



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:57 PM UTC

PDB ID : 7MHP / pdb_00007mhp
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 298 K at high humidity
Authors : Ebrahim, A.; Riley, B.T.; Kumaran, D.; Andi, B.; Fuchs, M.R.; McSweeney, S.; Keedy, D.A.
Deposited on : 2021-04-15
Resolution : 2.00 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
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

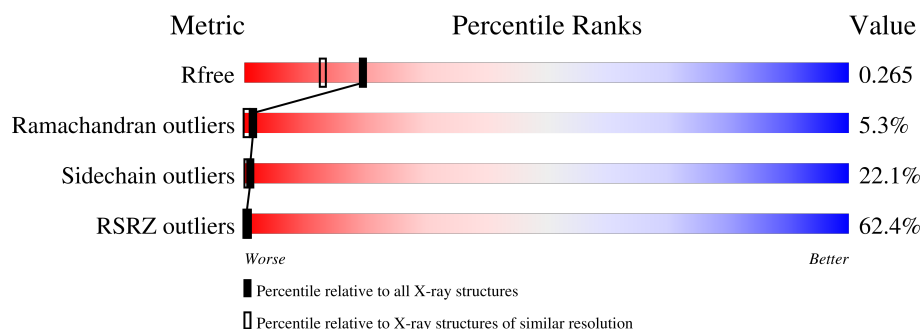
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	62% 76% 21% ..
1	10-A	306	76% 21% ..
1	11-A	306	75% 21% .
1	12-A	306	74% 24% .
1	13-A	306	76% 21% ..
1	14-A	306	75% 23% ..
1	15-A	306	75% 22% .

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Mol	Chain	Length	Quality of chain
1	16-A	306	 77% 21% .
1	17-A	306	 78% 20% .
1	18-A	306	 77% 20% .
1	19-A	306	 79% 20% .
1	2-A	306	 76% 20% . .
1	20-A	306	 77% 21% .
1	21-A	306	 77% 20% .
1	22-A	306	 77% 21% .
1	23-A	306	 76% 21% .
1	24-A	306	 77% 20% .
1	25-A	306	 76% 21% .
1	26-A	306	 77% 22% .
1	27-A	306	 77% 20% .
1	28-A	306	 76% 21% .
1	3-A	306	 77% 20% .
1	4-A	306	 77% 19% .
1	5-A	306	 77% 19% .
1	6-A	306	 78% 19% . .
1	7-A	306	 75% 22% .
1	8-A	306	 76% 21% .
1	9-A	306	 76% 21% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 132023 atoms, of which 64764 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	2-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	3-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	4-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	5-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	6-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	7-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	8-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	9-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	10-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	11-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	12-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	13-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	14-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	15-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	16-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	18-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	19-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	20-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	21-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	22-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	23-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	24-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	25-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	26-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	27-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			
1	28-A	306	Total	C	H	N	O	S	0	0	0
			4680	1499	2313	402	444	22			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	1	Total	Zn	0	0
			1	1		
2	2-A	1	Total	Zn	0	0
			1	1		
2	3-A	1	Total	Zn	0	0
			1	1		
2	4-A	1	Total	Zn	0	0
			1	1		
2	5-A	1	Total	Zn	0	0
			1	1		
2	6-A	1	Total	Zn	0	0
			1	1		
2	7-A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	8-A	1	Total 1	Zn 1	0	0
2	9-A	1	Total 1	Zn 1	0	0
2	10-A	1	Total 1	Zn 1	0	0
2	11-A	1	Total 1	Zn 1	0	0
2	12-A	1	Total 1	Zn 1	0	0
2	13-A	1	Total 1	Zn 1	0	0
2	14-A	1	Total 1	Zn 1	0	0
2	15-A	1	Total 1	Zn 1	0	0
2	16-A	1	Total 1	Zn 1	0	0
2	17-A	1	Total 1	Zn 1	0	0
2	18-A	1	Total 1	Zn 1	0	0
2	19-A	1	Total 1	Zn 1	0	0
2	20-A	1	Total 1	Zn 1	0	0
2	21-A	1	Total 1	Zn 1	0	0
2	22-A	1	Total 1	Zn 1	0	0
2	23-A	1	Total 1	Zn 1	0	0
2	24-A	1	Total 1	Zn 1	0	0
2	25-A	1	Total 1	Zn 1	0	0
2	26-A	1	Total 1	Zn 1	0	0
2	27-A	1	Total 1	Zn 1	0	0
2	28-A	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	34	Total O 34 34	0	0
3	2-A	29	Total O 29 29	0	0
3	3-A	24	Total O 24 24	0	0
3	4-A	37	Total O 37 37	0	0
3	5-A	46	Total O 46 46	0	0
3	6-A	30	Total O 30 30	0	0
3	7-A	45	Total O 45 45	0	0
3	8-A	30	Total O 30 30	0	0
3	9-A	35	Total O 35 35	0	0
3	10-A	38	Total O 38 38	0	0
3	11-A	41	Total O 41 41	0	0
3	12-A	34	Total O 34 34	0	0
3	13-A	36	Total O 36 36	0	0
3	14-A	29	Total O 29 29	0	0
3	15-A	29	Total O 29 29	0	0
3	16-A	36	Total O 36 36	0	0
3	17-A	33	Total O 33 33	0	0
3	18-A	29	Total O 29 29	0	0
3	19-A	31	Total O 31 31	0	0
3	20-A	29	Total O 29 29	0	0
3	21-A	34	Total O 34 34	0	0

