



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:31 AM UTC

PDB ID : 7MHM / pdb_00007mhm
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 240 K
Authors : Ebrahim, A.; Riley, B.T.; Kumaran, D.; Andi, B.; Fuchs, M.R.; McSweeney, S.; Keedy, D.A.
Deposited on : 2021-04-15
Resolution : 1.53 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

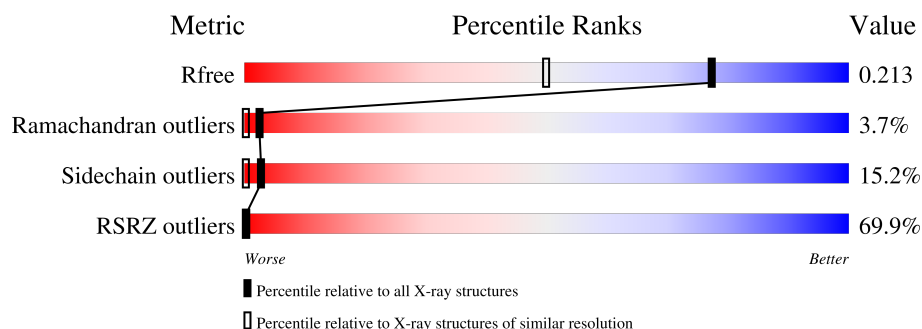
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1003 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	70% 84% 14% .
1	10-A	306	84% 14% .
1	11-A	306	83% 14% .
1	12-A	306	85% 13% .
1	13-A	306	85% 14% .
1	14-A	306	85% 14% .
1	15-A	306	84% 13% ..

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	39-A	306	 82% 15% .
1	4-A	306	 83% 13% .
1	40-A	306	 85% 14% .
1	41-A	306	 83% 14% .
1	42-A	306	 82% 16% .
1	43-A	306	 83% 14% .
1	5-A	306	 83% 14% .
1	6-A	306	 84% 14% .
1	7-A	306	 82% 17% .
1	8-A	306	 83% 15% .
1	9-A	306	 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	405	-	-	-	X
2	DMS	1-A	406	-	-	-	X
2	DMS	12-A	402	-	X	-	-
2	DMS	23-A	402	-	X	-	-
2	DMS	3-A	406	-	X	-	-
2	DMS	39-A	402	-	X	-	-
2	DMS	4-A	404	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 210185 atoms, of which 101308 are hydrogens and 0 are deuteriums.

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

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

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

Continued on next page...

Continued from previous page...

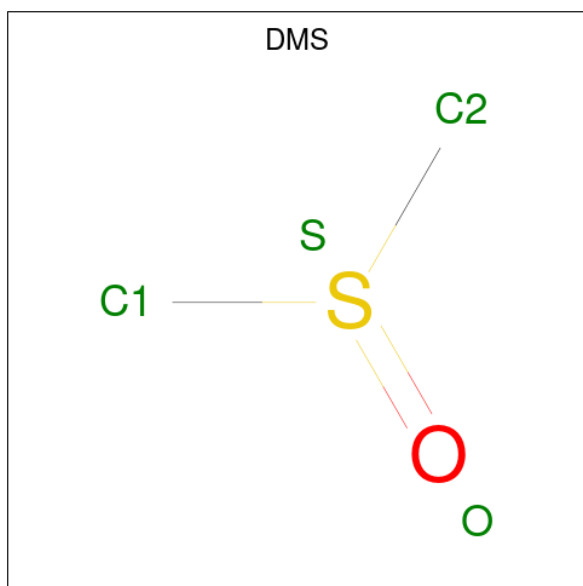
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	18-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	19-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	20-A	306	Total 4681	C 1499	H 2314	N 402	O 444	S 22	0	0	0
1	21-A	306	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: 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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

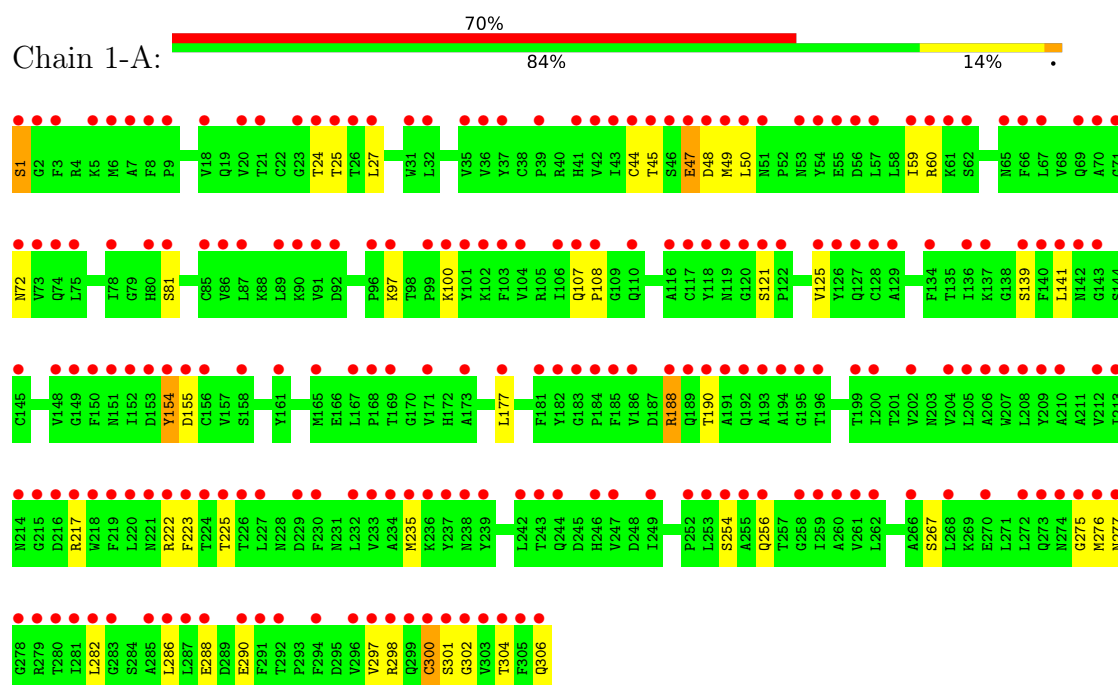
Continued from previous page...

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

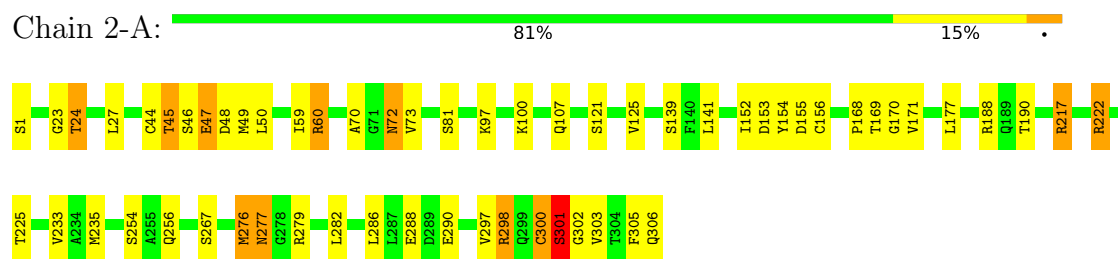
3 Residue-property plots

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.

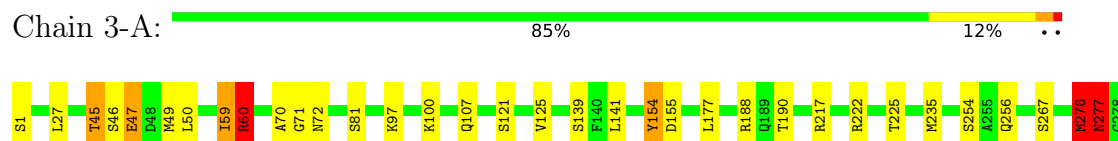
• Molecule 1: 3C-like proteinase



• Molecule 1: 3C-like proteinase

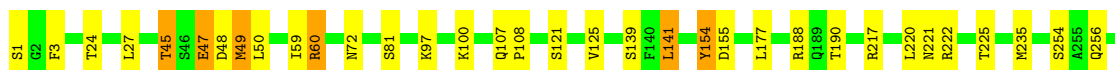
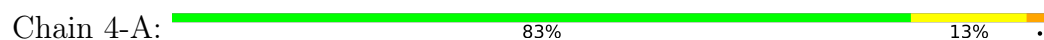


• Molecule 1: 3C-like proteinase

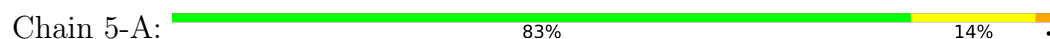




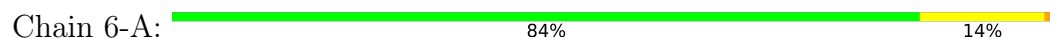
- Molecule 1: 3C-like proteinase



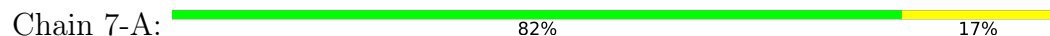
- Molecule 1: 3C-like proteinase



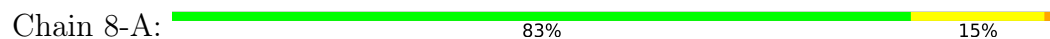
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase

Chain 9-A: 83% 15% .



- Molecule 1: 3C-like proteinase

Chain 10-A: 84% 14% .



- Molecule 1: 3C-like proteinase

Chain 11-A: 83% 14% .



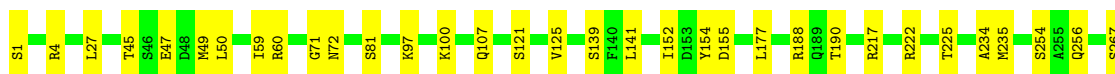
- Molecule 1: 3C-like proteinase

Chain 12-A: 85% 13% .



- Molecule 1: 3C-like proteinase

Chain 13-A: 85% 14% .





- Molecule 1: 3C-like proteinase

Chain 14-A: 85% 14%



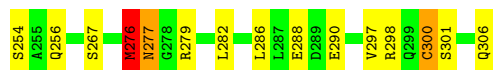
- Molecule 1: 3C-like proteinase

Chain 15-A: 84% 13%



- Molecule 1: 3C-like proteinase

Chain 16-A: 84% 14%



- Molecule 1: 3C-like proteinase

Chain 17-A: 85% 14%



- Molecule 1: 3C-like proteinase

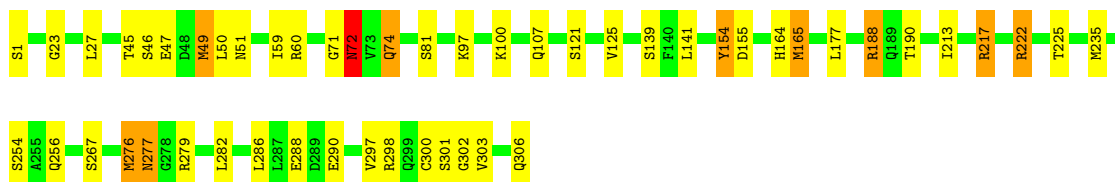
Chain 18-A: 84% 15%





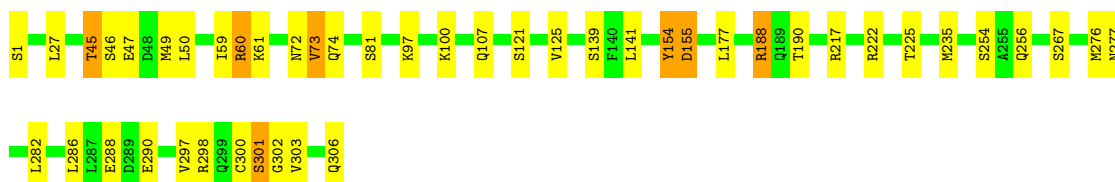
- Molecule 1: 3C-like proteinase

Chain 19-A: 83% 13% .



