)	15 (5%)	20 (7%)	1	0
1	35-A	304/306 (99%)	268 (88%)	22 (7%)	14 (5%)	2	0
1	36-A	304/306 (99%)	267 (88%)	20 (7%)	17 (6%)	2	0
1	37-A	304/306 (99%)	277 (91%)	13 (4%)	14 (5%)	2	0
1	38-A	304/306 (99%)	270 (89%)	23 (8%)	11 (4%)	3	0
1	39-A	304/306 (99%)	267 (88%)	23 (8%)	14 (5%)	2	0
1	40-A	304/306 (99%)	266 (88%)	23 (8%)	15 (5%)	2	0
1	41-A	304/306 (99%)	262 (86%)	26 (9%)	16 (5%)	2	0
1	42-A	304/306 (99%)	266 (88%)	25 (8%)	13 (4%)	2	0
1	43-A	304/306 (99%)	270 (89%)	20 (7%)	14 (5%)	2	0
1	44-A	304/306 (99%)	266 (88%)	21 (7%)	17 (6%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	45-A	304/306 (99%)	269 (88%)	21 (7%)	14 (5%)	2	0
1	46-A	304/306 (99%)	268 (88%)	26 (9%)	10 (3%)	4	0
1	47-A	304/306 (99%)	266 (88%)	23 (8%)	15 (5%)	2	0
1	48-A	304/306 (99%)	268 (88%)	16 (5%)	20 (7%)	1	0
1	49-A	304/306 (99%)	266 (88%)	23 (8%)	15 (5%)	2	0
1	50-A	304/306 (99%)	264 (87%)	22 (7%)	18 (6%)	1	0
1	51-A	304/306 (99%)	270 (89%)	18 (6%)	16 (5%)	2	0
1	52-A	304/306 (99%)	271 (89%)	21 (7%)	12 (4%)	3	0
1	53-A	304/306 (99%)	278 (91%)	15 (5%)	11 (4%)	3	0
1	54-A	304/306 (99%)	267 (88%)	23 (8%)	14 (5%)	2	0
All	All	16416/16524 (99%)	14479 (88%)	1100 (7%)	837 (5%)	2	0

5 of 837 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	51	ASN
1	1-A	53	ASN
1	1-A	155	ASP
1	1-A	193	ALA
1	2-A	46	SER

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%)	228 (87%)	35 (13%)	4	0
1	2-A	263/263 (100%)	232 (88%)	31 (12%)	5	0
1	3-A	263/263 (100%)	235 (89%)	28 (11%)	6	0
1	4-A	263/263 (100%)	230 (88%)	33 (12%)	4	0
1	5-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	6-A	263/263 (100%)	225 (86%)	38 (14%)	3	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-A	263/263 (100%)	231 (88%)	32 (12%)	5	0
1	8-A	263/263 (100%)	233 (89%)	30 (11%)	5	0
1	9-A	263/263 (100%)	233 (89%)	30 (11%)	5	0
1	10-A	263/263 (100%)	226 (86%)	37 (14%)	3	0
1	11-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	12-A	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	13-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	14-A	263/263 (100%)	228 (87%)	35 (13%)	4	0
1	15-A	263/263 (100%)	229 (87%)	34 (13%)	4	0
1	16-A	263/263 (100%)	236 (90%)	27 (10%)	7	0
1	17-A	263/263 (100%)	222 (84%)	41 (16%)	2	0
1	18-A	263/263 (100%)	226 (86%)	37 (14%)	3	0
1	19-A	263/263 (100%)	225 (86%)	38 (14%)	3	0
1	20-A	263/263 (100%)	219 (83%)	44 (17%)	2	0