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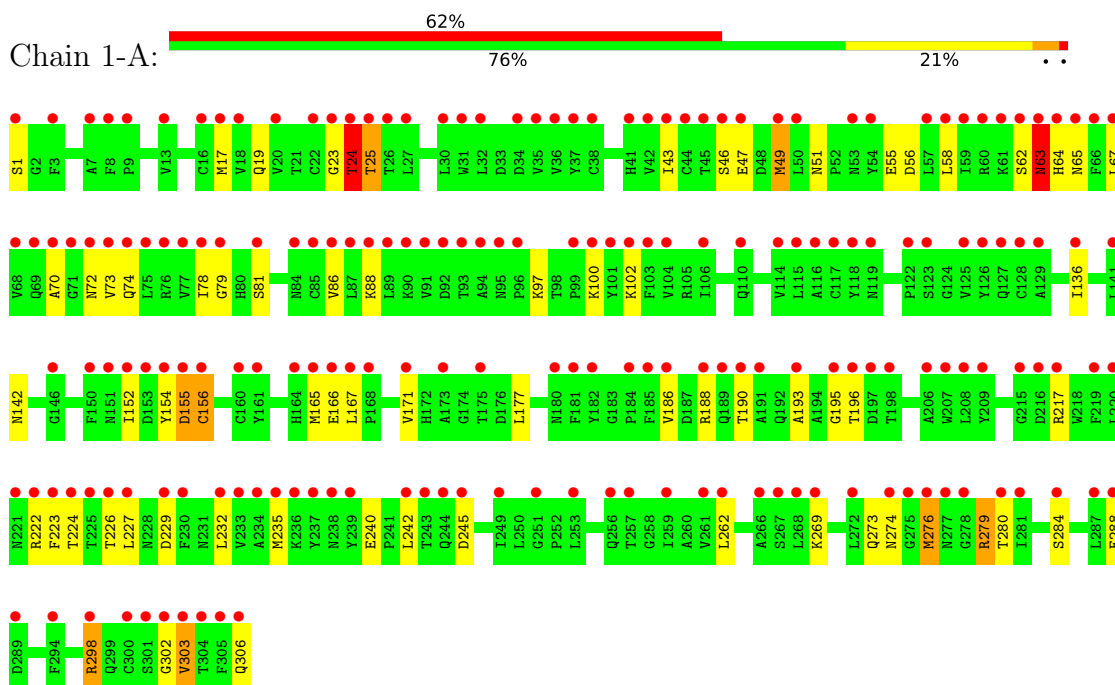
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	22-A	37	Total 37	O 37	0	0
3	23-A	37	Total 37	O 37	0	0
3	24-A	38	Total 38	O 38	0	0
3	25-A	40	Total 40	O 40	0	0
3	26-A	33	Total 33	O 33	0	0
3	27-A	30	Total 30	O 30	0	0
3	28-A	31	Total 31	O 31	0	0

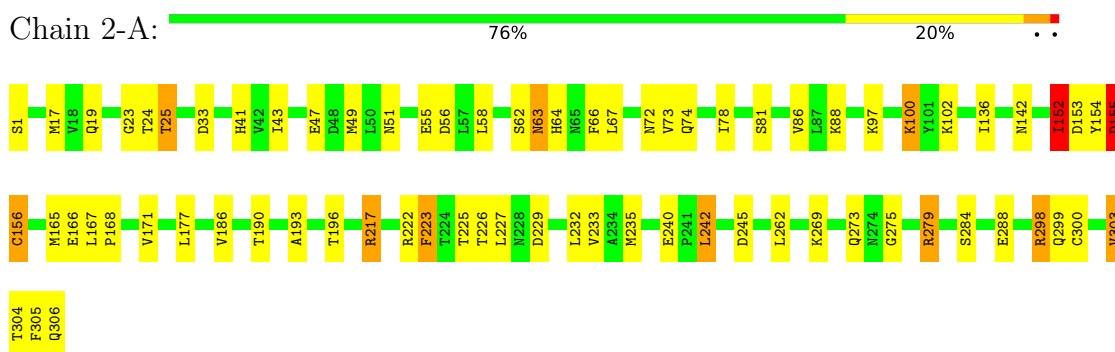
3 Residue-property plots [i](#)

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.

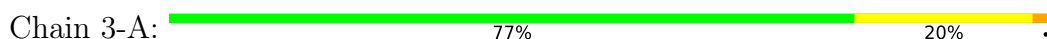
• Molecule 1: 3C-like proteinase

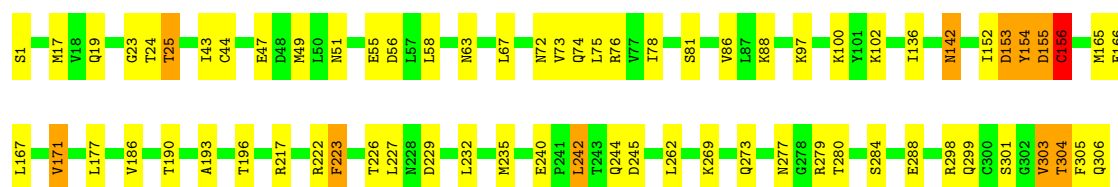


• Molecule 1: 3C-like proteinase

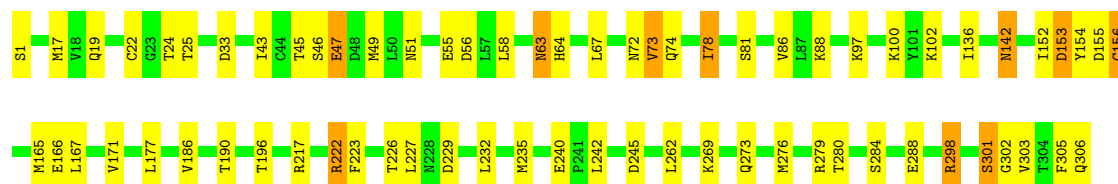
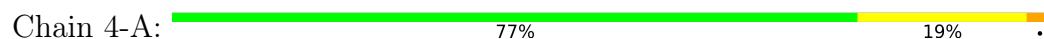