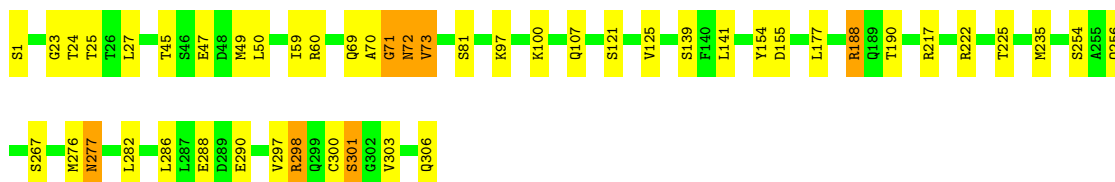
- Molecule 1: 3C-like proteinase

Chain 20-A: 85% 13% .



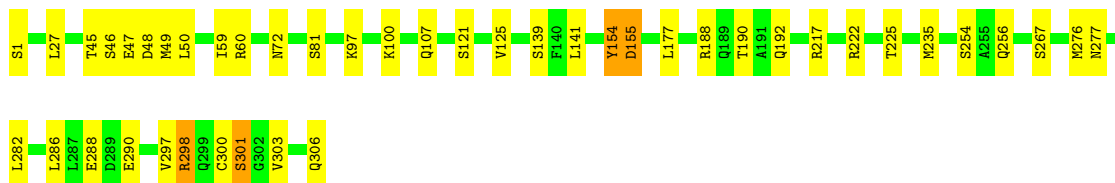
- Molecule 1: 3C-like proteinase

Chain 21-A: 84% 13% .



- Molecule 1: 3C-like proteinase

Chain 22-A: 86% 13% .



- Molecule 1: 3C-like proteinase

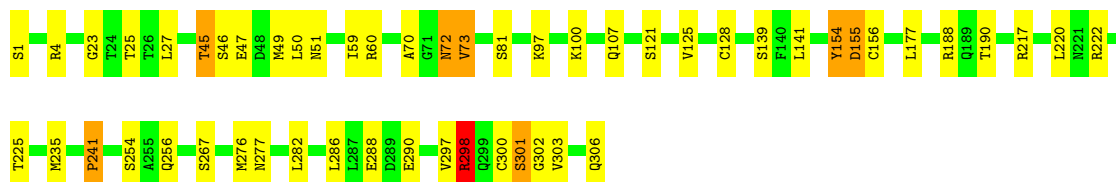
Chain 23-A: 84% 15% .





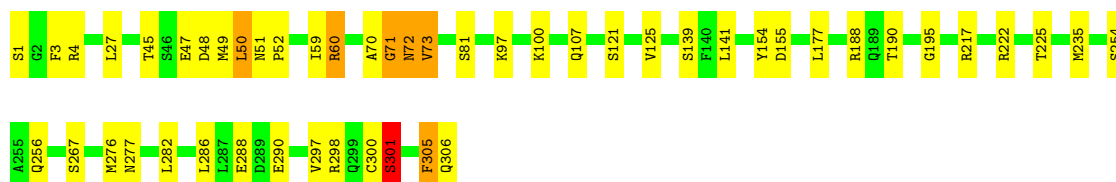
- Molecule 1: 3C-like proteinase

Chain 24-A: 83% 15% .



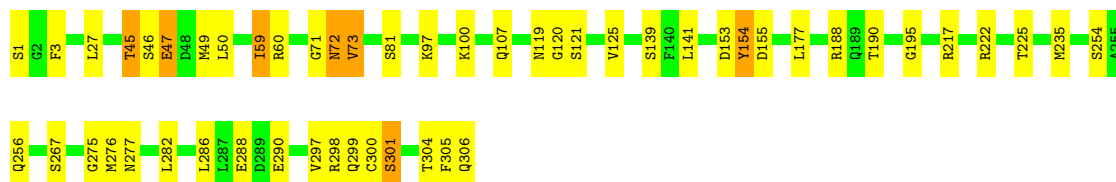
- Molecule 1: 3C-like proteinase

Chain 25-A: 84% 14% .



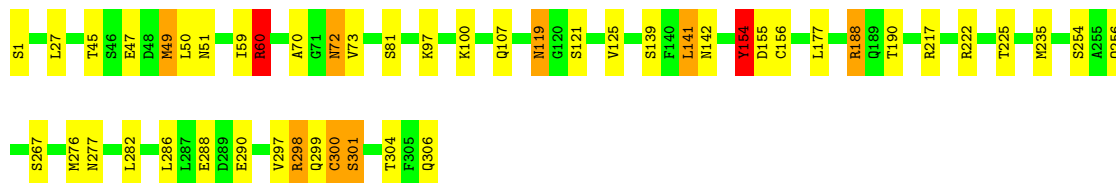
- Molecule 1: 3C-like proteinase

Chain 26-A: 83% 15% .



- Molecule 1: 3C-like proteinase

Chain 27-A: 84% 12% . .



- Molecule 1: 3C-like proteinase

Chain 28-A: 84% 13% . .





- Molecule 1: 3C-like proteinase

Chain 29-A: 83% 15% .



- Molecule 1: 3C-like proteinase

Chain 30-A: 84% 14% ..



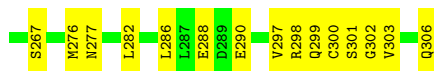
- Molecule 1: 3C-like proteinase

Chain 31-A: 85% 14% .



- Molecule 1: 3C-like proteinase

Chain 32-A: 83% 14% .



- Molecule 1: 3C-like proteinase

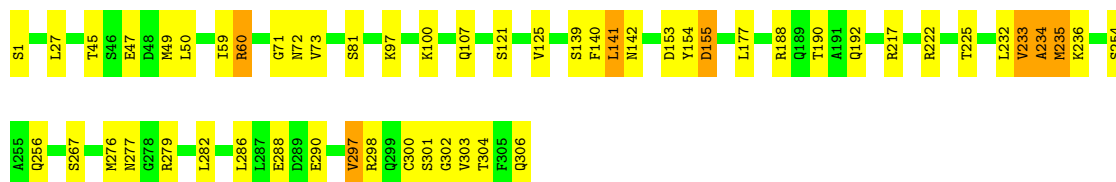
Chain 33-A: 82% 15% ..





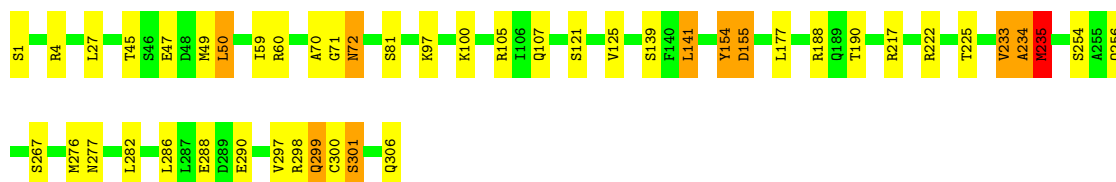
- Molecule 1: 3C-like proteinase

Chain 34-A: 82% 15% .



- Molecule 1: 3C-like proteinase

Chain 35-A: 85% 12% .



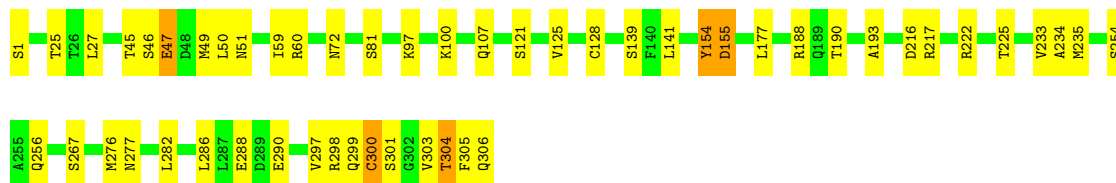
- Molecule 1: 3C-like proteinase

Chain 36-A: 84% 13% .



- Molecule 1: 3C-like proteinase

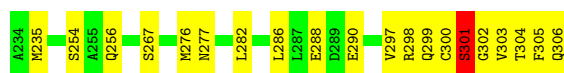
Chain 37-A: 83% 15% .



- Molecule 1: 3C-like proteinase

Chain 38-A: 82% 16% ..





- Molecule 1: 3C-like proteinase

Chain 39-A: 82% 15% .



- Molecule 1: 3C-like proteinase

Chain 40-A: 85% 14% .



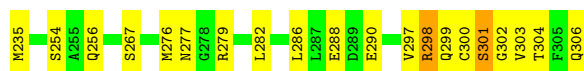
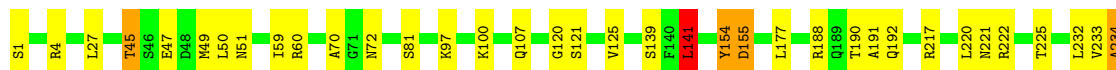
- Molecule 1: 3C-like proteinase

Chain 41-A: 83% 14% .



- Molecule 1: 3C-like proteinase

Chain 42-A: 82% 16% .



- Molecule 1: 3C-like proteinase

Chain 43-A: 83% 14% .



S254	A255	Q256	S267	M276	M277	L282	L286	L287	E288	D289	E290	V297	R298	Q299	C300	S301	G302	V303	T304	F305	Q306
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.19Å 53.49Å 45.00Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	48.20 – 1.53 48.20 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.20-1.53) 89.1 (48.20-1.53)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 1.53Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.158 , 0.197 0.173 , 0.213	Depositor DCC
R_{free} test set	2007 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 19.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	210185	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.12	0/2420	0.16	0/3289
1	2-A	0.12	0/2420	0.16	0/3289
1	3-A	0.12	0/2420	0.16	0/3289
1	4-A	0.12	0/2420	0.16	0/3289
1	5-A	0.12	0/2420	0.16	0/3289
1	6-A	0.12	0/2420	0.16	0/3289
1	7-A	0.12	0/2420	0.16	0/3289
1	8-A	0.12	0/2420	0.16	0/3289
1	9-A	0.12	0/2420	0.16	0/3289
1	10-A	0.12	0/2420	0.16	0/3289
1	11-A	0.12	0/2420	0.16	0/3289
1	12-A	0.12	0/2420	0.16	0/3289
1	13-A	0.12	0/2420	0.16	0/3289
1	14-A	0.12	0/2420	0.16	0/3289
1	15-A	0.12	0/2420	0.16	0/3289
1	16-A	0.12	0/2420	0.16	0/3289
1	17-A	0.12	0/2420	0.16	0/3289
1	18-A	0.12	0/2420	0.16	0/3289
1	19-A	0.12	0/2420	0.16	0/3289
1	20-A	0.12	0/2420	0.16	0/3289
1	21-A	0.12	0/2420	0.16	0/3289
1	22-A	0.12	0/2420	0.16	0/3289
1	23-A	0.12	0/2420	0.16	0/3289
1	24-A	0.12	0/2420	0.16	0/3289
1	25-A	0.12	0/2420	0.16	0/3289
1	26-A	0.12	0/2420	0.16	0/3289
1	27-A	0.12	0/2420	0.16	0/3289
1	28-A	0.12	0/2420	0.16	0/3289
1	29-A	0.12	0/2420	0.16	0/3289
1	30-A	0.12	0/2420	0.16	0/3289
1	31-A	0.12	0/2420	0.16	0/3289
1	32-A	0.12	0/2420	0.16	0/3289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.12	0/2420	0.16	0/3289
1	34-A	0.12	0/2420	0.16	0/3289
1	35-A	0.12	0/2420	0.16	0/3289
1	36-A	0.12	0/2420	0.16	0/3289
1	37-A	0.12	0/2420	0.16	0/3289
1	38-A	0.12	0/2420	0.16	0/3289
1	39-A	0.12	0/2420	0.16	0/3289
1	40-A	0.12	0/2420	0.16	0/3289
1	41-A	0.12	0/2420	0.16	0/3289
1	42-A	0.12	0/2420	0.16	0/3289
1	43-A	0.12	0/2420	0.16	0/3289
All	All	0.12	0/104060	0.16	0/141427

