



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:18 am GMT

PDB ID : 2ZLE  
EMDB ID: : EMD-1505  
Title : Cryo-EM structure of DegP12/OMP  
Authors : Schaefer, E.; Saibil, H.R.  
Deposited on : 2008-04-09  
Resolution : 28.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

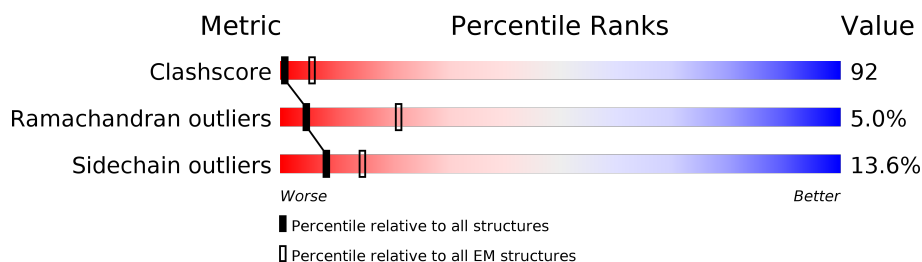
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


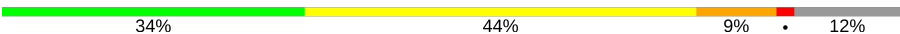



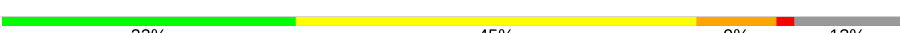
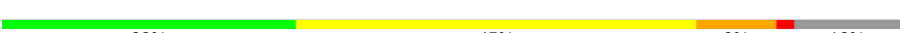


The reported resolution of this entry is 28.00 Å.

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.





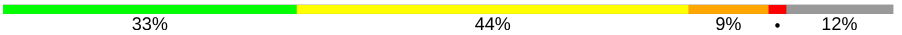
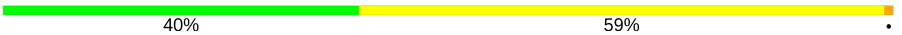
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	448	
1	B	448	
1	C	448	
1	E	448	
1	F	448	
1	G	448	
1	H	448	
1	I	448	
1	J	448	

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Mol	Chain	Length	Quality of chain
1	K	448	
1	L	448	
1	M	448	
2	D	346	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37730 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protease do.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	B	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	C	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	E	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	F	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	G	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	H	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	I	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	J	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	K	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	L	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		
1	M	396	Total	C	N	O	S	0	0
			2918	1818	519	568	13		

- Molecule 2 is a protein called Outer membrane protein C.

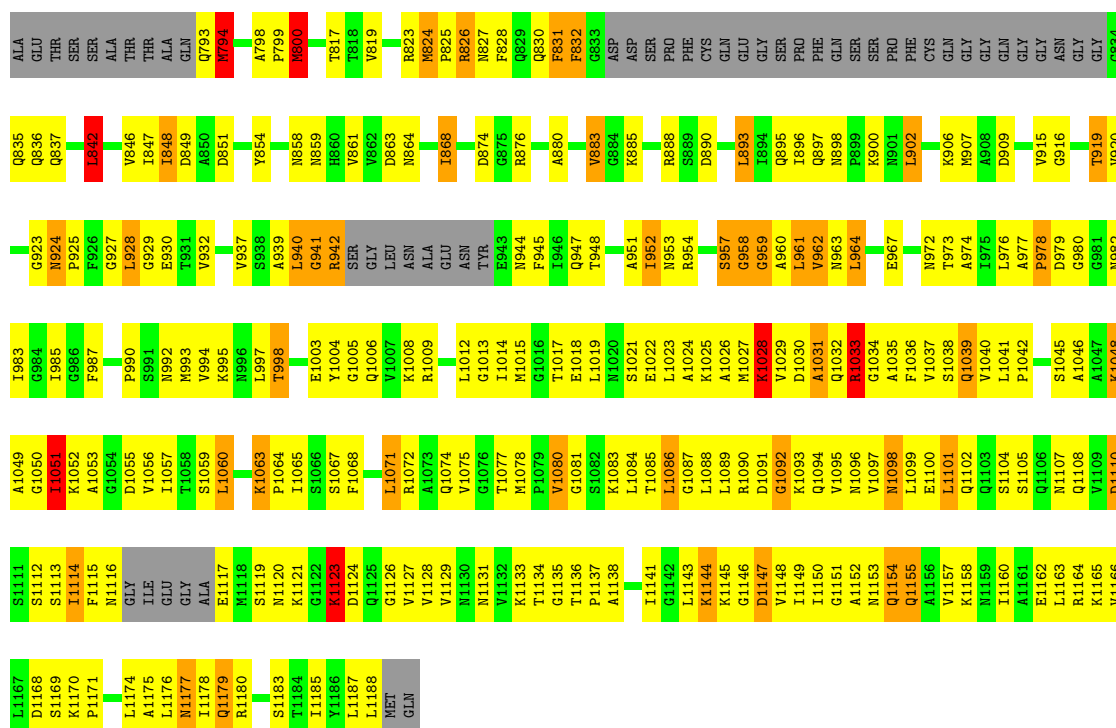
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	346	Total	C	N	O	S	0	0
			2714	1699	458	554	3		