• Molecule 1: 3C-like proteinase

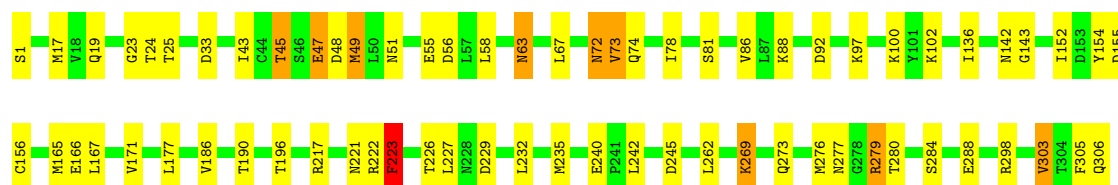
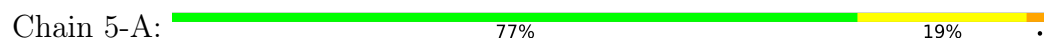




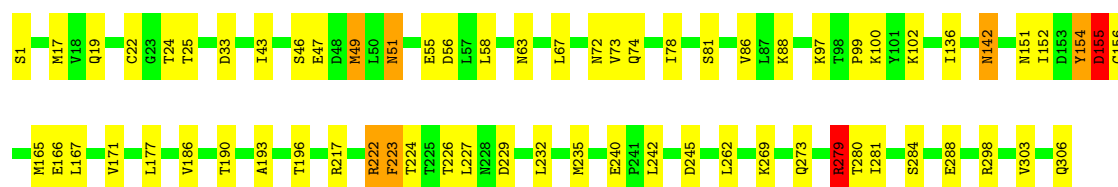
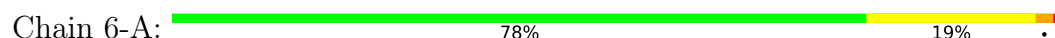
- Molecule 1: 3C-like proteinase



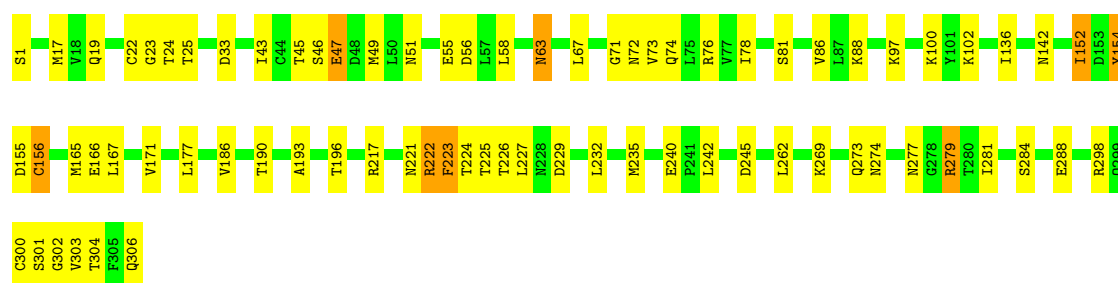
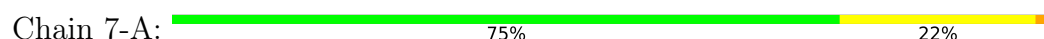
- Molecule 1: 3C-like proteinase