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	5
1	2-A	0	12
1	3-A	0	10
1	4-A	0	8
1	5-A	0	14
1	6-A	0	4
1	7-A	0	7
1	8-A	0	5
1	9-A	0	7
1	10-A	0	4
1	11-A	0	7
1	12-A	0	6
1	13-A	0	5
1	14-A	0	6
1	15-A	0	8
1	16-A	0	6
1	17-A	0	5
1	18-A	0	2
1	19-A	0	11
1	20-A	0	5
1	21-A	0	4
1	22-A	0	1
1	23-A	0	6

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 292 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	1	SER	Peptide
1	1-A	188	ARG	Sidechain
1	1-A	25	THR	Peptide
1	1-A	300	CYS	Peptide
1	1-A	44	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2367	2314	2313	0	0
1	2-A	2367	2314	2313	0	0
1	3-A	2367	2314	2313	0	0
1	4-A	2367	2314	2313	0	0
1	5-A	2367	2314	2313	0	0
1	6-A	2367	2314	2314	0	0
1	7-A	2367	2314	2313	0	0
1	8-A	2367	2314	2313	0	0
1	9-A	2367	2314	2313	0	0
1	10-A	2367	2314	2313	0	0
1	11-A	2367	2314	2314	0	0
1	12-A	2367	2314	2313	0	0
1	13-A	2367	2314	2313	0	0
1	14-A	2367	2314	2313	0	0
1	15-A	2367	2314	2313	0	0
1	16-A	2367	2314	2313	0	0
1	17-A	2367	2314	2314	0	0
1	18-A	2367	2314	2313	0	0
1	19-A	2367	2314	2313	0	0
1	20-A	2367	2314	2313	0	0
1	21-A	2367	2314	2313	0	0
1	22-A	2367	2314	2313	0	0
1	23-A	2367	2314	2313	0	0
1	24-A	2367	2314	2314	0	0
1	25-A	2367	2314	2313	0	0
1	26-A	2367	2314	2313	0	0
1	27-A	2367	2314	2313	0	0
1	28-A	2367	2314	2314	0	0
1	29-A	2367	2314	2313	0	0
1	30-A	2367	2314	2313	0	0
1	31-A	2367	2314	2313	0	0
1	32-A	2367	2314	2313	0	0
1	33-A	2367	2314	2313	0	0
1	34-A	2367	2314	2313	0	0
1	35-A	2367	2314	2313	0	0
1	36-A	2367	2314	2313	0	0
1	37-A	2367	2314	2313	0	0
1	38-A	2367	2314	2313	0	0
1	39-A	2367	2314	2313	0	0
1	40-A	2367	2314	2313	0	0
1	41-A	2367	2314	2313	0	0
1	42-A	2367	2314	2314	0	0
1	43-A	2367	2314	2313	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	43-A	28	42	42	0	0
3	1-A	1	0	0	0	0
3	2-A	1	0	0	0	0
3	3-A	1	0	0	0	0
3	4-A	1	0	0	0	0
3	5-A	1	0	0	0	0
3	6-A	1	0	0	0	0
3	7-A	1	0	0	0	0
3	8-A	1	0	0	0	0
3	9-A	1	0	0	0	0
3	10-A	1	0	0	0	0
3	11-A	1	0	0	0	0
3	12-A	1	0	0	0	0
3	13-A	1	0	0	0	0
3	14-A	1	0	0	0	0
3	15-A	1	0	0	0	0
3	16-A	1	0	0	0	0
3	17-A	1	0	0	0	0
3	18-A	1	0	0	0	0
3	19-A	1	0	0	0	0
3	20-A	1	0	0	0	0
3	21-A	1	0	0	0	0
3	22-A	1	0	0	0	0
3	23-A	1	0	0	0	0
3	24-A	1	0	0	0	0
3	25-A	1	0	0	0	0
3	26-A	1	0	0	0	0
3	27-A	1	0	0	0	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	42-A	1	0	0	0	0
3	43-A	1	0	0	0	0
4	1-A	148	0	0	0	0
4	2-A	135	0	0	0	0
4	3-A	134	0	0	0	0
4	4-A	142	0	0	0	0
4	5-A	140	0	0	0	0
4	6-A	145	0	0	0	0
4	7-A	133	0	0	0	0
4	8-A	131	0	0	0	0
4	9-A	147	0	0	0	0
4	10-A	146	0	0	0	0
4	11-A	137	0	0	0	0
4	12-A	141	0	0	0	0
4	13-A	130	0	0	0	0
4	14-A	135	0	0	0	0
4	15-A	136	0	0	0	0
4	16-A	121	0	0	0	0
4	17-A	152	0	0	0	0
4	18-A	122	0	0	0	0
4	19-A	141	0	0	0	0
4	20-A	131	0	0	0	0
4	21-A	142	0	0	0	0
4	22-A	139	0	0	0	0
4	23-A	134	0	0	0	0
4	24-A	138	0	0	0	0
4	25-A	145	0	0	0	0
4	26-A	125	0	0	0	0
4	27-A	144	0	0	0	0
4	28-A	135	0	0	0	0
4	29-A	144	0	0	0	0
4	30-A	146	0	0	0	0
4	31-A	136	0	0	0	0
4	32-A	122	0	0	0	0
4	33-A	134	0	0	0	0
4	34-A	123	0	0	0	0
4	35-A	130	0	0	0	0
4	36-A	139	0	0	0	0
4	37-A	140	0	0	0	0
4	38-A	120	0	0	0	0
4	39-A	145	0	0	0	0
4	40-A	121	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	41-A	127	0	0	0	0
4	42-A	133	0	0	0	0
4	43-A	140	0	0	0	0
All	All	108877	101308	101271	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	304/306 (99%)	274 (90%)	21 (7%)	9 (3%)	3	0
1	2-A	304/306 (99%)	269 (88%)	15 (5%)	20 (7%)	1	0
1	3-A	304/306 (99%)	274 (90%)	20 (7%)	10 (3%)	3	0
1	4-A	304/306 (99%)	269 (88%)	20 (7%)	15 (5%)	1	0
1	5-A	304/306 (99%)	274 (90%)	21 (7%)	9 (3%)	3	0
1	6-A	304/306 (99%)	277 (91%)	12 (4%)	15 (5%)	1	0
1	7-A	304/306 (99%)	272 (90%)	21 (7%)	11 (4%)	2	0
1	8-A	304/306 (99%)	275 (90%)	15 (5%)	14 (5%)	2	0
1	9-A	304/306 (99%)	275 (90%)	17 (6%)	12 (4%)	2	0
1	10-A	304/306 (99%)	281 (92%)	13 (4%)	10 (3%)	3	0
1	11-A	304/306 (99%)	274 (90%)	19 (6%)	11 (4%)	2	0
1	12-A	304/306 (99%)	282 (93%)	17 (6%)	5 (2%)	7	1
1	13-A	304/306 (99%)	288 (95%)	13 (4%)	3 (1%)	12	2
1	14-A	304/306 (99%)	289 (95%)	9 (3%)	6 (2%)	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	15-A	304/306 (99%)	274 (90%)	16 (5%)	14 (5%)	2	0
1	16-A	304/306 (99%)	285 (94%)	10 (3%)	9 (3%)	3	0
1	17-A	304/306 (99%)	282 (93%)	16 (5%)	6 (2%)	6	0
1	18-A	304/306 (99%)	276 (91%)	19 (6%)	9 (3%)	3	0
1	19-A	304/306 (99%)	274 (90%)	19 (6%)	11 (4%)	2	0
1	20-A	304/306 (99%)	288 (95%)	8 (3%)	8 (3%)	4	0
1	21-A	304/306 (99%)	281 (92%)	12 (4%)	11 (4%)	2	0
1	22-A	304/306 (99%)	277 (91%)	20 (7%)	7 (2%)	5	0
1	23-A	304/306 (99%)	271 (89%)	23 (8%)	10 (3%)	3	0
1	24-A	304/306 (99%)	272 (90%)	19 (6%)	13 (4%)	2	0
1	25-A	304/306 (99%)	279 (92%)	15 (5%)	10 (3%)	3	0
1	26-A	304/306 (99%)	268 (88%)	19 (6%)	17 (6%)	1	0
1	27-A	304/306 (99%)	279 (92%)	14 (5%)	11 (4%)	2	0
1	28-A	304/306 (99%)	277 (91%)	17 (6%)	10 (3%)	3	0
1	29-A	304/306 (99%)	271 (89%)	21 (7%)	12 (4%)	2	0
1	30-A	304/306 (99%)	279 (92%)	16 (5%)	9 (3%)	3	0
1	31-A	304/306 (99%)	268 (88%)	27 (9%)	9 (3%)	3	0
1	32-A	304/306 (99%)	273 (90%)	19 (6%)	12 (4%)	2	0
1	33-A	304/306 (99%)	268 (88%)	16 (5%)	20 (7%)	1	0
1	34-A	304/306 (99%)	275 (90%)	17 (6%)	12 (4%)	2	0
1	35-A	304/306 (99%)	278 (91%)	14 (5%)	12 (4%)	2	0
1	36-A	304/306 (99%)	277 (91%)	18 (6%)	9 (3%)	3	0
1	37-A	304/306 (99%)	272 (90%)	18 (6%)	14 (5%)	2	0
1	38-A	304/306 (99%)	268 (88%)	20 (7%)	16 (5%)	1	0
1	39-A	304/306 (99%)	270 (89%)	19 (6%)	15 (5%)	1	0
1	40-A	304/306 (99%)	287 (94%)	10 (3%)	7 (2%)	5	0
1	41-A	304/306 (99%)	273 (90%)	15 (5%)	16 (5%)	1	0
1	42-A	304/306 (99%)	275 (90%)	17 (6%)	12 (4%)	2	0
1	43-A	304/306 (99%)	270 (89%)	21 (7%)	13 (4%)	2	0
All	All	13072/13158 (99%)	11860 (91%)	728 (6%)	484 (4%)	2	0

5 of 484 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	2-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	3-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	4-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	5-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	6-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	7-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	8-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	9-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	10-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	11-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	12-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	13-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	14-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	15-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	16-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	17-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	18-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	19-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	20-A	263/263 (100%)	223 (85%)	40 (15%)	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	21-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	22-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	23-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	24-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	25-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	26-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	27-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	28-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	29-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	30-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	31-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	32-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	33-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	34-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	35-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	36-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	37-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	38-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	39-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	40-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	41-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	42-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
1	43-A	263/263 (100%)	223 (85%)	40 (15%)	3	0
All	All	11309/11309 (100%)	9589 (85%)	1720 (15%)	3	0