1	21-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	22-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	23-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	24-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	25-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	26-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	27-A	263/263 (100%)	209 (80%)	54 (20%)	1	0
1	28-A	263/263 (100%)	220 (84%)	43 (16%)	2	0
1	29-A	263/263 (100%)	231 (88%)	32 (12%)	5	0
1	30-A	263/263 (100%)	237 (90%)	26 (10%)	8	0
1	31-A	263/263 (100%)	227 (86%)	36 (14%)	3	0
1	32-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	33-A	263/263 (100%)	225 (86%)	38 (14%)	3	0
1	34-A	263/263 (100%)	233 (89%)	30 (11%)	5	0
1	35-A	263/263 (100%)	221 (84%)	42 (16%)	2	0
1	36-A	263/263 (100%)	224 (85%)	39 (15%)	3	0
1	37-A	263/263 (100%)	227 (86%)	36 (14%)	3	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	38-A	263/263 (100%)	228 (87%)	35 (13%)	4 0
1	39-A	263/263 (100%)	229 (87%)	34 (13%)	4 0
1	40-A	263/263 (100%)	227 (86%)	36 (14%)	3 0
1	41-A	263/263 (100%)	223 (85%)	40 (15%)	3 0
1	42-A	263/263 (100%)	234 (89%)	29 (11%)	6 0
1	43-A	263/263 (100%)	232 (88%)	31 (12%)	5 0
1	44-A	263/263 (100%)	233 (89%)	30 (11%)	5 0
1	45-A	263/263 (100%)	229 (87%)	34 (13%)	4 0
1	46-A	263/263 (100%)	238 (90%)	25 (10%)	8 0
1	47-A	263/263 (100%)	225 (86%)	38 (14%)	3 0
1	48-A	263/263 (100%)	227 (86%)	36 (14%)	3 0
1	49-A	263/263 (100%)	230 (88%)	33 (12%)	4 0
1	50-A	263/263 (100%)	229 (87%)	34 (13%)	4 0
1	51-A	263/263 (100%)	240 (91%)	23 (9%)	10 1
1	52-A	263/263 (100%)	226 (86%)	37 (14%)	3 0
1	53-A	263/263 (100%)	223 (85%)	40 (15%)	3 0
1	54-A	263/263 (100%)	236 (90%)	27 (10%)	7 0
All	All	14202/14202 (100%)	12290 (86%)	1912 (14%)	4 0

5 of 1912 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	26-A	276	MET
1	50-A	229	ASP
1	32-A	167	LEU
1	50-A	27	LEU
1	54-A	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 440 such sidechains are listed below:

Mol	Chain	Res	Type
1	31-A	110	GLN
1	37-A	273	GLN
1	54-A	273	GLN
1	50-A	192	GLN

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Mol	Chain	Res	Type
1	32-A	19	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 324 ligands modelled in this entry, 54 are monoatomic - leaving 270 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	49-A	405	-	3,3,3	0.55	0	3,3,3	1.28	0
2	DMS	33-A	403	-	3,3,3	0.59	0	3,3,3	1.13	0
2	DMS	9-A	405	-	3,3,3	0.79	0	3,3,3	3.20	3 (100%)
2	DMS	48-A	403	-	3,3,3	0.65	0	3,3,3	1.09	0
2	DMS	52-A	401	-	3,3,3	0.41	0	3,3,3	0.93	0
2	DMS	44-A	401	-	3,3,3	0.48	0	3,3,3	1.73	1 (33%)