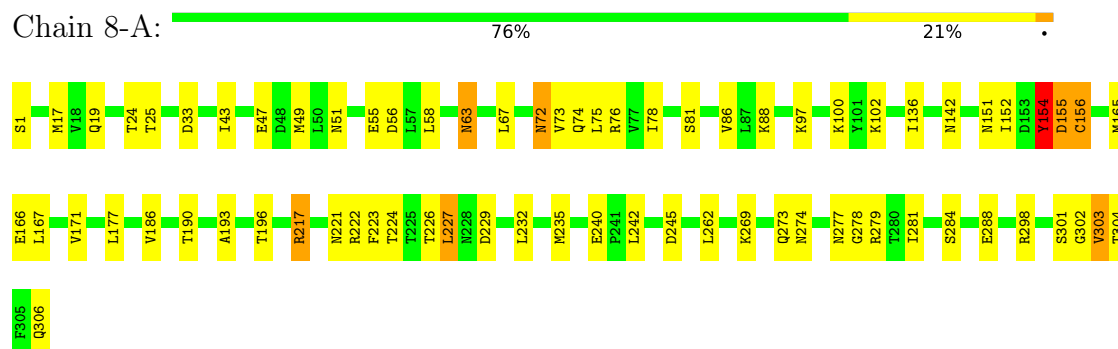
- Molecule 1: 3C-like proteinase



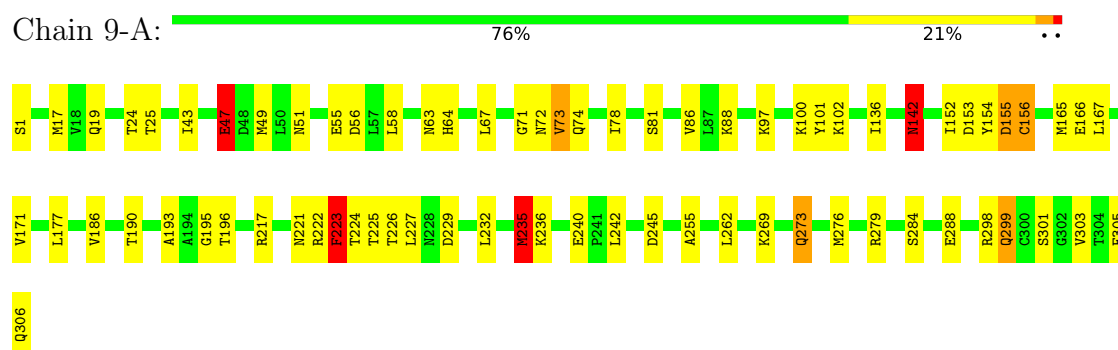
- Molecule 1: 3C-like proteinase



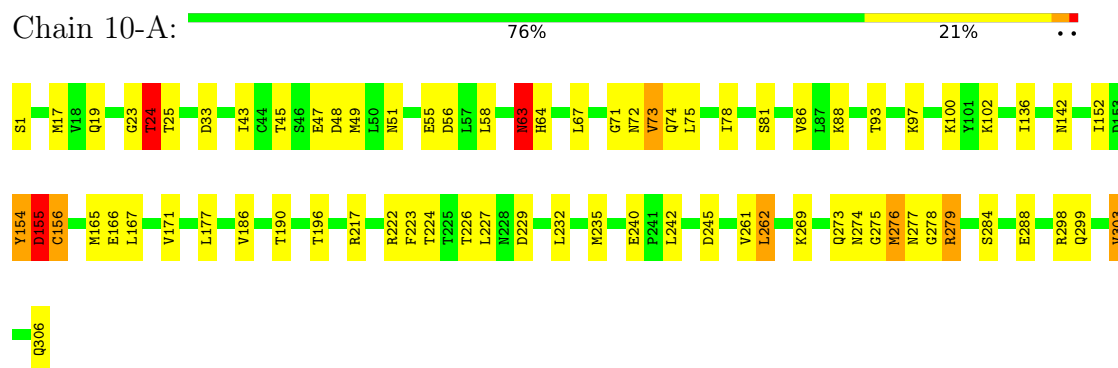
- Molecule 1: 3C-like proteinase



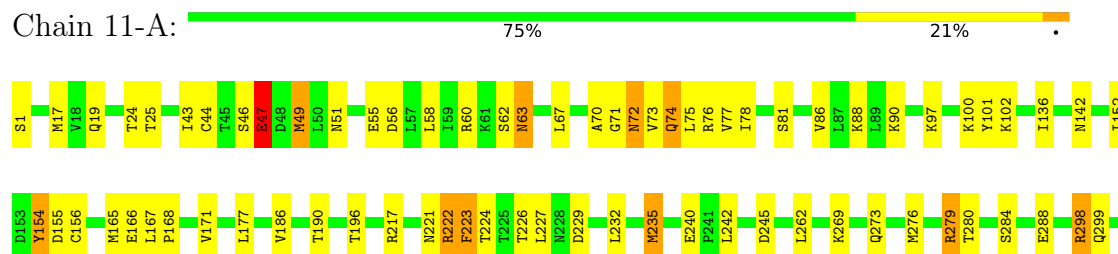
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



V303
T304
F305
Q306

- Molecule 1: 3C-like proteinase

Chain 12-A:  74% 24% .

S1 M17 V18 Q19 T24 T25 D33 D34 V35 I43 E47 D48 M49 M50 M51 E55 D56 D57 L57 L58 K61 S62 N63 L67 G71 M72 V73 Q74 L75 R76 V77 I78 S81 V86 L87 K88 L89 P96 K97 K100 Y101 K102 I136 L141 N142

I152 D153 Y154 D155 C156 M165 E166 L167 V171 L177 V186 T190 T196 R217 L220 N221 R222 F223 T224 T225 T226 L227 N228 D229 L232 M235 E240 F241 L242 D245 L262 K269 Q273 Q274 G275 N276 K279 T280 S284 E288 R298

Q299 C300 S301 G302 V303 T304 F305 Q306

- Molecule 1: 3C-like proteinase

Chain 13-A:  76% 21% ..

S1 M17 V18 Q19 T24 T25 V35 I43 E47 D48 M49 M50 M51 E55 D56 D57 L57 L58 N63 L67 N72 V73 Q74 I78 S81 V86 L87 K88 K97 T98 P99 K100 Y101 K102 R105 I136 N142 G143 I152 D153 Y154 C156

M165 E166 L167 V171 L177 P184 F185 V186 T190 T196 R217 R221 N222 F223 T224 T225 T226 L227 N228 D229 L232 M235 K236 Y237 E240 P241 L242 D245 L262 K269 Q273 N274 G275 M276 R279 S284 E288 R298 Q299 C300 V303

Q306

- Molecule 1: 3C-like proteinase

Chain 14-A:  75% 23% ..