5 of 1720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	24-A	59	ILE
1	29-A	254	SER
1	40-A	306	GLN
1	24-A	288	GLU
1	24-A	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 356 such sidechains are listed below:

Mol	Chain	Res	Type
1	30-A	214	ASN
1	37-A	64	HIS
1	31-A	64	HIS
1	33-A	228	ASN
1	38-A	214	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DMS	29-A	402	-	3,3,3	0.68	0	3,3,3	1.60	1 (33%)
2	DMS	32-A	406	-	3,3,3	0.77	0	3,3,3	1.72	1 (33%)
2	DMS	17-A	407	-	3,3,3	0.86	0	3,3,3	2.54	2 (66%)
2	DMS	41-A	402	-	3,3,3	0.80	0	3,3,3	1.41	1 (33%)
2	DMS	27-A	401	-	3,3,3	0.52	0	3,3,3	0.51	0
2	DMS	33-A	405	-	3,3,3	0.79	0	3,3,3	1.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	30-A	404	-	3,3,3	0.64	0	3,3,3	0.92	0
2	DMS	6-A	407	-	3,3,3	0.91	0	3,3,3	1.12	0
2	DMS	23-A	403	-	3,3,3	0.62	0	3,3,3	1.16	0
2	DMS	11-A	407	-	3,3,3	0.67	0	3,3,3	1.19	0
2	DMS	25-A	407	-	3,3,3	0.99	0	3,3,3	1.17	0
2	DMS	16-A	406	-	3,3,3	0.99	0	3,3,3	0.50	0
2	DMS	20-A	407	-	3,3,3	0.73	0	3,3,3	0.98	0
2	DMS	10-A	401	-	3,3,3	0.61	0	3,3,3	1.05	0
2	DMS	41-A	405	-	3,3,3	0.67	0	3,3,3	1.90	1 (33%)
2	DMS	30-A	406	-	3,3,3	0.87	0	3,3,3	0.27	0
2	DMS	32-A	404	-	3,3,3	0.65	0	3,3,3	2.43	2 (66%)
2	DMS	22-A	405	-	3,3,3	0.77	0	3,3,3	1.62	1 (33%)
2	DMS	36-A	404	-	3,3,3	0.84	0	3,3,3	2.20	2 (66%)
2	DMS	37-A	406	-	3,3,3	0.86	0	3,3,3	1.22	0
2	DMS	9-A	407	-	3,3,3	0.72	0	3,3,3	0.86	0
2	DMS	10-A	402	-	3,3,3	0.69	0	3,3,3	2.60	2 (66%)
2	DMS	26-A	401	-	3,3,3	0.49	0	3,3,3	1.53	1 (33%)
2	DMS	20-A	406	-	3,3,3	0.83	0	3,3,3	0.38	0
2	DMS	6-A	401	-	3,3,3	0.73	0	3,3,3	2.62	2 (66%)
2	DMS	14-A	407	-	3,3,3	0.76	0	3,3,3	1.40	0
2	DMS	13-A	402	-	3,3,3	0.85	0	3,3,3	1.46	0
2	DMS	16-A	401	-	3,3,3	0.67	0	3,3,3	0.90	0
2	DMS	17-A	405	-	3,3,3	0.72	0	3,3,3	1.29	0
2	DMS	31-A	407	-	3,3,3	0.71	0	3,3,3	1.56	1 (33%)
2	DMS	32-A	407	-	3,3,3	0.90	0	3,3,3	0.96	0
2	DMS	9-A	404	-	3,3,3	0.78	0	3,3,3	0.53	0
2	DMS	21-A	402	-	3,3,3	0.78	0	3,3,3	1.73	1 (33%)
2	DMS	25-A	403	-	3,3,3	0.74	0	3,3,3	0.82	0
2	DMS	27-A	405	-	3,3,3	0.80	0	3,3,3	1.23	0
2	DMS	43-A	404	-	3,3,3	0.68	0	3,3,3	0.74	0
2	DMS	42-A	405	-	3,3,3	0.77	0	3,3,3	0.84	0
2	DMS	20-A	401	-	3,3,3	0.45	0	3,3,3	0.68	0
2	DMS	23-A	402	-	3,3,3	0.89	0	3,3,3	2.51	3 (100%)
2	DMS	14-A	406	-	3,3,3	0.74	0	3,3,3	1.01	0
2	DMS	6-A	404	-	3,3,3	0.87	0	3,3,3	0.86	0
2	DMS	39-A	406	-	3,3,3	0.77	0	3,3,3	1.55	0
2	DMS	2-A	407	-	3,3,3	0.66	0	3,3,3	1.69	1 (33%)
2	DMS	11-A	404	-	3,3,3	0.74	0	3,3,3	1.56	1 (33%)
2	DMS	8-A	407	-	3,3,3	0.73	0	3,3,3	1.96	2 (66%)
2	DMS	12-A	407	-	3,3,3	0.81	0	3,3,3	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	16-A	407	-	3,3,3	0.63	0	3,3,3	1.88	1 (33%)
2	DMS	22-A	407	-	3,3,3	0.76	0	3,3,3	1.21	0
2	DMS	9-A	406	-	3,3,3	0.72	0	3,3,3	1.02	0
2	DMS	36-A	403	-	3,3,3	0.76	0	3,3,3	1.68	1 (33%)
2	DMS	35-A	403	-	3,3,3	0.81	0	3,3,3	1.23	0
2	DMS	24-A	402	-	3,3,3	0.79	0	3,3,3	1.62	1 (33%)
2	DMS	34-A	401	-	3,3,3	0.85	0	3,3,3	1.07	0
2	DMS	11-A	402	-	3,3,3	0.86	0	3,3,3	0.49	0
2	DMS	4-A	404	-	3,3,3	0.66	0	3,3,3	3.04	3 (100%)
2	DMS	33-A	404	-	3,3,3	0.75	0	3,3,3	1.89	1 (33%)
2	DMS	38-A	404	-	3,3,3	0.80	0	3,3,3	1.35	0
2	DMS	25-A	406	-	3,3,3	0.94	0	3,3,3	1.38	1 (33%)
2	DMS	43-A	405	-	3,3,3	0.56	0	3,3,3	1.21	1 (33%)
2	DMS	25-A	404	-	3,3,3	0.83	0	3,3,3	3.05	1 (33%)
2	DMS	42-A	407	-	3,3,3	0.62	0	3,3,3	1.68	1 (33%)
2	DMS	3-A	407	-	3,3,3	0.71	0	3,3,3	1.64	1 (33%)
2	DMS	40-A	403	-	3,3,3	0.81	0	3,3,3	2.02	1 (33%)
2	DMS	21-A	401	-	3,3,3	0.62	0	3,3,3	0.36	0
2	DMS	31-A	404	-	3,3,3	0.80	0	3,3,3	2.45	2 (66%)
2	DMS	28-A	404	-	3,3,3	0.71	0	3,3,3	1.46	1 (33%)
2	DMS	13-A	405	-	3,3,3	0.77	0	3,3,3	1.59	1 (33%)
2	DMS	34-A	403	-	3,3,3	0.74	0	3,3,3	1.89	1 (33%)
2	DMS	19-A	405	-	3,3,3	0.67	0	3,3,3	1.10	0
2	DMS	29-A	407	-	3,3,3	0.74	0	3,3,3	2.37	2 (66%)
2	DMS	19-A	401	-	3,3,3	0.67	0	3,3,3	0.56	0
2	DMS	25-A	402	-	3,3,3	0.77	0	3,3,3	1.82	1 (33%)
2	DMS	40-A	402	-	3,3,3	0.74	0	3,3,3	0.48	0
2	DMS	21-A	406	-	3,3,3	0.79	0	3,3,3	1.47	0
2	DMS	18-A	401	-	3,3,3	0.59	0	3,3,3	0.21	0
2	DMS	31-A	402	-	3,3,3	0.67	0	3,3,3	2.57	2 (66%)
2	DMS	7-A	407	-	3,3,3	0.79	0	3,3,3	1.05	0
2	DMS	4-A	403	-	3,3,3	0.80	0	3,3,3	0.56	0
2	DMS	33-A	403	-	3,3,3	0.95	0	3,3,3	2.66	1 (33%)
2	DMS	28-A	402	-	3,3,3	0.95	0	3,3,3	2.23	1 (33%)
2	DMS	8-A	404	-	3,3,3	0.86	0	3,3,3	1.60	1 (33%)
2	DMS	12-A	404	-	3,3,3	0.82	0	3,3,3	2.10	2 (66%)
2	DMS	1-A	407	-	3,3,3	0.63	0	3,3,3	1.30	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	2-A	405	-	3,3,3	0.77	0	3,3,3	2.10	1 (33%)
2	DMS	31-A	406	-	3,3,3	0.66	0	3,3,3	0.29	0
2	DMS	28-A	407	-	3,3,3	0.62	0	3,3,3	0.66	0
2	DMS	5-A	402	-	3,3,3	0.69	0	3,3,3	1.68	1 (33%)
2	DMS	40-A	406	-	3,3,3	0.79	0	3,3,3	1.08	0
2	DMS	35-A	405	-	3,3,3	0.65	0	3,3,3	1.79	1 (33%)
2	DMS	5-A	404	-	3,3,3	0.50	0	3,3,3	2.14	2 (66%)
2	DMS	12-A	402	-	3,3,3	0.77	0	3,3,3	2.45	3 (100%)
2	DMS	34-A	404	-	3,3,3	0.59	0	3,3,3	1.53	1 (33%)
2	DMS	2-A	406	-	3,3,3	0.68	0	3,3,3	1.94	1 (33%)
2	DMS	8-A	406	-	3,3,3	0.65	0	3,3,3	1.42	1 (33%)
2	DMS	12-A	406	-	3,3,3	0.84	0	3,3,3	2.21	1 (33%)
2	DMS	27-A	407	-	3,3,3	0.77	0	3,3,3	1.05	0
2	DMS	17-A	403	-	3,3,3	0.87	0	3,3,3	1.34	0
2	DMS	43-A	407	-	3,3,3	0.60	0	3,3,3	1.28	1 (33%)
2	DMS	22-A	406	-	3,3,3	0.82	0	3,3,3	1.08	0
2	DMS	21-A	405	-	3,3,3	0.48	0	3,3,3	0.92	0
2	DMS	41-A	401	-	3,3,3	0.63	0	3,3,3	1.01	0
2	DMS	4-A	401	-	3,3,3	0.78	0	3,3,3	2.07	1 (33%)
2	DMS	10-A	407	-	3,3,3	0.67	0	3,3,3	0.77	0
2	DMS	19-A	403	-	3,3,3	0.61	0	3,3,3	0.47	0
2	DMS	27-A	406	-	3,3,3	0.80	0	3,3,3	2.94	1 (33%)
2	DMS	27-A	403	-	3,3,3	0.88	0	3,3,3	1.18	0
2	DMS	3-A	403	-	3,3,3	0.66	0	3,3,3	0.85	0
2	DMS	18-A	405	-	3,3,3	0.73	0	3,3,3	1.55	1 (33%)
2	DMS	37-A	405	-	3,3,3	0.87	0	3,3,3	1.35	0
2	DMS	42-A	406	-	3,3,3	0.57	0	3,3,3	0.42	0
2	DMS	9-A	402	-	3,3,3	0.82	0	3,3,3	1.62	1 (33%)
2	DMS	38-A	407	-	3,3,3	0.74	0	3,3,3	1.98	1 (33%)
2	DMS	3-A	406	-	3,3,3	0.79	0	3,3,3	2.53	3 (100%)
2	DMS	13-A	404	-	3,3,3	0.91	0	3,3,3	1.46	0
2	DMS	1-A	401	-	3,3,3	0.65	0	3,3,3	1.38	1 (33%)
2	DMS	26-A	406	-	3,3,3	0.75	0	3,3,3	0.63	0
2	DMS	32-A	403	-	3,3,3	0.69	0	3,3,3	1.41	0
2	DMS	7-A	406	-	3,3,3	0.68	0	3,3,3	0.48	0
2	DMS	24-A	401	-	3,3,3	0.42	0	3,3,3	0.67	0
2	DMS	17-A	402	-	3,3,3	0.91	0	3,3,3	0.74	0
2	DMS	27-A	404	-	3,3,3	1.01	0	3,3,3	2.50	1 (33%)
2	DMS	39-A	404	-	3,3,3	0.80	0	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	5-A	401	-	3,3,3	0.70	0	3,3,3	1.51	1 (33%)
2	DMS	3-A	404	-	3,3,3	0.90	0	3,3,3	0.81	0
2	DMS	23-A	405	-	3,3,3	0.91	0	3,3,3	0.73	0
2	DMS	3-A	401	-	3,3,3	0.74	0	3,3,3	0.61	0
2	DMS	28-A	406	-	3,3,3	0.90	0	3,3,3	0.70	0
2	DMS	41-A	406	-	3,3,3	0.59	0	3,3,3	1.09	0
2	DMS	12-A	403	-	3,3,3	0.88	0	3,3,3	0.94	0
2	DMS	38-A	405	-	3,3,3	0.71	0	3,3,3	1.47	1 (33%)
2	DMS	15-A	405	-	3,3,3	0.84	0	3,3,3	0.62	0
2	DMS	35-A	404	-	3,3,3	0.65	0	3,3,3	1.01	0
2	DMS	15-A	401	-	3,3,3	0.59	0	3,3,3	1.86	1 (33%)
2	DMS	39-A	405	-	3,3,3	0.83	0	3,3,3	1.90	1 (33%)
2	DMS	3-A	402	-	3,3,3	0.68	0	3,3,3	0.96	0
2	DMS	40-A	407	-	3,3,3	0.80	0	3,3,3	3.37	2 (66%)
2	DMS	21-A	404	-	3,3,3	0.55	0	3,3,3	1.22	0
2	DMS	14-A	403	-	3,3,3	0.71	0	3,3,3	1.72	1 (33%)
2	DMS	36-A	401	-	3,3,3	0.74	0	3,3,3	0.72	0
2	DMS	43-A	406	-	3,3,3	0.77	0	3,3,3	1.58	1 (33%)
2	DMS	1-A	406	-	3,3,3	0.94	0	3,3,3	1.37	1 (33%)
2	DMS	30-A	405	-	3,3,3	0.88	0	3,3,3	0.74	0
2	DMS	34-A	407	-	3,3,3	0.96	0	3,3,3	1.26	0
2	DMS	35-A	402	-	3,3,3	0.76	0	3,3,3	1.27	0
2	DMS	11-A	401	-	3,3,3	0.56	0	3,3,3	0.91	0
2	DMS	10-A	406	-	3,3,3	0.78	0	3,3,3	1.37	0