2	DMS	54-A	403	-	3,3,3	0.72	0	3,3,3	0.95	0
2	DMS	18-A	404	-	3,3,3	0.74	0	3,3,3	1.95	1 (33%)
2	DMS	13-A	404	-	3,3,3	0.82	0	3,3,3	1.16	0
2	DMS	49-A	403	-	3,3,3	0.65	0	3,3,3	1.02	0
2	DMS	52-A	402	-	3,3,3	0.66	0	3,3,3	0.86	0
2	DMS	44-A	402	-	3,3,3	0.75	0	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	51-A	403	-	3,3,3	0.71	0	3,3,3	0.82	0
2	DMS	11-A	401	-	3,3,3	0.83	0	3,3,3	1.50	1 (33%)
2	DMS	9-A	403	-	3,3,3	0.59	0	3,3,3	3.14	3 (100%)
2	DMS	15-A	403	-	3,3,3	0.88	0	3,3,3	1.25	0
2	DMS	1-A	405	-	3,3,3	0.70	0	3,3,3	2.55	2 (66%)
2	DMS	45-A	401	-	3,3,3	0.73	0	3,3,3	3.38	2 (66%)
2	DMS	4-A	401	-	3,3,3	0.80	0	3,3,3	1.12	0
2	DMS	37-A	402	-	3,3,3	0.84	0	3,3,3	0.23	0
2	DMS	14-A	403	-	3,3,3	0.65	0	3,3,3	1.42	0
2	DMS	48-A	405	-	3,3,3	0.89	0	3,3,3	1.56	1 (33%)
2	DMS	46-A	404	-	3,3,3	0.65	0	3,3,3	1.19	0
2	DMS	54-A	405	-	3,3,3	0.83	0	3,3,3	2.18	2 (66%)
2	DMS	16-A	403	-	3,3,3	0.68	0	3,3,3	1.29	0
2	DMS	35-A	401	-	3,3,3	0.49	0	3,3,3	0.75	0
2	DMS	22-A	403	-	3,3,3	0.65	0	3,3,3	1.12	0
2	DMS	21-A	404	-	3,3,3	0.82	0	3,3,3	0.38	0
2	DMS	7-A	401	-	3,3,3	0.58	0	3,3,3	0.43	0
2	DMS	12-A	404	-	3,3,3	0.81	0	3,3,3	0.73	0
2	DMS	39-A	402	-	3,3,3	0.69	0	3,3,3	1.15	0
2	DMS	26-A	402	-	3,3,3	0.72	0	3,3,3	0.31	0
2	DMS	11-A	404	-	3,3,3	0.72	0	3,3,3	0.44	0
2	DMS	32-A	401	-	3,3,3	0.51	0	3,3,3	1.06	0
2	DMS	9-A	402	-	3,3,3	0.70	0	3,3,3	1.63	1 (33%)
2	DMS	18-A	405	-	3,3,3	0.76	0	3,3,3	0.62	0
2	DMS	30-A	405	-	3,3,3	0.67	0	3,3,3	0.39	0
2	DMS	46-A	405	-	3,3,3	0.80	0	3,3,3	0.52	0
2	DMS	18-A	401	-	3,3,3	0.42	0	3,3,3	0.59	0
2	DMS	11-A	403	-	3,3,3	0.77	0	3,3,3	0.11	0
2	DMS	47-A	401	-	3,3,3	0.59	0	3,3,3	0.89	0
2	DMS	10-A	403	-	3,3,3	0.50	0	3,3,3	1.44	0
2	DMS	14-A	405	-	3,3,3	0.55	0	3,3,3	2.06	1 (33%)
2	DMS	31-A	401	-	3,3,3	0.41	0	3,3,3	1.11	0
2	DMS	42-A	405	-	3,3,3	0.82	0	3,3,3	0.73	0
2	DMS	13-A	402	-	3,3,3	0.69	0	3,3,3	1.34	1 (33%)
2	DMS	34-A	402	-	3,3,3	0.68	0	3,3,3	1.49	1 (33%)
2	DMS	45-A	403	-	3,3,3	0.69	0	3,3,3	1.26	0
2	DMS	21-A	405	-	3,3,3	0.62	0	3,3,3	2.35	2 (66%)
2	DMS	20-A	403	-	3,3,3	0.80	0	3,3,3	1.17	0
2	DMS	35-A	404	-	3,3,3	0.64	0	3,3,3	0.68	0
2	DMS	47-A	402	-	3,3,3	0.82	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	5-A	405	-	3,3,3	0.67	0	3,3,3	0.60	0
2	DMS	25-A	401	-	3,3,3	0.47	0	3,3,3	0.55	0
2	DMS	37-A	404	-	3,3,3	0.62	0	3,3,3	0.93	0
2	DMS	22-A	402	-	3,3,3	0.66	0	3,3,3	1.31	0
2	DMS	41-A	401	-	3,3,3	0.46	0	3,3,3	1.59	1 (33%)
2	DMS	35-A	403	-	3,3,3	0.76	0	3,3,3	1.20	0