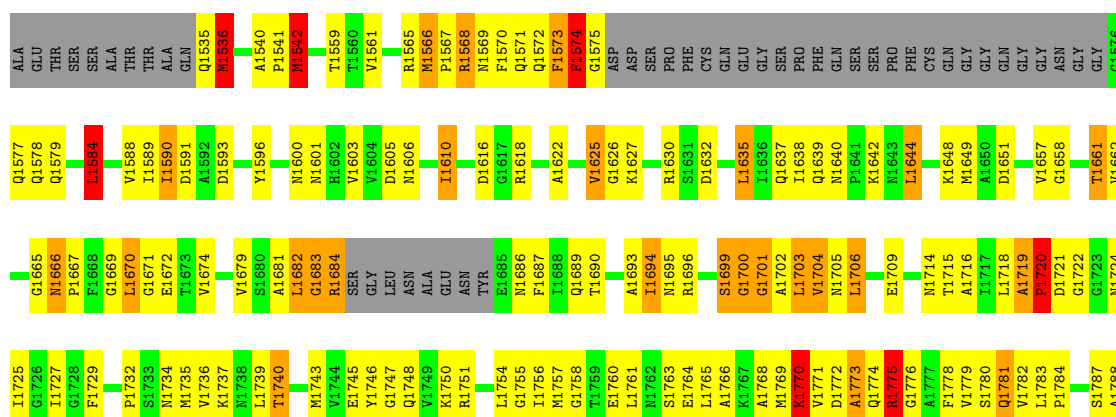
• Molecule 1: Protease do

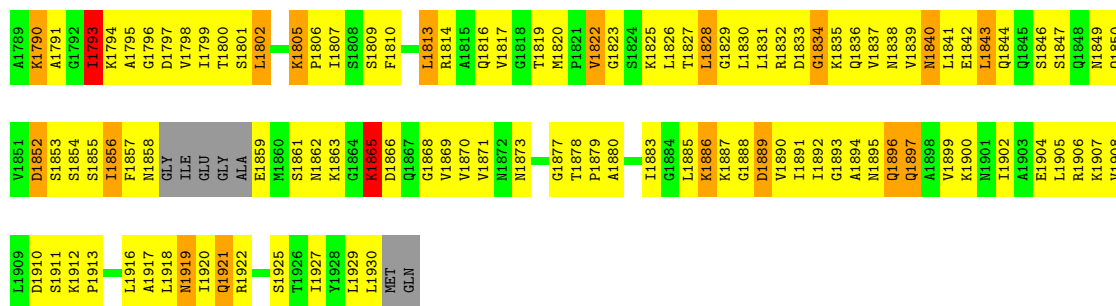
Chain C: 33% 44% 10% 12%



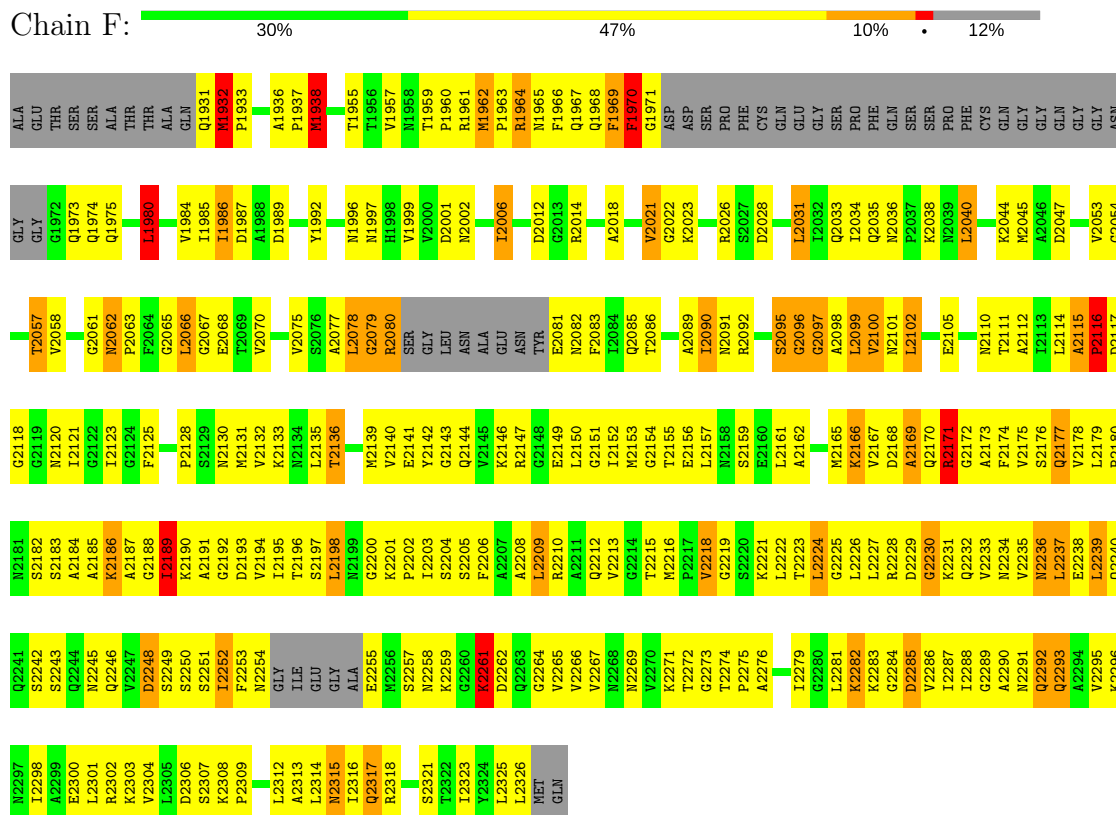