2	DMS	41-A	407	-	3,3,3	0.87	0	3,3,3	1.35	1 (33%)
2	DMS	8-A	402	-	3,3,3	0.70	0	3,3,3	1.28	0
2	DMS	39-A	407	-	3,3,3	0.79	0	3,3,3	2.33	1 (33%)
2	DMS	32-A	405	-	3,3,3	0.58	0	3,3,3	1.26	1 (33%)
2	DMS	32-A	402	-	3,3,3	0.73	0	3,3,3	1.33	0
2	DMS	16-A	403	-	3,3,3	0.67	0	3,3,3	1.48	1 (33%)
2	DMS	26-A	405	-	3,3,3	0.72	0	3,3,3	2.03	1 (33%)
2	DMS	2-A	404	-	3,3,3	0.75	0	3,3,3	0.89	0
2	DMS	16-A	402	-	3,3,3	0.60	0	3,3,3	1.27	1 (33%)
2	DMS	37-A	407	-	3,3,3	0.68	0	3,3,3	1.82	1 (33%)
2	DMS	30-A	401	-	3,3,3	0.68	0	3,3,3	1.91	1 (33%)
2	DMS	39-A	403	-	3,3,3	0.81	0	3,3,3	1.04	0
2	DMS	18-A	407	-	3,3,3	0.67	0	3,3,3	0.50	0
2	DMS	16-A	404	-	3,3,3	0.69	0	3,3,3	2.81	1 (33%)
2	DMS	10-A	405	-	3,3,3	0.57	0	3,3,3	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	14-A	404	-	3,3,3	0.72	0	3,3,3	1.41	1 (33%)
2	DMS	11-A	406	-	3,3,3	0.85	0	3,3,3	1.11	0
2	DMS	14-A	401	-	3,3,3	0.56	0	3,3,3	0.92	0
2	DMS	2-A	402	-	3,3,3	0.74	0	3,3,3	1.82	1 (33%)
2	DMS	29-A	406	-	3,3,3	0.64	0	3,3,3	0.52	0
2	DMS	40-A	401	-	3,3,3	0.77	0	3,3,3	0.44	0
2	DMS	30-A	402	-	3,3,3	0.79	0	3,3,3	1.07	0
2	DMS	39-A	401	-	3,3,3	0.67	0	3,3,3	1.53	1 (33%)
2	DMS	31-A	401	-	3,3,3	1.12	0	3,3,3	1.57	1 (33%)
2	DMS	42-A	402	-	3,3,3	0.75	0	3,3,3	1.45	0
2	DMS	9-A	403	-	3,3,3	0.77	0	3,3,3	0.73	0
2	DMS	9-A	405	-	3,3,3	0.90	0	3,3,3	1.17	0
2	DMS	28-A	405	-	3,3,3	0.61	0	3,3,3	1.01	0
2	DMS	37-A	403	-	3,3,3	0.65	0	3,3,3	0.31	0
2	DMS	17-A	406	-	3,3,3	0.87	0	3,3,3	1.76	1 (33%)
2	DMS	14-A	402	-	3,3,3	0.63	0	3,3,3	0.88	0
2	DMS	6-A	406	-	3,3,3	0.81	0	3,3,3	1.04	0
2	DMS	19-A	407	-	3,3,3	0.82	0	3,3,3	3.14	1 (33%)
2	DMS	37-A	401	-	3,3,3	0.97	0	3,3,3	0.33	0
2	DMS	20-A	405	-	3,3,3	0.87	0	3,3,3	2.22	1 (33%)
2	DMS	6-A	403	-	3,3,3	0.65	0	3,3,3	0.26	0
2	DMS	9-A	401	-	3,3,3	0.55	0	3,3,3	1.85	1 (33%)
2	DMS	8-A	401	-	3,3,3	0.91	0	3,3,3	0.94	0
2	DMS	41-A	404	-	3,3,3	0.99	0	3,3,3	1.27	0
2	DMS	22-A	404	-	3,3,3	0.76	0	3,3,3	0.79	0
2	DMS	7-A	402	-	3,3,3	0.71	0	3,3,3	1.20	0
2	DMS	34-A	402	-	3,3,3	0.85	0	3,3,3	0.11	0
2	DMS	22-A	401	-	3,3,3	0.55	0	3,3,3	0.98	0
2	DMS	5-A	406	-	3,3,3	0.61	0	3,3,3	1.01	0
2	DMS	35-A	407	-	3,3,3	0.91	0	3,3,3	1.18	0
2	DMS	38-A	402	-	3,3,3	0.80	0	3,3,3	0.86	0
2	DMS	7-A	404	-	3,3,3	0.71	0	3,3,3	1.57	0
2	DMS	5-A	403	-	3,3,3	0.73	0	3,3,3	1.61	1 (33%)
2	DMS	34-A	406	-	3,3,3	0.91	0	3,3,3	1.45	0
2	DMS	1-A	404	-	3,3,3	0.62	0	3,3,3	0.95	0
2	DMS	23-A	406	-	3,3,3	0.83	0	3,3,3	1.03	0
2	DMS	33-A	406	-	3,3,3	0.73	0	3,3,3	1.69	1 (33%)
2	DMS	37-A	404	-	3,3,3	0.51	0	3,3,3	1.30	1 (33%)
2	DMS	4-A	405	-	3,3,3	0.69	0	3,3,3	1.08	0
2	DMS	4-A	402	-	3,3,3	0.81	0	3,3,3	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	18-A	404	-	3,3,3	0.48	0	3,3,3	1.50	1 (33%)
2	DMS	42-A	404	-	3,3,3	0.68	0	3,3,3	0.91	0
2	DMS	42-A	401	-	3,3,3	0.87	0	3,3,3	1.51	1 (33%)
2	DMS	11-A	405	-	3,3,3	0.77	0	3,3,3	2.09	1 (33%)
2	DMS	24-A	405	-	3,3,3	0.65	0	3,3,3	0.93	0
2	DMS	40-A	405	-	3,3,3	0.89	0	3,3,3	0.93	0
2	DMS	27-A	402	-	3,3,3	0.85	0	3,3,3	2.10	1 (33%)
2	DMS	43-A	402	-	3,3,3	0.84	0	3,3,3	3.04	2 (66%)
2	DMS	26-A	403	-	3,3,3	0.88	0	3,3,3	0.75	0
2	DMS	31-A	403	-	3,3,3	0.66	0	3,3,3	1.41	1 (33%)
2	DMS	1-A	402	-	3,3,3	0.84	0	3,3,3	0.50	0
2	DMS	18-A	402	-	3,3,3	0.77	0	3,3,3	1.51	0
2	DMS	35-A	401	-	3,3,3	0.93	0	3,3,3	1.60	0
2	DMS	18-A	403	-	3,3,3	0.89	0	3,3,3	2.24	1 (33%)
2	DMS	29-A	405	-	3,3,3	0.62	0	3,3,3	0.49	0
2	DMS	19-A	404	-	3,3,3	0.84	0	3,3,3	0.19	0
2	DMS	7-A	405	-	3,3,3	0.80	0	3,3,3	1.02	0
2	DMS	6-A	405	-	3,3,3	0.92	0	3,3,3	1.09	0
2	DMS	18-A	406	-	3,3,3	0.71	0	3,3,3	0.97	0
2	DMS	24-A	407	-	3,3,3	0.64	0	3,3,3	1.21	0
2	DMS	2-A	403	-	3,3,3	0.65	0	3,3,3	1.16	0
2	DMS	8-A	403	-	3,3,3	0.79	0	3,3,3	0.68	0
2	DMS	25-A	405	-	3,3,3	0.87	0	3,3,3	0.68	0
2	DMS	25-A	401	-	3,3,3	0.78	0	3,3,3	1.76	1 (33%)
2	DMS	12-A	405	-	3,3,3	0.52	0	3,3,3	1.10	0
2	DMS	26-A	402	-	3,3,3	0.81	0	3,3,3	1.53	0
2	DMS	22-A	403	-	3,3,3	0.63	0	3,3,3	1.65	1 (33%)
2	DMS	19-A	406	-	3,3,3	0.75	0	3,3,3	0.97	0
2	DMS	28-A	401	-	3,3,3	0.82	0	3,3,3	1.13	0
2	DMS	23-A	401	-	3,3,3	0.67	0	3,3,3	0.70	0
2	DMS	5-A	405	-	3,3,3	0.54	0	3,3,3	1.42	1 (33%)
2	DMS	26-A	404	-	3,3,3	0.55	0	3,3,3	1.90	1 (33%)
2	DMS	1-A	403	-	3,3,3	0.74	0	3,3,3	1.19	0
2	DMS	10-A	403	-	3,3,3	0.60	0	3,3,3	2.06	2 (66%)
2	DMS	34-A	405	-	3,3,3	0.87	0	3,3,3	1.76	1 (33%)
2	DMS	36-A	407	-	3,3,3	0.80	0	3,3,3	1.51	1 (33%)
2	DMS	42-A	403	-	3,3,3	0.72	0	3,3,3	1.43	1 (33%)
2	DMS	43-A	401	-	3,3,3	0.83	0	3,3,3	0.64	0
2	DMS	21-A	407	-	3,3,3	0.79	0	3,3,3	1.66	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	6-A	402	-	3,3,3	0.75	0	3,3,3	0.98	0
2	DMS	13-A	401	-	3,3,3	0.60	0	3,3,3	0.42	0
2	DMS	20-A	402	-	3,3,3	0.67	0	3,3,3	2.03	1 (33%)
2	DMS	35-A	406	-	3,3,3	0.73	0	3,3,3	0.57	0
2	DMS	41-A	403	-	3,3,3	0.67	0	3,3,3	0.79	0
2	DMS	36-A	406	-	3,3,3	0.86	0	3,3,3	1.27	1 (33%)
2	DMS	15-A	407	-	3,3,3	0.76	0	3,3,3	2.02	1 (33%)
2	DMS	39-A	402	-	3,3,3	0.73	0	3,3,3	3.24	3 (100%)
2	DMS	20-A	403	-	3,3,3	0.83	0	3,3,3	1.84	1 (33%)
2	DMS	8-A	405	-	3,3,3	0.84	0	3,3,3	2.81	2 (66%)
2	DMS	13-A	406	-	3,3,3	0.81	0	3,3,3	1.23	0
2	DMS	24-A	404	-	3,3,3	0.73	0	3,3,3	1.21	0
2	DMS	30-A	407	-	3,3,3	0.87	0	3,3,3	1.39	1 (33%)
2	DMS	4-A	407	-	3,3,3	0.81	0	3,3,3	1.52	1 (33%)
2	DMS	33-A	407	-	3,3,3	0.60	0	3,3,3	0.64	0
2	DMS	13-A	403	-	3,3,3	0.69	0	3,3,3	2.70	2 (66%)
2	DMS	10-A	404	-	3,3,3	0.69	0	3,3,3	0.26	0
2	DMS	28-A	403	-	3,3,3	0.72	0	3,3,3	0.70	0
2	DMS	40-A	404	-	3,3,3	0.76	0	3,3,3	0.57	0
2	DMS	24-A	403	-	3,3,3	0.71	0	3,3,3	1.52	0
2	DMS	5-A	407	-	3,3,3	0.98	0	3,3,3	0.87	0
2	DMS	1-A	405	-	3,3,3	0.64	0	3,3,3	1.67	1 (33%)
2	DMS	17-A	401	-	3,3,3	0.70	0	3,3,3	2.09	1 (33%)
2	DMS	24-A	406	-	3,3,3	0.77	0	3,3,3	1.09	0
2	DMS	4-A	406	-	3,3,3	0.82	0	3,3,3	0.92	0
2	DMS	2-A	401	-	3,3,3	0.79	0	3,3,3	0.86	0
2	DMS	23-A	407	-	3,3,3	0.74	0	3,3,3	1.84	1 (33%)
2	DMS	43-A	403	-	3,3,3	0.70	0	3,3,3	0.68	0
2	DMS	26-A	407	-	3,3,3	0.72	0	3,3,3	1.55	1 (33%)
2	DMS	20-A	404	-	3,3,3	0.74	0	3,3,3	0.44	0
2	DMS	3-A	405	-	3,3,3	0.75	0	3,3,3	1.50	1 (33%)
2	DMS	15-A	403	-	3,3,3	0.79	0	3,3,3	2.37	1 (33%)
2	DMS	38-A	401	-	3,3,3	0.86	0	3,3,3	2.44	1 (33%)
2	DMS	29-A	403	-	3,3,3	0.75	0	3,3,3	1.95	1 (33%)
2	DMS	7-A	403	-	3,3,3	0.76	0	3,3,3	1.77	1 (33%)
2	DMS	33-A	402	-	3,3,3	0.76	0	3,3,3	0.52	0
2	DMS	37-A	402	-	3,3,3	0.78	0	3,3,3	0.53	0
2	DMS	38-A	406	-	3,3,3	0.78	0	3,3,3	1.28	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	11-A	403	-	3,3,3	0.99	0	3,3,3	2.11	1 (33%)
2	DMS	7-A	401	-	3,3,3	0.75	0	3,3,3	1.18	0
2	DMS	33-A	401	-	3,3,3	0.64	0	3,3,3	1.76	1 (33%)
2	DMS	38-A	403	-	3,3,3	0.55	0	3,3,3	0.90	0
2	DMS	19-A	402	-	3,3,3	0.88	0	3,3,3	0.40	0
2	DMS	21-A	403	-	3,3,3	0.99	0	3,3,3	1.24	0
2	DMS	31-A	405	-	3,3,3	0.68	0	3,3,3	0.88	0
2	DMS	22-A	402	-	3,3,3	0.84	0	3,3,3	1.74	0
2	DMS	29-A	401	-	3,3,3	0.68	0	3,3,3	0.45	0
2	DMS	15-A	406	-	3,3,3	0.76	0	3,3,3	1.15	0
2	DMS	32-A	401	-	3,3,3	0.85	0	3,3,3	1.30	0
2	DMS	13-A	407	-	3,3,3	0.76	0	3,3,3	1.01	0
2	DMS	15-A	404	-	3,3,3	0.70	0	3,3,3	2.05	1 (33%)
2	DMS	30-A	403	-	3,3,3	0.68	0	3,3,3	1.19	0
2	DMS	29-A	404	-	3,3,3	0.49	0	3,3,3	1.39	0
2	DMS	17-A	404	-	3,3,3	0.80	0	3,3,3	2.49	1 (33%)
2	DMS	36-A	405	-	3,3,3	0.73	0	3,3,3	0.57	0
2	DMS	23-A	404	-	3,3,3	0.77	0	3,3,3	0.86	0
2	DMS	36-A	402	-	3,3,3	0.75	0	3,3,3	1.65	1 (33%)
2	DMS	12-A	401	-	3,3,3	0.83	0	3,3,3	0.99	0
2	DMS	16-A	405	-	3,3,3	0.69	0	3,3,3	0.82	0
2	DMS	15-A	402	-	3,3,3	0.77	0	3,3,3	1.58	1 (33%)
2	DMS	14-A	405	-	3,3,3	0.72	0	3,3,3	1.27	0