2	DMS	38-A	404	-	3,3,3	0.68	0	3,3,3	1.07	0
2	DMS	25-A	402	-	3,3,3	0.78	0	3,3,3	0.19	0
2	DMS	24-A	402	-	3,3,3	0.74	0	3,3,3	1.05	0
2	DMS	12-A	403	-	3,3,3	0.77	0	3,3,3	0.40	0
2	DMS	32-A	403	-	3,3,3	0.77	0	3,3,3	0.79	0
2	DMS	10-A	405	-	3,3,3	0.75	0	3,3,3	0.70	0
2	DMS	38-A	405	-	3,3,3	0.85	0	3,3,3	0.55	0
2	DMS	12-A	401	-	3,3,3	0.56	0	3,3,3	0.88	0
2	DMS	3-A	404	-	3,3,3	0.68	0	3,3,3	0.62	0
2	DMS	51-A	405	-	3,3,3	0.77	0	3,3,3	1.55	1 (33%)
2	DMS	1-A	401	-	3,3,3	0.50	0	3,3,3	0.39	0
2	DMS	20-A	405	-	3,3,3	0.75	0	3,3,3	1.92	1 (33%)
2	DMS	23-A	403	-	3,3,3	0.57	0	3,3,3	1.07	0
2	DMS	45-A	405	-	3,3,3	0.63	0	3,3,3	1.00	0
2	DMS	9-A	401	-	3,3,3	0.56	0	3,3,3	0.88	0
2	DMS	53-A	403	-	3,3,3	0.70	0	3,3,3	2.33	1 (33%)
2	DMS	36-A	402	-	3,3,3	0.73	0	3,3,3	2.07	2 (66%)
2	DMS	2-A	404	-	3,3,3	0.55	0	3,3,3	1.35	1 (33%)
2	DMS	27-A	405	-	3,3,3	0.73	0	3,3,3	0.97	0
2	DMS	1-A	402	-	3,3,3	0.74	0	3,3,3	0.31	0
2	DMS	53-A	402	-	3,3,3	0.63	0	3,3,3	1.14	0
2	DMS	54-A	401	-	3,3,3	0.48	0	3,3,3	0.39	0
2	DMS	31-A	404	-	3,3,3	0.55	0	3,3,3	0.66	0
2	DMS	39-A	403	-	3,3,3	0.63	0	3,3,3	0.88	0
2	DMS	50-A	404	-	3,3,3	0.76	0	3,3,3	1.25	0
2	DMS	32-A	402	-	3,3,3	0.79	0	3,3,3	1.02	0
2	DMS	41-A	403	-	3,3,3	0.64	0	3,3,3	0.76	0
2	DMS	32-A	405	-	3,3,3	0.70	0	3,3,3	1.74	1 (33%)
2	DMS	54-A	402	-	3,3,3	0.55	0	3,3,3	1.92	1 (33%)
2	DMS	11-A	402	-	3,3,3	0.84	0	3,3,3	1.88	1 (33%)
2	DMS	43-A	402	-	3,3,3	0.79	0	3,3,3	0.82	0
2	DMS	2-A	401	-	3,3,3	0.58	0	3,3,3	0.28	0
2	DMS	13-A	405	-	3,3,3	0.75	0	3,3,3	0.86	0
2	DMS	36-A	401	-	3,3,3	0.46	0	3,3,3	0.47	0
2	DMS	31-A	405	-	3,3,3	0.88	0	3,3,3	1.74	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	2-A	402	-	3,3,3	0.57	0	3,3,3	0.71	0
2	DMS	15-A	402	-	3,3,3	0.89	0	3,3,3	0.44	0
2	DMS	1-A	403	-	3,3,3	0.68	0	3,3,3	0.43	0
2	DMS	6-A	404	-	3,3,3	0.78	0	3,3,3	1.19	0
2	DMS	18-A	402	-	3,3,3	0.59	0	3,3,3	3.10	3 (100%)
2	DMS	30-A	402	-	3,3,3	0.69	0	3,3,3	1.26	1 (33%)
2	DMS	52-A	404	-	3,3,3	0.67	0	3,3,3	1.82	1 (33%)
2	DMS	17-A	402	-	3,3,3	0.73	0	3,3,3	1.07	0
2	DMS	36-A	403	-	3,3,3	0.80	0	3,3,3	0.89	0
2	DMS	42-A	402	-	3,3,3	0.90	0	3,3,3	0.99	0
2	DMS	36-A	404	-	3,3,3	0.67	0	3,3,3	1.42	0
2	DMS	21-A	402	-	3,3,3	0.74	0	3,3,3	1.35	0
2	DMS	15-A	404	-	3,3,3	0.68	0	3,3,3	1.81	1 (33%)
2	DMS	23-A	404	-	3,3,3	0.78	0	3,3,3	1.29	0
2	DMS	27-A	401	-	3,3,3	0.65	0	3,3,3	1.60	1 (33%)
2	DMS	6-A	402	-	3,3,3	0.67	0	3,3,3	1.21	0
2	DMS	39-A	404	-	3,3,3	0.59	0	3,3,3	0.84	0
2	DMS	40-A	404	-	3,3,3	0.75	0	3,3,3	1.14	0
2	DMS	29-A	404	-	3,3,3	0.73	0	3,3,3	1.10	0