S1 M17 V18 Q19 T24 T25 V35 I43 E47 D48 M49 M50 M51 E55 D56 D57 L57 L58 N63 L67 V68 Q69 A70 G71 N72 V73 Q74 I78 S81 V86 L87 K88 L89 K90 K97 T98 P99 K100 Y101 K102 I136 N142 I152 D153 Y154 D155

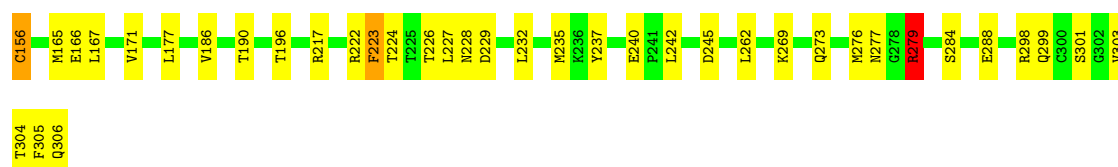
C156 M165 E166 L167 P168 V171 L177 V186 T190 T196 R217 N221 R222 F223 T224 T225 T226 L227 N228 D229 L232 M235 E240 P241 L242 D245 L262 K269 Q273 R274 G275 M276 N277 G278 R279 S284 E288 R298 Q299 C300 S301 G302

V303
T304
F305
Q306

- Molecule 1: 3C-like proteinase

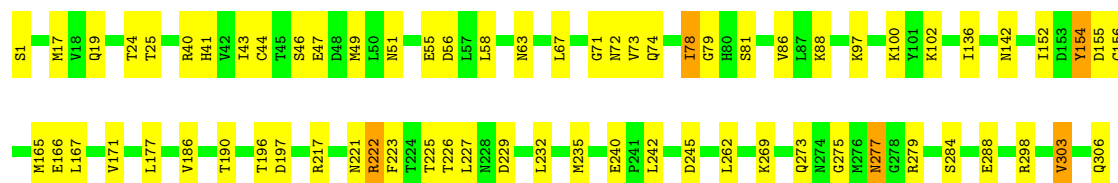
Chain 15-A:  75% 22% .

S1 M17 V18 Q19 Q23 T24 T25 R40 R41 V42 V43 S46 E47 D48 M49 M50 M51 E55 D56 D57 L57 L58 N63 H64 L67 N72 V73 Q74 I78 S81 V86 L87 K88 L89 K90 K97 K100 Y101 K102 I136 N142 I152 D153 Y154 D155



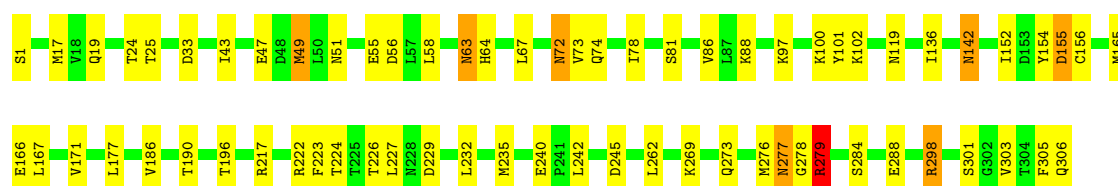
- Molecule 1: 3C-like proteinase

Chain 16-A: 77% 21% .



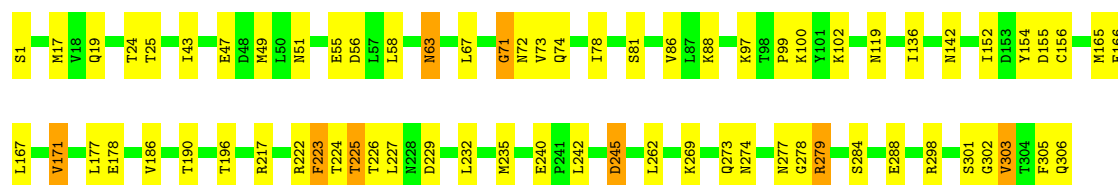
- Molecule 1: 3C-like proteinase

Chain 17-A: 78% 20% .



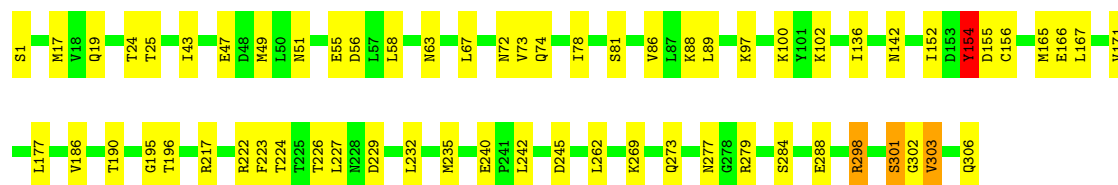
- Molecule 1: 3C-like proteinase

Chain 18-A: 77% 20% .



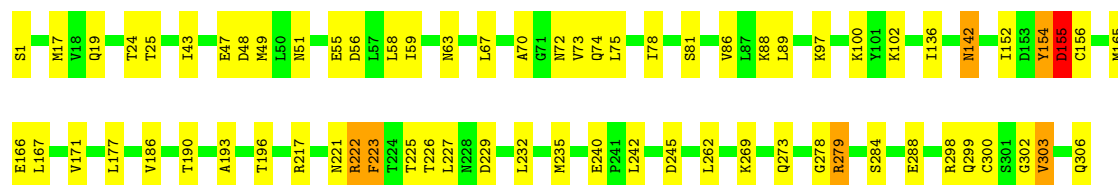
- Molecule 1: 3C-like proteinase

Chain 19-A: 79% 20% .