There are no bond length outliers.

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	25-A	404	DMS	O-S-C2	5.16	132.31	106.49
2	19-A	407	DMS	O-S-C2	5.12	132.14	106.49
2	40-A	407	DMS	O-S-C2	4.73	130.15	106.49
2	27-A	406	DMS	O-S-C2	4.56	129.31	106.49
2	16-A	404	DMS	C2-S-C1	4.29	120.40	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	3.23	214 (69%) 0 0	0, 0, 0, 0	306 (100%)
1	2-A	0/306	-	-	-	-
1	3-A	0/306	-	-	-	-
1	4-A	0/306	-	-	-	-
1	5-A	0/306	-	-	-	-
1	6-A	0/306	-	-	-	-
1	7-A	0/306	-	-	-	-
1	8-A	0/306	-	-	-	-
1	9-A	0/306	-	-	-	-
1	10-A	0/306	-	-	-	-
1	11-A	0/306	-	-	-	-
1	12-A	0/306	-	-	-	-
1	13-A	0/306	-	-	-	-
1	14-A	0/306	-	-	-	-
1	15-A	0/306	-	-	-	-
1	16-A	0/306	-	-	-	-
1	17-A	0/306	-	-	-	-
1	18-A	0/306	-	-	-	-
1	19-A	0/306	-	-	-	-
1	20-A	0/306	-	-	-	-
1	21-A	0/306	-	-	-	-
1	22-A	0/306	-	-	-	-
1	23-A	0/306	-	-	-	-
1	24-A	0/306	-	-	-	-
1	25-A	0/306	-	-	-	-
1	26-A	0/306	-	-	-	-
1	27-A	0/306	-	-	-	-
1	28-A	0/306	-	-	-	-
1	29-A	0/306	-	-	-	-
1	30-A	0/306	-	-	-	-
1	31-A	0/306	-	-	-	-
1	32-A	0/306	-	-	-	-

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/306	-	-	-	-
1	34-A	0/306	-	-	-	-
1	35-A	0/306	-	-	-	-
1	36-A	0/306	-	-	-	-
1	37-A	0/306	-	-	-	-
1	38-A	0/306	-	-	-	-
1	39-A	0/306	-	-	-	-
1	40-A	0/306	-	-	-	-
1	41-A	0/306	-	-	-	-
1	42-A	0/306	-	-	-	-
1	43-A	0/306	-	-	-	-
All	All	306/13158 (2%)	3.23	214 (69%) 0 0	0, 0, 0, 0	306 (100%)

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	305	PHE	19.9
1	1-A	300	CYS	16.1
1	1-A	302	GLY	13.7
1	1-A	303	VAL	11.5
1	1-A	191	ALA	11.3