2	DMS	40-A	405	-	3,3,3	0.91	0	3,3,3	1.53	1 (33%)
2	DMS	5-A	402	-	3,3,3	0.60	0	3,3,3	1.74	1 (33%)
2	DMS	30-A	401	-	3,3,3	0.50	0	3,3,3	0.24	0
2	DMS	8-A	403	-	3,3,3	0.73	0	3,3,3	1.51	1 (33%)
2	DMS	17-A	404	-	3,3,3	0.80	0	3,3,3	1.19	0
2	DMS	24-A	401	-	3,3,3	0.69	0	3,3,3	0.74	0
2	DMS	8-A	402	-	3,3,3	0.62	0	3,3,3	1.58	0
2	DMS	48-A	402	-	3,3,3	0.54	0	3,3,3	0.92	0
2	DMS	28-A	401	-	3,3,3	0.36	0	3,3,3	1.46	0
2	DMS	7-A	403	-	3,3,3	0.66	0	3,3,3	2.04	1 (33%)
2	DMS	26-A	403	-	3,3,3	0.80	0	3,3,3	0.99	0
2	DMS	11-A	405	-	3,3,3	0.82	0	3,3,3	0.66	0
2	DMS	12-A	405	-	3,3,3	0.63	0	3,3,3	1.04	0
2	DMS	20-A	401	-	3,3,3	0.46	0	3,3,3	0.87	0
2	DMS	25-A	405	-	3,3,3	0.57	0	3,3,3	1.31	0
2	DMS	34-A	403	-	3,3,3	0.79	0	3,3,3	0.33	0
2	DMS	10-A	402	-	3,3,3	0.64	0	3,3,3	1.92	1 (33%)
2	DMS	9-A	404	-	3,3,3	0.60	0	3,3,3	0.49	0
2	DMS	14-A	404	-	3,3,3	0.80	0	3,3,3	1.44	0
2	DMS	33-A	401	-	3,3,3	0.45	0	3,3,3	0.67	0
2	DMS	28-A	402	-	3,3,3	0.77	0	3,3,3	1.49	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	51-A	402	-	3,3,3	0.81	0	3,3,3	1.91	1 (33%)
2	DMS	41-A	404	-	3,3,3	0.76	0	3,3,3	1.08	0
2	DMS	38-A	401	-	3,3,3	0.45	0	3,3,3	1.32	1 (33%)
2	DMS	3-A	403	-	3,3,3	0.70	0	3,3,3	1.53	0
2	DMS	44-A	403	-	3,3,3	0.69	0	3,3,3	1.62	1 (33%)
2	DMS	16-A	405	-	3,3,3	0.59	0	3,3,3	1.75	1 (33%)
2	DMS	8-A	405	-	3,3,3	0.65	0	3,3,3	1.83	2 (66%)
2	DMS	16-A	401	-	3,3,3	0.92	0	3,3,3	1.77	1 (33%)
2	DMS	10-A	404	-	3,3,3	0.75	0	3,3,3	2.48	1 (33%)
2	DMS	24-A	404	-	3,3,3	0.72	0	3,3,3	0.82	0
2	DMS	28-A	404	-	3,3,3	0.86	0	3,3,3	0.33	0
2	DMS	20-A	404	-	3,3,3	0.77	0	3,3,3	0.92	0
2	DMS	50-A	402	-	3,3,3	0.80	0	3,3,3	1.07	0
2	DMS	45-A	404	-	3,3,3	0.79	0	3,3,3	0.81	0
2	DMS	22-A	405	-	3,3,3	0.63	0	3,3,3	1.16	0
2	DMS	23-A	401	-	3,3,3	0.49	0	3,3,3	0.41	0
2	DMS	7-A	402	-	3,3,3	0.81	0	3,3,3	0.65	0
2	DMS	29-A	403	-	3,3,3	0.74	0	3,3,3	0.43	0
2	DMS	13-A	401	-	3,3,3	0.65	0	3,3,3	1.11	0
2	DMS	25-A	403	-	3,3,3	0.80	0	3,3,3	0.80	0
2	DMS	36-A	405	-	3,3,3	0.65	0	3,3,3	1.36	0
2	DMS	17-A	401	-	3,3,3	0.57	0	3,3,3	1.09	0
2	DMS	6-A	403	-	3,3,3	0.69	0	3,3,3	2.09	1 (33%)
2	DMS	4-A	404	-	3,3,3	0.67	0	3,3,3	0.31	0
2	DMS	31-A	402	-	3,3,3	0.85	0	3,3,3	1.04	0
2	DMS	43-A	401	-	3,3,3	0.75	0	3,3,3	0.64	0
2	DMS	21-A	401	-	3,3,3	0.37	0	3,3,3	1.08	0
2	DMS	38-A	403	-	3,3,3	0.67	0	3,3,3	0.93	0
2	DMS	32-A	404	-	3,3,3	0.81	0	3,3,3	0.76	0
2	DMS	3-A	402	-	3,3,3	0.79	0	3,3,3	0.77	0
2	DMS	49-A	402	-	3,3,3	0.73	0	3,3,3	0.96	0
2	DMS	2-A	405	-	3,3,3	0.66	0	3,3,3	0.92	0