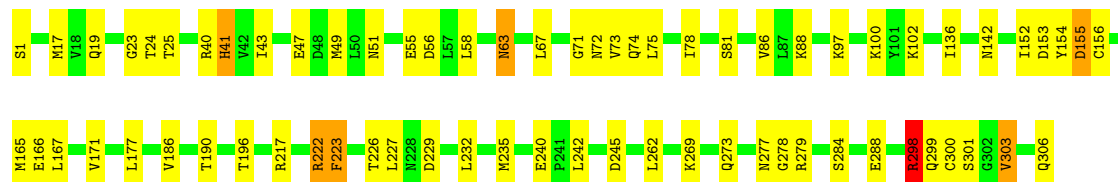
- Molecule 1: 3C-like proteinase

Chain 20-A: 77% 21% .



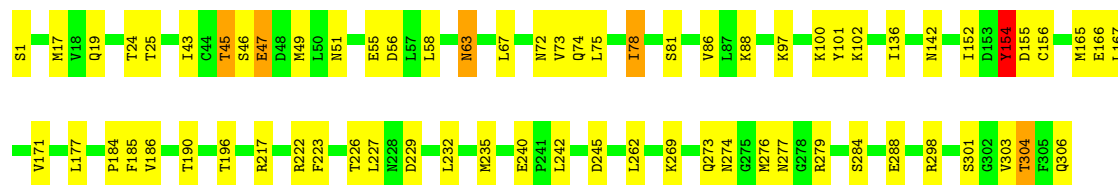
- Molecule 1: 3C-like proteinase

Chain 21-A: 77% 20% .



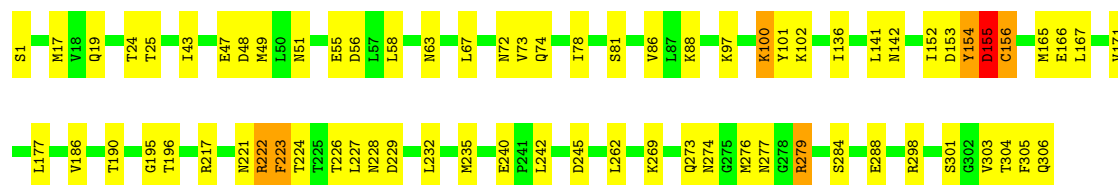
- Molecule 1: 3C-like proteinase

Chain 22-A: 77% 21% .



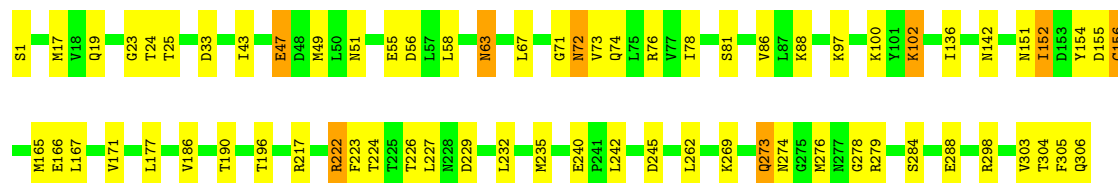
- Molecule 1: 3C-like proteinase

Chain 23-A: 76% 21% .



- Molecule 1: 3C-like proteinase

Chain 24-A: 77% 20% .



- Molecule 1: 3C-like proteinase

Chain 25-A: 76% 21% .

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.88Å 54.74Å 45.24Å 90.00° 101.42° 90.00°	Depositor
Resolution (Å)	56.30 – 2.00 56.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (56.30-2.00) 88.6 (56.30-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.19.2_4158)	Depositor
R, R_{free}	0.159 , 0.221 0.189 , 0.265	Depositor DCC
R_{free} test set	924 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	132023	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.00% 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

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	0.10	0/2420	0.14	0/3289
1	2-A	0.10	0/2420	0.14	0/3289
1	3-A	0.10	0/2420	0.14	0/3289
1	4-A	0.10	0/2420	0.14	0/3289
1	5-A	0.10	0/2420	0.14	0/3289
1	6-A	0.10	0/2420	0.14	0/3289
1	7-A	0.10	0/2420	0.14	0/3289
1	8-A	0.10	0/2420	0.14	0/3289
1	9-A	0.10	0/2420	0.14	0/3289
1	10-A	0.10	0/2420	0.14	0/3289
1	11-A	0.10	0/2420	0.14	0/3289
1	12-A	0.10	0/2420	0.14	0/3289
1	13-A	0.10	0/2420	0.14	0/3289
1	14-A	0.10	0/2420	0.14	0/3289
1	15-A	0.10	0/2420	0.14	0/3289
1	16-A	0.10	0/2420	0.14	0/3289
1	17-A	0.10	0/2420	0.14	0/3289
1	18-A	0.10	0/2420	0.14	0/3289
1	19-A	0.10	0/2420	0.14	0/3289
1	20-A	0.10	0/2420	0.14	0/3289
1	21-A	0.10	0/2420	0.14	0/3289
1	22-A	0.10	0/2420	0.14	0/3289
1	23-A	0.10	0/2420	0.14	0/3289
1	24-A	0.10	0/2420	0.14	0/3289
1	25-A	0.10	0/2420	0.14	0/3289
1	26-A	0.10	0/2420	0.14	0/3289
1	27-A	0.10	0/2420	0.14	0/3289
1	28-A	0.10	0/2420	0.14	0/3289
All	All	0.10	0/67760	0.14	0/92092