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 oligosaccharides 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, 95th 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	405	4/4	0.45	0.46	19,20,20,20	10
2	DMS	2-A	401	4/4	-	-	20,20,21,21	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	3-A	401	4/4	-	-	20,20,21,21	10
2	DMS	4-A	401	4/4	-	-	20,20,21,21	10
2	DMS	5-A	401	4/4	-	-	20,20,21,21	10
2	DMS	6-A	401	4/4	-	-	20,20,21,21	10
2	DMS	7-A	401	4/4	-	-	20,20,21,21	10
2	DMS	8-A	401	4/4	-	-	20,20,21,21	10
2	DMS	9-A	401	4/4	-	-	20,20,21,21	10
2	DMS	10-A	401	4/4	-	-	20,20,21,21	10
2	DMS	11-A	401	4/4	-	-	20,20,21,21	10
2	DMS	12-A	401	4/4	-	-	20,20,21,21	10
2	DMS	13-A	401	4/4	-	-	20,20,21,21	10
2	DMS	14-A	401	4/4	-	-	20,20,21,21	10
2	DMS	15-A	401	4/4	-	-	20,20,21,21	10
2	DMS	16-A	401	4/4	-	-	20,20,21,21	10
2	DMS	17-A	401	4/4	-	-	20,20,21,21	10
2	DMS	18-A	401	4/4	-	-	20,20,21,21	10
2	DMS	19-A	401	4/4	-	-	20,20,21,21	10
2	DMS	20-A	401	4/4	-	-	20,20,21,21	10
2	DMS	21-A	401	4/4	-	-	20,20,21,21	10
2	DMS	22-A	401	4/4	-	-	20,20,21,21	10
2	DMS	23-A	401	4/4	-	-	20,20,21,21	10
2	DMS	24-A	401	4/4	-	-	20,20,21,21	10
2	DMS	25-A	401	4/4	-	-	20,20,21,21	10
2	DMS	26-A	401	4/4	-	-	20,20,21,21	10
2	DMS	27-A	401	4/4	-	-	20,20,21,21	10
2	DMS	28-A	401	4/4	-	-	20,20,21,21	10
2	DMS	29-A	401	4/4	-	-	20,20,21,21	10
2	DMS	30-A	401	4/4	-	-	20,20,21,21	10
2	DMS	31-A	401	4/4	-	-	20,20,21,21	10
2	DMS	32-A	401	4/4	-	-	20,20,21,21	10
2	DMS	33-A	401	4/4	-	-	20,20,21,21	10
2	DMS	34-A	401	4/4	-	-	20,20,21,21	10
2	DMS	35-A	401	4/4	-	-	20,20,21,21	10
2	DMS	36-A	401	4/4	-	-	20,20,21,21	10
2	DMS	37-A	401	4/4	-	-	20,20,21,21	10
2	DMS	38-A	401	4/4	-	-	20,20,21,21	10
2	DMS	39-A	401	4/4	-	-	20,20,21,21	10
2	DMS	40-A	401	4/4	-	-	20,20,21,21	10
2	DMS	41-A	401	4/4	-	-	20,20,21,21	10
2	DMS	42-A	401	4/4	-	-	20,20,21,21	10
2	DMS	43-A	401	4/4	-	-	20,20,21,21	10
2	DMS	1-A	406	4/4	0.45	0.47	19,19,20,20	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	2-A	402	4/4	-	-	18,19,19,19	10
2	DMS	3-A	402	4/4	-	-	18,19,19,19	10
2	DMS	4-A	402	4/4	-	-	18,19,19,19	10
2	DMS	5-A	402	4/4	-	-	18,19,19,19	10
2	DMS	6-A	402	4/4	-	-	18,19,19,19	10
2	DMS	7-A	402	4/4	-	-	18,19,19,19	10
2	DMS	8-A	402	4/4	-	-	18,19,19,19	10
2	DMS	9-A	402	4/4	-	-	18,19,19,19	10
2	DMS	10-A	402	4/4	-	-	18,19,19,19	10
2	DMS	11-A	402	4/4	-	-	18,19,19,19	10
2	DMS	12-A	402	4/4	-	-	18,19,19,19	10
2	DMS	13-A	402	4/4	-	-	18,19,19,19	10
2	DMS	14-A	402	4/4	-	-	18,19,19,19	10
2	DMS	15-A	402	4/4	-	-	18,19,19,19	10
2	DMS	16-A	402	4/4	-	-	18,19,19,19	10
2	DMS	17-A	402	4/4	-	-	18,19,19,19	10
2	DMS	18-A	402	4/4	-	-	18,19,19,19	10
2	DMS	19-A	402	4/4	-	-	18,19,19,19	10
2	DMS	20-A	402	4/4	-	-	18,19,19,19	10
2	DMS	21-A	402	4/4	-	-	18,19,19,19	10
2	DMS	22-A	402	4/4	-	-	18,19,19,19	10
2	DMS	23-A	402	4/4	-	-	18,19,19,19	10
2	DMS	24-A	402	4/4	-	-	18,19,19,19	10
2	DMS	25-A	402	4/4	-	-	18,19,19,19	10
2	DMS	26-A	402	4/4	-	-	18,19,19,19	10
2	DMS	27-A	402	4/4	-	-	18,19,19,19	10
2	DMS	28-A	402	4/4	-	-	18,19,19,19	10
2	DMS	29-A	402	4/4	-	-	18,19,19,19	10
2	DMS	30-A	402	4/4	-	-	18,19,19,19	10
2	DMS	31-A	402	4/4	-	-	18,19,19,19	10
2	DMS	32-A	402	4/4	-	-	18,19,19,19	10
2	DMS	33-A	402	4/4	-	-	18,19,19,19	10
2	DMS	34-A	402	4/4	-	-	18,19,19,19	10
2	DMS	35-A	402	4/4	-	-	18,19,19,19	10
2	DMS	36-A	402	4/4	-	-	18,19,19,19	10
2	DMS	37-A	402	4/4	-	-	18,19,19,19	10
2	DMS	38-A	402	4/4	-	-	18,19,19,19	10
2	DMS	39-A	402	4/4	-	-	18,19,19,19	10
2	DMS	40-A	402	4/4	-	-	18,19,19,19	10
2	DMS	41-A	402	4/4	-	-	18,19,19,19	10
2	DMS	42-A	402	4/4	-	-	18,19,19,19	10
2	DMS	43-A	402	4/4	-	-	18,19,19,19	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	1-A	403	4/4	0.48	0.44	19,19,19,19	10
2	DMS	2-A	403	4/4	-	-	19,19,19,19	10
2	DMS	3-A	403	4/4	-	-	19,19,19,19	10
2	DMS	4-A	403	4/4	-	-	19,19,19,19	10
2	DMS	5-A	403	4/4	-	-	19,19,19,19	10
2	DMS	6-A	403	4/4	-	-	19,19,19,19	10
2	DMS	7-A	403	4/4	-	-	19,19,19,19	10
2	DMS	8-A	403	4/4	-	-	19,19,19,19	10
2	DMS	9-A	403	4/4	-	-	19,19,19,19	10
2	DMS	10-A	403	4/4	-	-	19,19,19,19	10
2	DMS	11-A	403	4/4	-	-	19,19,19,19	10
2	DMS	12-A	403	4/4	-	-	19,19,19,19	10
2	DMS	13-A	403	4/4	-	-	19,19,19,19	10
2	DMS	14-A	403	4/4	-	-	19,19,19,19	10
2	DMS	15-A	403	4/4	-	-	19,19,19,19	10
2	DMS	16-A	403	4/4	-	-	19,19,19,19	10
2	DMS	17-A	403	4/4	-	-	19,19,19,19	10
2	DMS	18-A	403	4/4	-	-	19,19,19,19	10
2	DMS	19-A	403	4/4	-	-	19,19,19,19	10
2	DMS	20-A	403	4/4	-	-	19,19,19,19	10
2	DMS	21-A	403	4/4	-	-	19,19,19,19	10
2	DMS	22-A	403	4/4	-	-	19,19,19,19	10
2	DMS	23-A	403	4/4	-	-	19,19,19,19	10
2	DMS	24-A	403	4/4	-	-	19,19,19,19	10
2	DMS	25-A	403	4/4	-	-	19,19,19,19	10
2	DMS	26-A	403	4/4	-	-	19,19,19,19	10
2	DMS	27-A	403	4/4	-	-	19,19,19,19	10
2	DMS	28-A	403	4/4	-	-	19,19,19,19	10
2	DMS	29-A	403	4/4	-	-	19,19,19,19	10
2	DMS	30-A	403	4/4	-	-	19,19,19,19	10
2	DMS	31-A	403	4/4	-	-	19,19,19,19	10
2	DMS	32-A	403	4/4	-	-	19,19,19,19	10
2	DMS	33-A	403	4/4	-	-	19,19,19,19	10
2	DMS	34-A	403	4/4	-	-	19,19,19,19	10
2	DMS	35-A	403	4/4	-	-	19,19,19,19	10
2	DMS	36-A	403	4/4	-	-	19,19,19,19	10
2	DMS	37-A	403	4/4	-	-	19,19,19,19	10
2	DMS	38-A	403	4/4	-	-	19,19,19,19	10
2	DMS	39-A	403	4/4	-	-	19,19,19,19	10
2	DMS	40-A	403	4/4	-	-	19,19,19,19	10
2	DMS	41-A	403	4/4	-	-	19,19,19,19	10
2	DMS	42-A	403	4/4	-	-	19,19,19,19	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	43-A	403	4/4	-	-	19,19,19,19	10
2	DMS	1-A	401	4/4	0.53	0.30	20,20,21,21	10
2	DMS	2-A	404	4/4	-	-	19,19,19,19	10
2	DMS	3-A	404	4/4	-	-	19,19,19,19	10
2	DMS	4-A	404	4/4	-	-	19,19,19,19	10
2	DMS	5-A	404	4/4	-	-	19,19,19,19	10
2	DMS	6-A	404	4/4	-	-	19,19,19,19	10
2	DMS	7-A	404	4/4	-	-	19,19,19,19	10
2	DMS	8-A	404	4/4	-	-	19,19,19,19	10
2	DMS	9-A	404	4/4	-	-	19,19,19,19	10
2	DMS	10-A	404	4/4	-	-	19,19,19,19	10
2	DMS	11-A	404	4/4	-	-	19,19,19,19	10
2	DMS	12-A	404	4/4	-	-	19,19,19,19	10
2	DMS	13-A	404	4/4	-	-	19,19,19,19	10
2	DMS	14-A	404	4/4	-	-	19,19,19,19	10
2	DMS	15-A	404	4/4	-	-	19,19,19,19	10
2	DMS	16-A	404	4/4	-	-	19,19,19,19	10
2	DMS	17-A	404	4/4	-	-	19,19,19,19	10
2	DMS	18-A	404	4/4	-	-	19,19,19,19	10
2	DMS	19-A	404	4/4	-	-	19,19,19,19	10
2	DMS	20-A	404	4/4	-	-	19,19,19,19	10
2	DMS	21-A	404	4/4	-	-	19,19,19,19	10
2	DMS	22-A	404	4/4	-	-	19,19,19,19	10
2	DMS	23-A	404	4/4	-	-	19,19,19,19	10
2	DMS	24-A	404	4/4	-	-	19,19,19,19	10
2	DMS	25-A	404	4/4	-	-	19,19,19,19	10
2	DMS	26-A	404	4/4	-	-	19,19,19,19	10
2	DMS	27-A	404	4/4	-	-	19,19,19,19	10
2	DMS	28-A	404	4/4	-	-	19,19,19,19	10
2	DMS	29-A	404	4/4	-	-	19,19,19,19	10
2	DMS	30-A	404	4/4	-	-	19,19,19,19	10
2	DMS	31-A	404	4/4	-	-	19,19,19,19	10
2	DMS	32-A	404	4/4	-	-	19,19,19,19	10
2	DMS	33-A	404	4/4	-	-	19,19,19,19	10
2	DMS	34-A	404	4/4	-	-	19,19,19,19	10
2	DMS	35-A	404	4/4	-	-	19,19,19,19	10
2	DMS	36-A	404	4/4	-	-	19,19,19,19	10
2	DMS	37-A	404	4/4	-	-	19,19,19,19	10
2	DMS	38-A	404	4/4	-	-	19,19,19,19	10
2	DMS	39-A	404	4/4	-	-	19,19,19,19	10
2	DMS	40-A	404	4/4	-	-	19,19,19,19	10