2	DMS	7-A	404	-	3,3,3	0.71	0	3,3,3	0.79	0
2	DMS	19-A	403	-	3,3,3	0.66	0	3,3,3	0.82	0
2	DMS	1-A	404	-	3,3,3	0.90	0	3,3,3	1.71	0
2	DMS	27-A	402	-	3,3,3	0.66	0	3,3,3	1.13	0
2	DMS	40-A	402	-	3,3,3	0.76	0	3,3,3	0.81	0
2	DMS	52-A	403	-	3,3,3	0.43	0	3,3,3	2.02	1 (33%)
2	DMS	42-A	403	-	3,3,3	0.67	0	3,3,3	0.75	0
2	DMS	34-A	404	-	3,3,3	0.66	0	3,3,3	1.88	1 (33%)
2	DMS	42-A	404	-	3,3,3	0.88	0	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	6-A	405	-	3,3,3	0.72	0	3,3,3	1.62	0
2	DMS	35-A	402	-	3,3,3	0.63	0	3,3,3	1.77	1 (33%)
2	DMS	26-A	405	-	3,3,3	0.69	0	3,3,3	2.31	2 (66%)
2	DMS	42-A	401	-	3,3,3	0.51	0	3,3,3	0.90	0
2	DMS	48-A	404	-	3,3,3	0.67	0	3,3,3	1.78	2 (66%)
2	DMS	43-A	403	-	3,3,3	0.70	0	3,3,3	0.82	0
2	DMS	54-A	404	-	3,3,3	0.75	0	3,3,3	1.25	0
2	DMS	5-A	404	-	3,3,3	1.07	0	3,3,3	1.56	0
2	DMS	27-A	404	-	3,3,3	0.61	0	3,3,3	3.00	3 (100%)
2	DMS	33-A	405	-	3,3,3	0.86	0	3,3,3	1.71	0
2	DMS	51-A	401	-	3,3,3	0.45	0	3,3,3	0.64	0
2	DMS	37-A	401	-	3,3,3	0.43	0	3,3,3	0.22	0
2	DMS	19-A	405	-	3,3,3	0.69	0	3,3,3	0.64	0
2	DMS	18-A	403	-	3,3,3	0.65	0	3,3,3	0.61	0
2	DMS	41-A	405	-	3,3,3	0.70	0	3,3,3	1.49	0
2	DMS	46-A	401	-	3,3,3	0.50	0	3,3,3	0.77	0
2	DMS	33-A	402	-	3,3,3	0.85	0	3,3,3	0.83	0
2	DMS	25-A	404	-	3,3,3	0.72	0	3,3,3	1.10	0
2	DMS	8-A	401	-	3,3,3	0.45	0	3,3,3	0.42	0
2	DMS	30-A	403	-	3,3,3	0.69	0	3,3,3	0.57	0
2	DMS	47-A	404	-	3,3,3	0.64	0	3,3,3	1.06	0
2	DMS	29-A	401	-	3,3,3	0.35	0	3,3,3	0.86	0
2	DMS	16-A	402	-	3,3,3	0.73	0	3,3,3	2.02	1 (33%)
2	DMS	5-A	401	-	3,3,3	0.71	0	3,3,3	0.97	0
2	DMS	15-A	405	-	3,3,3	0.74	0	3,3,3	0.55	0
2	DMS	33-A	404	-	3,3,3	0.43	0	3,3,3	2.35	1 (33%)
2	DMS	23-A	405	-	3,3,3	0.51	0	3,3,3	1.68	1 (33%)
2	DMS	39-A	405	-	3,3,3	0.83	0	3,3,3	1.01	0
2	DMS	43-A	405	-	3,3,3	0.96	0	3,3,3	1.73	1 (33%)
2	DMS	53-A	404	-	3,3,3	0.68	0	3,3,3	1.22	0
2	DMS	41-A	402	-	3,3,3	0.81	0	3,3,3	0.78	0
2	DMS	29-A	405	-	3,3,3	0.65	0	3,3,3	1.88	1 (33%)
2	DMS	53-A	405	-	3,3,3	0.95	0	3,3,3	2.13	1 (33%)
2	DMS	17-A	405	-	3,3,3	0.73	0	3,3,3	2.30	2 (66%)
2	DMS	19-A	404	-	3,3,3	0.67	0	3,3,3	2.30	2 (66%)
2	DMS	16-A	404	-	3,3,3	0.70	0	3,3,3	1.35	1 (33%)
2	DMS	8-A	404	-	3,3,3	0.62	0	3,3,3	1.31	0
2	DMS	34-A	401	-	3,3,3	0.73	0	3,3,3	0.93	0
2	DMS	4-A	402	-	3,3,3	0.72	0	3,3,3	1.29	0
2	DMS	37-A	403	-	3,3,3	0.71	0	3,3,3	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	10-A	401	-	3,3,3	0.87	0	3,3,3	1.41	1 (33%)
2	DMS	21-A	403	-	3,3,3	0.73	0	3,3,3	1.12	0
2	DMS	43-A	404	-	3,3,3	0.56	0	3,3,3	1.92	1 (33%)