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	11
1	2-A	0	8
1	3-A	0	7
1	4-A	0	4
1	5-A	0	7
1	6-A	0	4
1	7-A	0	5
1	8-A	0	8
1	9-A	0	9
1	10-A	0	7
1	11-A	0	11
1	12-A	0	9
1	13-A	0	14
1	14-A	0	5
1	15-A	0	6
1	16-A	0	4
1	17-A	0	5
1	18-A	0	7
1	19-A	0	5
1	20-A	0	7
1	21-A	0	8
1	22-A	0	5
1	23-A	0	6
1	24-A	0	4
1	25-A	0	8
1	26-A	0	4
1	27-A	0	8
1	28-A	0	7
All	All	0	193

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 193 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	23	GLY	Peptide
1	1-A	24	THR	Peptide

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Mol	Chain	Res	Type	Group
1	1-A	62	SER	Peptide
1	1-A	63	ASN	Peptide
1	1-A	79	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2367	2313	2313	0	0
1	2-A	2367	2313	2313	0	0
1	3-A	2367	2313	2313	0	0
1	4-A	2367	2313	2313	0	0
1	5-A	2367	2313	2313	0	0
1	6-A	2367	2313	2313	0	0
1	7-A	2367	2313	2313	0	0
1	8-A	2367	2313	2313	0	0
1	9-A	2367	2313	2313	0	0
1	10-A	2367	2313	2313	0	0
1	11-A	2367	2313	2313	0	0
1	12-A	2367	2313	2313	0	0
1	13-A	2367	2313	2313	0	0
1	14-A	2367	2313	2313	0	0
1	15-A	2367	2313	2313	0	0
1	16-A	2367	2313	2313	0	0
1	17-A	2367	2313	2313	0	0
1	18-A	2367	2313	2313	0	0
1	19-A	2367	2313	2313	0	0
1	20-A	2367	2313	2313	0	0
1	21-A	2367	2313	2313	0	0
1	22-A	2367	2313	2313	0	0
1	23-A	2367	2313	2313	0	0
1	24-A	2367	2313	2313	0	0
1	25-A	2367	2313	2313	0	0
1	26-A	2367	2313	2313	0	0
1	27-A	2367	2313	2313	0	0
1	28-A	2367	2313	2313	0	0
2	1-A	1	0	0	0	0
2	2-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3-A	1	0	0	0	0
2	4-A	1	0	0	0	0
2	5-A	1	0	0	0	0
2	6-A	1	0	0	0	0
2	7-A	1	0	0	0	0
2	8-A	1	0	0	0	0
2	9-A	1	0	0	0	0
2	10-A	1	0	0	0	0
2	11-A	1	0	0	0	0
2	12-A	1	0	0	0	0
2	13-A	1	0	0	0	0
2	14-A	1	0	0	0	0
2	15-A	1	0	0	0	0
2	16-A	1	0	0	0	0
2	17-A	1	0	0	0	0
2	18-A	1	0	0	0	0
2	19-A	1	0	0	0	0
2	20-A	1	0	0	0	0
2	21-A	1	0	0	0	0
2	22-A	1	0	0	0	0
2	23-A	1	0	0	0	0
2	24-A	1	0	0	0	0
2	25-A	1	0	0	0	0
2	26-A	1	0	0	0	0
2	27-A	1	0	0	0	0
2	28-A	1	0	0	0	0
3	1-A	34	0	0	0	0
3	2-A	29	0	0	0	0
3	3-A	24	0	0	0	0
3	4-A	37	0	0	0	0
3	5-A	46	0	0	0	0
3	6-A	30	0	0	0	0
3	7-A	45	0	0	0	0
3	8-A	30	0	0	0	0
3	9-A	35	0	0	0	0
3	10-A	38	0	0	0	0
3	11-A	41	0	0	0	0
3	12-A	34	0	0	0	0
3	13-A	36	0	0	0	0
3	14-A	29	0	0	0	0
3	15-A	29	0	0	0	0
3	16-A	36	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	17-A	33	0	0	0	0
3	18-A	29	0	0	0	0
3	19-A	31	0	0	0	0
3	20-A	29	0	0	0	0
3	21-A	34	0	0	0	0
3	22-A	37	0	0	0	0
3	23-A	37	0	0	0	0
3	24-A	38	0	0	0	0
3	25-A	40	0	0	0	0
3	26-A	33	0	0	0	0
3	27-A	30	0	0	0	0
3	28-A	31	0	0	0	0
All	All	67259	64764	64764	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%)	253 (83%)	35 (12%)	16 (5%)	1	0
1	2-A	304/306 (99%)	246 (81%)	36 (12%)	22 (7%)	1	0
1	3-A	304/306 (99%)	257 (84%)	29 (10%)	18 (6%)	1	0
1	4-A	304/306 (99%)	262 (86%)	25 (8%)	17 (6%)	1	0
1	5-A	304/306 (99%)	256 (84%)	33 (11%)	15 (5%)	1	0
1	6-A	304/306 (99%)	261 (86%)	28 (9%)	15 (5%)	1	0
1	7-A	304/306 (99%)	255 (84%)	28 (9%)	21 (7%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-A	304/306 (99%)	253 (83%)	36 (12%)	15 (5%)	1	0
1	9-A	304/306 (99%)	243 (80%)	42 (14%)	19 (6%)	1	0
1	10-A	304/306 (99%)	256 (84%)	26 (9%)	22 (7%)	1	0
1	11-A	304/306 (99%)	251 (83%)	34 (11%)	19 (6%)	1	0
1	12-A	304/306 (99%)	258 (85%)	26 (9%)	20 (7%)	1	0
1	13-A	304/306 (99%)	259 (85%)	32 (10%)	13 (4%)	2	0
1	14-A	304/306 (99%)	260 (86%)	23 (8%)	21 (7%)	1	0
1	15-A	304/306 (99%)	258 (85%)	26 (9%)	20 (7%)	1	0
1	16-A	304/306 (99%)	262 (86%)	30 (10%)	12 (4%)	2	1
1	17-A	304/306 (99%)	253 (83%)	37 (12%)	14 (5%)	2	0
1	18-A	304/306 (99%)	266 (88%)	25 (8%)	13 (4%)	2	0
1	19-A	304/306 (99%)	268 (88%)	30 (10%)	6 (2%)	6	2
1	20-A	304/306 (99%)	267 (88%)	24 (8%)	13 (4%)	2	0
1	21-A	304/306 (99%)	265 (87%)	28 (9%)	11 (4%)	2	1
1	22-A	304/306 (99%)	258 (85%)	33 (11%)	13 (4%)	2	0
1	23-A	304/306 (99%)	263 (86%)	25 (8%)	16 (5%)	1	0
1	24-A	304/306 (99%)	250 (82%)	39 (13%)	15 (5%)	1	0
1	25-A	304/306 (99%)	261 (86%)	29 (10%)	14 (5%)	2	0
1	26-A	304/306 (99%)	263 (86%)	27 (9%)	14 (5%)	2	0
1	27-A	304/306 (99%)	262 (86%)	26 (9%)	16 (5%)	1	0
1	28-A	304/306 (99%)	248 (82%)	39 (13%)	17 (6%)	1	0
All	All	8512/8568 (99%)	7214 (85%)	851 (10%)	447 (5%)	1	0