2	DMS	41-A	404	4/4	-	-	19,19,19,19	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	42-A	404	4/4	-	-	19,19,19,19	10
2	DMS	43-A	404	4/4	-	-	19,19,19,19	10
2	DMS	1-A	407	4/4	0.70	0.32	20,20,21,21	10
2	DMS	2-A	405	4/4	-	-	19,20,20,20	10
2	DMS	3-A	405	4/4	-	-	19,20,20,20	10
2	DMS	4-A	405	4/4	-	-	19,20,20,20	10
2	DMS	5-A	405	4/4	-	-	19,20,20,20	10
2	DMS	6-A	405	4/4	-	-	19,20,20,20	10
2	DMS	7-A	405	4/4	-	-	19,20,20,20	10
2	DMS	8-A	405	4/4	-	-	19,20,20,20	10
2	DMS	9-A	405	4/4	-	-	19,20,20,20	10
2	DMS	10-A	405	4/4	-	-	19,20,20,20	10
2	DMS	11-A	405	4/4	-	-	19,20,20,20	10
2	DMS	12-A	405	4/4	-	-	19,20,20,20	10
2	DMS	13-A	405	4/4	-	-	19,20,20,20	10
2	DMS	14-A	405	4/4	-	-	19,20,20,20	10
2	DMS	15-A	405	4/4	-	-	19,20,20,20	10
2	DMS	16-A	405	4/4	-	-	19,20,20,20	10
2	DMS	17-A	405	4/4	-	-	19,20,20,20	10
2	DMS	18-A	405	4/4	-	-	19,20,20,20	10
2	DMS	19-A	405	4/4	-	-	19,20,20,20	10
2	DMS	20-A	405	4/4	-	-	19,20,20,20	10
2	DMS	21-A	405	4/4	-	-	19,20,20,20	10
2	DMS	22-A	405	4/4	-	-	19,20,20,20	10
2	DMS	23-A	405	4/4	-	-	19,20,20,20	10
2	DMS	24-A	405	4/4	-	-	19,20,20,20	10
2	DMS	25-A	405	4/4	-	-	19,20,20,20	10
2	DMS	26-A	405	4/4	-	-	19,20,20,20	10
2	DMS	27-A	405	4/4	-	-	19,20,20,20	10
2	DMS	28-A	405	4/4	-	-	19,20,20,20	10
2	DMS	29-A	405	4/4	-	-	19,20,20,20	10
2	DMS	30-A	405	4/4	-	-	19,20,20,20	10
2	DMS	31-A	405	4/4	-	-	19,20,20,20	10
2	DMS	32-A	405	4/4	-	-	19,20,20,20	10
2	DMS	33-A	405	4/4	-	-	19,20,20,20	10
2	DMS	34-A	405	4/4	-	-	19,20,20,20	10
2	DMS	35-A	405	4/4	-	-	19,20,20,20	10
2	DMS	36-A	405	4/4	-	-	19,20,20,20	10
2	DMS	37-A	405	4/4	-	-	19,20,20,20	10
2	DMS	38-A	405	4/4	-	-	19,20,20,20	10
2	DMS	39-A	405	4/4	-	-	19,20,20,20	10
2	DMS	40-A	405	4/4	-	-	19,20,20,20	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	41-A	405	4/4	-	-	19,20,20,20	10
2	DMS	42-A	405	4/4	-	-	19,20,20,20	10
2	DMS	43-A	405	4/4	-	-	19,20,20,20	10
2	DMS	1-A	402	4/4	0.71	0.61	18,19,19,19	10
2	DMS	2-A	406	4/4	-	-	19,19,20,20	10
2	DMS	3-A	406	4/4	-	-	19,19,20,20	10
2	DMS	4-A	406	4/4	-	-	19,19,20,20	10
2	DMS	5-A	406	4/4	-	-	19,19,20,20	10
2	DMS	6-A	406	4/4	-	-	19,19,20,20	10
2	DMS	7-A	406	4/4	-	-	19,19,20,20	10
2	DMS	8-A	406	4/4	-	-	19,19,20,20	10
2	DMS	9-A	406	4/4	-	-	19,19,20,20	10
2	DMS	10-A	406	4/4	-	-	19,19,20,20	10
2	DMS	11-A	406	4/4	-	-	19,19,20,20	10
2	DMS	12-A	406	4/4	-	-	19,19,20,20	10
2	DMS	13-A	406	4/4	-	-	19,19,20,20	10
2	DMS	14-A	406	4/4	-	-	19,19,20,20	10
2	DMS	15-A	406	4/4	-	-	19,19,20,20	10
2	DMS	16-A	406	4/4	-	-	19,19,20,20	10
2	DMS	17-A	406	4/4	-	-	19,19,20,20	10
2	DMS	18-A	406	4/4	-	-	19,19,20,20	10
2	DMS	19-A	406	4/4	-	-	19,19,20,20	10
2	DMS	20-A	406	4/4	-	-	19,19,20,20	10
2	DMS	21-A	406	4/4	-	-	19,19,20,20	10
2	DMS	22-A	406	4/4	-	-	19,19,20,20	10
2	DMS	23-A	406	4/4	-	-	19,19,20,20	10
2	DMS	24-A	406	4/4	-	-	19,19,20,20	10
2	DMS	25-A	406	4/4	-	-	19,19,20,20	10
2	DMS	26-A	406	4/4	-	-	19,19,20,20	10
2	DMS	27-A	406	4/4	-	-	19,19,20,20	10
2	DMS	28-A	406	4/4	-	-	19,19,20,20	10
2	DMS	29-A	406	4/4	-	-	19,19,20,20	10
2	DMS	30-A	406	4/4	-	-	19,19,20,20	10
2	DMS	31-A	406	4/4	-	-	19,19,20,20	10
2	DMS	32-A	406	4/4	-	-	19,19,20,20	10
2	DMS	33-A	406	4/4	-	-	19,19,20,20	10
2	DMS	34-A	406	4/4	-	-	19,19,20,20	10
2	DMS	35-A	406	4/4	-	-	19,19,20,20	10
2	DMS	36-A	406	4/4	-	-	19,19,20,20	10
2	DMS	37-A	406	4/4	-	-	19,19,20,20	10
2	DMS	38-A	406	4/4	-	-	19,19,20,20	10
2	DMS	39-A	406	4/4	-	-	19,19,20,20	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	40-A	406	4/4	-	-	19,19,20,20	10
2	DMS	41-A	406	4/4	-	-	19,19,20,20	10
2	DMS	42-A	406	4/4	-	-	19,19,20,20	10
2	DMS	43-A	406	4/4	-	-	19,19,20,20	10
2	DMS	1-A	404	4/4	0.72	0.34	19,19,19,19	10
2	DMS	2-A	407	4/4	-	-	20,20,21,21	10
2	DMS	3-A	407	4/4	-	-	20,20,21,21	10
2	DMS	4-A	407	4/4	-	-	20,20,21,21	10
2	DMS	5-A	407	4/4	-	-	20,20,21,21	10
2	DMS	6-A	407	4/4	-	-	20,20,21,21	10
2	DMS	7-A	407	4/4	-	-	20,20,21,21	10
2	DMS	8-A	407	4/4	-	-	20,20,21,21	10
2	DMS	9-A	407	4/4	-	-	20,20,21,21	10
2	DMS	10-A	407	4/4	-	-	20,20,21,21	10
2	DMS	11-A	407	4/4	-	-	20,20,21,21	10
2	DMS	12-A	407	4/4	-	-	20,20,21,21	10
2	DMS	13-A	407	4/4	-	-	20,20,21,21	10
2	DMS	14-A	407	4/4	-	-	20,20,21,21	10
2	DMS	15-A	407	4/4	-	-	20,20,21,21	10
2	DMS	16-A	407	4/4	-	-	20,20,21,21	10
2	DMS	17-A	407	4/4	-	-	20,20,21,21	10
2	DMS	18-A	407	4/4	-	-	20,20,21,21	10
2	DMS	19-A	407	4/4	-	-	20,20,21,21	10
2	DMS	20-A	407	4/4	-	-	20,20,21,21	10
2	DMS	21-A	407	4/4	-	-	20,20,21,21	10
2	DMS	22-A	407	4/4	-	-	20,20,21,21	10
2	DMS	23-A	407	4/4	-	-	20,20,21,21	10
2	DMS	24-A	407	4/4	-	-	20,20,21,21	10
2	DMS	25-A	407	4/4	-	-	20,20,21,21	10
2	DMS	26-A	407	4/4	-	-	20,20,21,21	10
2	DMS	27-A	407	4/4	-	-	20,20,21,21	10
2	DMS	28-A	407	4/4	-	-	20,20,21,21	10
2	DMS	29-A	407	4/4	-	-	20,20,21,21	10
2	DMS	30-A	407	4/4	-	-	20,20,21,21	10
2	DMS	31-A	407	4/4	-	-	20,20,21,21	10
2	DMS	32-A	407	4/4	-	-	20,20,21,21	10
2	DMS	33-A	407	4/4	-	-	20,20,21,21	10
2	DMS	34-A	407	4/4	-	-	20,20,21,21	10
2	DMS	35-A	407	4/4	-	-	20,20,21,21	10
2	DMS	36-A	407	4/4	-	-	20,20,21,21	10
2	DMS	37-A	407	4/4	-	-	20,20,21,21	10
2	DMS	38-A	407	4/4	-	-	20,20,21,21	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	39-A	407	4/4	-	-	20,20,21,21	10
2	DMS	40-A	407	4/4	-	-	20,20,21,21	10
2	DMS	41-A	407	4/4	-	-	20,20,21,21	10
2	DMS	42-A	407	4/4	-	-	20,20,21,21	10
2	DMS	43-A	407	4/4	-	-	20,20,21,21	10
3	ZN	1-A	408	1/1	0.93	0.46	19,19,19,19	1
3	ZN	2-A	408	1/1	-	-	19,19,19,19	1
3	ZN	3-A	408	1/1	-	-	19,19,19,19	1
3	ZN	4-A	408	1/1	-	-	19,19,19,19	1
3	ZN	5-A	408	1/1	-	-	19,19,19,19	1
3	ZN	6-A	408	1/1	-	-	19,19,19,19	1
3	ZN	7-A	408	1/1	-	-	19,19,19,19	1
3	ZN	8-A	408	1/1	-	-	19,19,19,19	1
3	ZN	9-A	408	1/1	-	-	19,19,19,19	1
3	ZN	10-A	408	1/1	-	-	19,19,19,19	1
3	ZN	11-A	408	1/1	-	-	19,19,19,19	1
3	ZN	12-A	408	1/1	-	-	19,19,19,19	1
3	ZN	13-A	408	1/1	-	-	19,19,19,19	1
3	ZN	14-A	408	1/1	-	-	19,19,19,19	1
3	ZN	15-A	408	1/1	-	-	19,19,19,19	1
3	ZN	16-A	408	1/1	-	-	19,19,19,19	1
3	ZN	17-A	408	1/1	-	-	19,19,19,19	1
3	ZN	18-A	408	1/1	-	-	19,19,19,19	1
3	ZN	19-A	408	1/1	-	-	19,19,19,19	1
3	ZN	20-A	408	1/1	-	-	19,19,19,19	1
3	ZN	21-A	408	1/1	-	-	19,19,19,19	1
3	ZN	22-A	408	1/1	-	-	19,19,19,19	1
3	ZN	23-A	408	1/1	-	-	19,19,19,19	1
3	ZN	24-A	408	1/1	-	-	19,19,19,19	1
3	ZN	25-A	408	1/1	-	-	19,19,19,19	1
3	ZN	26-A	408	1/1	-	-	19,19,19,19	1
3	ZN	27-A	408	1/1	-	-	19,19,19,19	1
3	ZN	28-A	408	1/1	-	-	19,19,19,19	1
3	ZN	29-A	408	1/1	-	-	19,19,19,19	1
3	ZN	30-A	408	1/1	-	-	19,19,19,19	1
3	ZN	31-A	408	1/1	-	-	19,19,19,19	1
3	ZN	32-A	408	1/1	-	-	19,19,19,19	1
3	ZN	33-A	408	1/1	-	-	19,19,19,19	1
3	ZN	34-A	408	1/1	-	-	19,19,19,19	1
3	ZN	35-A	408	1/1	-	-	19,19,19,19	1
3	ZN	36-A	408	1/1	-	-	19,19,19,19	1
3	ZN	37-A	408	1/1	-	-	19,19,19,19	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	38-A	408	1/1	-	-	19,19,19,19	1
3	ZN	39-A	408	1/1	-	-	19,19,19,19	1
3	ZN	40-A	408	1/1	-	-	19,19,19,19	1
3	ZN	41-A	408	1/1	-	-	19,19,19,19	1
3	ZN	42-A	408	1/1	-	-	19,19,19,19	1
3	ZN	43-A	408	1/1	-	-	19,19,19,19	1

6.5 Other polymers [i](#)

There are no such residues in this entry.