2	DMS	28-A	403	-	3,3,3	0.82	0	3,3,3	0.77	0
2	DMS	22-A	401	-	3,3,3	0.63	0	3,3,3	0.98	0
2	DMS	4-A	403	-	3,3,3	0.79	0	3,3,3	0.36	0
2	DMS	24-A	403	-	3,3,3	0.85	0	3,3,3	0.73	0
2	DMS	47-A	403	-	3,3,3	0.88	0	3,3,3	0.90	0
2	DMS	24-A	405	-	3,3,3	0.73	0	3,3,3	2.04	2 (66%)
2	DMS	52-A	405	-	3,3,3	0.81	0	3,3,3	0.85	0
2	DMS	5-A	403	-	3,3,3	0.73	0	3,3,3	1.63	1 (33%)
2	DMS	44-A	404	-	3,3,3	0.57	0	3,3,3	0.74	0
2	DMS	26-A	401	-	3,3,3	0.51	0	3,3,3	1.01	0
2	DMS	44-A	405	-	3,3,3	0.69	0	3,3,3	1.31	0
2	DMS	50-A	405	-	3,3,3	0.86	0	3,3,3	1.52	1 (33%)
2	DMS	50-A	401	-	3,3,3	0.37	0	3,3,3	0.38	0
2	DMS	37-A	405	-	3,3,3	0.70	0	3,3,3	1.42	1 (33%)
2	DMS	6-A	401	-	3,3,3	0.83	0	3,3,3	1.45	0
2	DMS	20-A	402	-	3,3,3	0.78	0	3,3,3	1.17	0
2	DMS	45-A	402	-	3,3,3	0.61	0	3,3,3	1.06	0
2	DMS	13-A	403	-	3,3,3	0.74	0	3,3,3	1.15	0
2	DMS	22-A	404	-	3,3,3	0.75	0	3,3,3	3.12	2 (66%)
2	DMS	31-A	403	-	3,3,3	0.70	0	3,3,3	0.76	0
2	DMS	4-A	405	-	3,3,3	0.68	0	3,3,3	3.13	3 (100%)
2	DMS	53-A	401	-	3,3,3	0.52	0	3,3,3	0.95	0
2	DMS	19-A	401	-	3,3,3	0.45	0	3,3,3	0.24	0
2	DMS	38-A	402	-	3,3,3	0.81	0	3,3,3	1.13	0
2	DMS	19-A	402	-	3,3,3	0.72	0	3,3,3	1.47	0
2	DMS	3-A	401	-	3,3,3	0.55	0	3,3,3	0.34	0
2	DMS	14-A	402	-	3,3,3	0.86	0	3,3,3	0.70	0
2	DMS	26-A	404	-	3,3,3	0.64	0	3,3,3	0.52	0
2	DMS	48-A	401	-	3,3,3	0.47	0	3,3,3	0.62	0
2	DMS	15-A	401	-	3,3,3	0.41	0	3,3,3	0.64	0
2	DMS	39-A	401	-	3,3,3	0.45	0	3,3,3	0.48	0
2	DMS	35-A	405	-	3,3,3	0.75	0	3,3,3	0.79	0
2	DMS	49-A	404	-	3,3,3	0.88	0	3,3,3	2.12	1 (33%)
2	DMS	49-A	401	-	3,3,3	0.44	0	3,3,3	0.34	0
2	DMS	40-A	403	-	3,3,3	0.74	0	3,3,3	0.86	0
2	DMS	27-A	403	-	3,3,3	0.72	0	3,3,3	0.71	0
2	DMS	51-A	404	-	3,3,3	0.79	0	3,3,3	1.19	0
2	DMS	7-A	405	-	3,3,3	0.92	0	3,3,3	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DMS	2-A	403	-	3,3,3	0.78	0	3,3,3	1.81	1 (33%)
2	DMS	40-A	401	-	3,3,3	0.50	0	3,3,3	0.31	0
2	DMS	23-A	402	-	3,3,3	0.68	0	3,3,3	0.98	0
2	DMS	12-A	402	-	3,3,3	0.67	0	3,3,3	3.15	3 (100%)
2	DMS	46-A	403	-	3,3,3	0.65	0	3,3,3	0.82	0
2	DMS	30-A	404	-	3,3,3	0.70	0	3,3,3	0.89	0
2	DMS	29-A	402	-	3,3,3	0.77	0	3,3,3	0.73	0
2	DMS	3-A	405	-	3,3,3	0.69	0	3,3,3	1.23	0
2	DMS	17-A	403	-	3,3,3	0.76	0	3,3,3	1.30	1 (33%)
2	DMS	50-A	403	-	3,3,3	0.80	0	3,3,3	0.72	0
2	DMS	28-A	405	-	3,3,3	0.79	0	3,3,3	1.63	1 (33%)
2	DMS	34-A	405	-	3,3,3	0.68	0	3,3,3	0.71	0
2	DMS	47-A	405	-	3,3,3	0.79	0	3,3,3	0.29	0
2	DMS	46-A	402	-	3,3,3	0.72	0	3,3,3	0.74	0
2	DMS	14-A	401	-	3,3,3	0.52	0	3,3,3	1.06	0

There are no bond length outliers.