5 of 447 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	25	THR
1	1-A	63	ASN
1	1-A	193	ALA
1	1-A	274	ASN
1	1-A	276	MET

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%)	205 (78%)	58 (22%)	1	0
1	2-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	3-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	4-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	5-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	6-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	7-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	8-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	9-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	10-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	11-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	12-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	13-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	14-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	15-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	16-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	17-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	18-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	19-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	20-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	21-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	22-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	23-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	24-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	25-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	26-A	263/263 (100%)	205 (78%)	58 (22%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	27-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
1	28-A	263/263 (100%)	205 (78%)	58 (22%)	1	0
All	All	7364/7364 (100%)	5740 (78%)	1624 (22%)	1	0

5 of 1624 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	16-A	303	VAL
1	20-A	232	LEU
1	28-A	171	VAL
1	17-A	142	ASN
1	16-A	298	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 260 such sidechains are listed below:

Mol	Chain	Res	Type
1	26-A	180	ASN
1	27-A	63	ASN
1	11-A	64	HIS
1	10-A	274	ASN
1	28-A	51	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 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	2.64	191 (62%) 0 0	2, 2, 2, 2	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	-	-	-	-
All	All	306/8568 (3%)	2.64	191 (62%) 0 0	2, 2, 2, 2	306 (100%)

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	275	GLY	9.6
1	1-A	302	GLY	9.3
1	1-A	305	PHE	8.3
1	1-A	62	SER	7.0
1	1-A	304	THR	7.0

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($\text{\AA}^2$)	Q<0.9
2	ZN	1-A	401	1/1	0.89	0.46	42,42,42,42	1
2	ZN	2-A	401	1/1	-	-	42,42,42,42	1
2	ZN	3-A	401	1/1	-	-	42,42,42,42	1
2	ZN	4-A	401	1/1	-	-	42,42,42,42	1
2	ZN	5-A	401	1/1	-	-	42,42,42,42	1
2	ZN	6-A	401	1/1	-	-	42,42,42,42	1
2	ZN	7-A	401	1/1	-	-	42,42,42,42	1
2	ZN	8-A	401	1/1	-	-	42,42,42,42	1
2	ZN	9-A	401	1/1	-	-	42,42,42,42	1
2	ZN	10-A	401	1/1	-	-	42,42,42,42	1
2	ZN	11-A	401	1/1	-	-	42,42,42,42	1
2	ZN	12-A	401	1/1	-	-	42,42,42,42	1
2	ZN	13-A	401	1/1	-	-	42,42,42,42	1
2	ZN	14-A	401	1/1	-	-	42,42,42,42	1
2	ZN	15-A	401	1/1	-	-	42,42,42,42	1
2	ZN	16-A	401	1/1	-	-	42,42,42,42	1
2	ZN	17-A	401	1/1	-	-	42,42,42,42	1
2	ZN	18-A	401	1/1	-	-	42,42,42,42	1
2	ZN	19-A	401	1/1	-	-	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	20-A	401	1/1	-	-	42,42,42,42	1
2	ZN	21-A	401	1/1	-	-	42,42,42,42	1
2	ZN	22-A	401	1/1	-	-	42,42,42,42	1
2	ZN	23-A	401	1/1	-	-	42,42,42,42	1
2	ZN	24-A	401	1/1	-	-	42,42,42,42	1
2	ZN	25-A	401	1/1	-	-	42,42,42,42	1
2	ZN	26-A	401	1/1	-	-	42,42,42,42	1
2	ZN	27-A	401	1/1	-	-	42,42,42,42	1
2	ZN	28-A	401	1/1	-	-	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.