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	45-A	401	DMS	O-S-C1	4.46	129.32	106.54
2	10-A	404	DMS	O-S-C1	-4.28	84.71	106.54
2	22-A	404	DMS	O-S-C1	4.19	127.94	106.54
2	9-A	403	DMS	O-S-C1	4.14	127.65	106.54
2	9-A	405	DMS	O-S-C1	3.85	126.17	106.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	18-A	1
1	27-A	1
1	31-A	1
1	38-A	1
1	40-A	1
1	20-A	1
1	39-A	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
18	A	106:ILE	C	107:GLN	N	1.20
27	A	106:ILE	C	107:GLN	N	1.19
31	A	106:ILE	C	107:GLN	N	1.19
38	A	106:ILE	C	107:GLN	N	1.17
40	A	106:ILE	C	107:GLN	N	1.17

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%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	2-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	3-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	4-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	5-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	6-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	7-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	8-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	9-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	10-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	11-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	12-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	13-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	14-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	15-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	16-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	17-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	18-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	19-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	20-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	21-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	22-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	23-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	24-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	25-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	26-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	27-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	28-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	29-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	30-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	31-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	32-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	33-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	34-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	35-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	36-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	37-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	38-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	39-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	40-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	41-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	42-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	43-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	44-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	45-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	46-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	47-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	48-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	49-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	50-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	51-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	52-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	53-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
1	54-A	306/306 (100%)	1.08	36 (11%)	4	4	16, 18, 19, 21	306 (100%)
All	All	16524/16524 (100%)	1.08	1944 (11%)	4	4	16, 18, 20, 21	16524 (100%)

The worst 5 of 1944 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	300	CYS	22.1
1	2-A	300	CYS	22.1
1	3-A	300	CYS	22.1
1	4-A	300	CYS	22.1
1	5-A	300	CYS	22.1

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	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	2-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	3-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	4-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	5-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	6-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	7-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	8-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	9-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	10-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	11-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	12-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	13-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	14-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	15-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	16-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	17-A	403	4/4	-0.01	0.69	16,17,17,17	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	18-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	19-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	20-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	21-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	22-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	23-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	24-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	25-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	26-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	27-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	28-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	29-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	30-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	31-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	32-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	33-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	34-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	35-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	36-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	37-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	38-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	39-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	40-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	41-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	42-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	43-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	44-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	45-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	46-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	47-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	48-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	49-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	50-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	51-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	52-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	53-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	54-A	403	4/4	-0.01	0.69	16,17,17,17	10
2	DMS	1-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	2-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	3-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	4-A	404	4/4	0.58	1.46	17,17,18,18	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	5-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	6-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	7-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	8-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	9-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	10-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	11-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	12-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	13-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	14-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	15-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	16-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	17-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	18-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	19-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	20-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	21-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	22-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	23-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	24-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	25-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	26-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	27-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	28-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	29-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	30-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	31-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	32-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	33-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	34-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	35-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	36-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	37-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	38-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	39-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	40-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	41-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	42-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	43-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	44-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	45-A	404	4/4	0.58	1.46	17,17,18,18	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	46-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	47-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	48-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	49-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	50-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	51-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	52-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	53-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	54-A	404	4/4	0.58	1.46	17,17,18,18	10
2	DMS	1-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	2-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	3-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	4-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	5-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	6-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	7-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	8-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	9-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	10-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	11-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	12-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	13-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	14-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	15-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	16-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	17-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	18-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	19-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	20-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	21-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	22-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	23-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	24-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	25-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	26-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	27-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	28-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	29-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	30-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	31-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	32-A	405	4/4	0.58	0.83	17,17,17,17	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	33-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	34-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	35-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	36-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	37-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	38-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	39-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	40-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	41-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	42-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	43-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	44-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	45-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	46-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	47-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	48-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	49-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	50-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	51-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	52-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	53-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	54-A	405	4/4	0.58	0.83	17,17,17,17	10
2	DMS	1-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	2-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	3-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	4-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	5-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	6-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	7-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	8-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	9-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	10-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	11-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	12-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	13-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	14-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	15-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	16-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	17-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	18-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	19-A	402	4/4	0.80	1.01	17,17,18,18	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	20-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	21-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	22-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	23-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	24-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	25-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	26-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	27-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	28-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	29-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	30-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	31-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	32-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	33-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	34-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	35-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	36-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	37-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	38-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	39-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	40-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	41-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	42-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	43-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	44-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	45-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	46-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	47-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	48-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	49-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	50-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	51-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	52-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	53-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	54-A	402	4/4	0.80	1.01	17,17,18,18	10
2	DMS	1-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	2-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	3-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	4-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	5-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	6-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	7-A	401	4/4	0.98	0.06	17,17,17,17	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	8-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	9-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	10-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	11-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	12-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	13-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	14-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	15-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	16-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	17-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	18-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	19-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	20-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	21-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	22-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	23-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	24-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	25-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	26-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	27-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	28-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	29-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	30-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	31-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	32-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	33-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	34-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	35-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	36-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	37-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	38-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	39-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	40-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	41-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	42-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	43-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	44-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	45-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	46-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	47-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	48-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	49-A	401	4/4	0.98	0.06	17,17,17,17	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMS	50-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	51-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	52-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	53-A	401	4/4	0.98	0.06	17,17,17,17	10
2	DMS	54-A	401	4/4	0.98	0.06	17,17,17,17	10
3	ZN	1-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	2-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	3-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	4-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	5-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	6-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	7-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	8-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	9-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	10-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	11-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	12-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	13-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	14-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	15-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	16-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	17-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	18-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	19-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	20-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	21-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	22-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	23-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	24-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	25-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	26-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	27-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	28-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	29-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	30-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	31-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	32-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	33-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	34-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	35-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	36-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	37-A	406	1/1	0.99	0.15	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	38-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	39-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	40-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	41-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	42-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	43-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	44-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	45-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	46-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	47-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	48-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	49-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	50-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	51-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	52-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	53-A	406	1/1	0.99	0.15	17,17,17,17	1
3	ZN	54-A	406	1/1	0.99	0.15	17,17,17,17	1

6.5 Other polymers (i)

There are no such residues in this entry.