• Molecule 1: Protease do

Chain E: 33% 44% 9% 12%

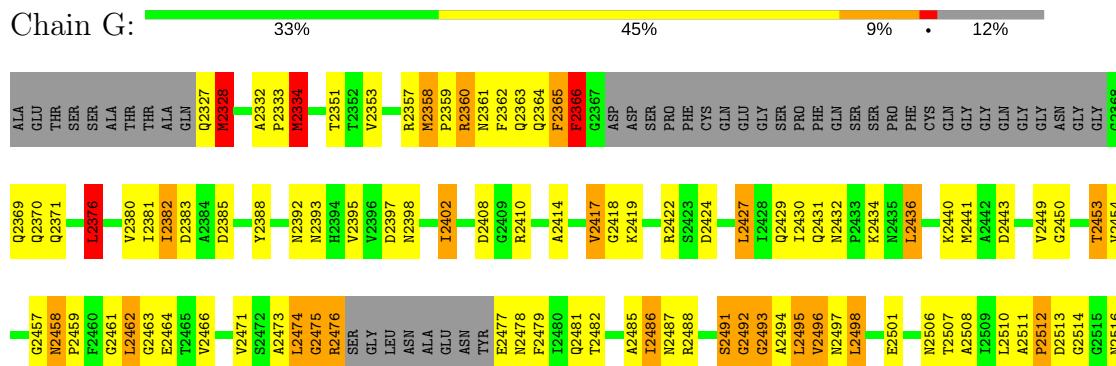


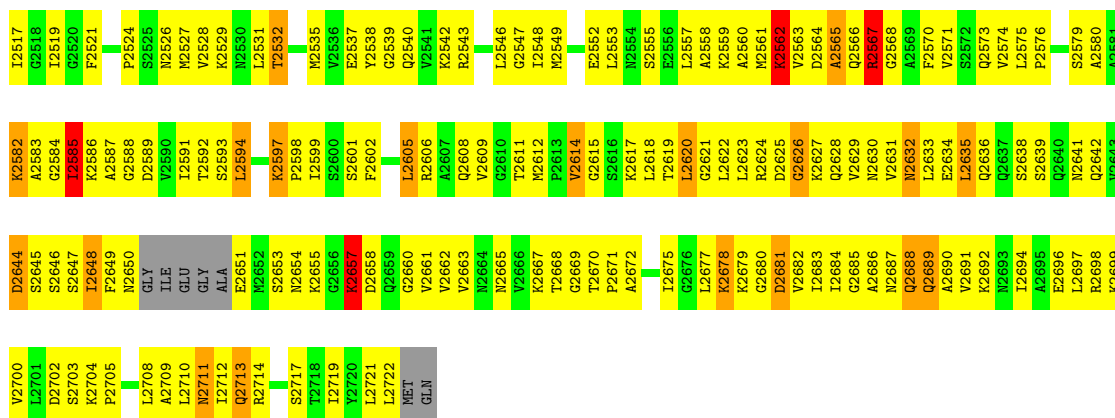


• Molecule 1: Protease do

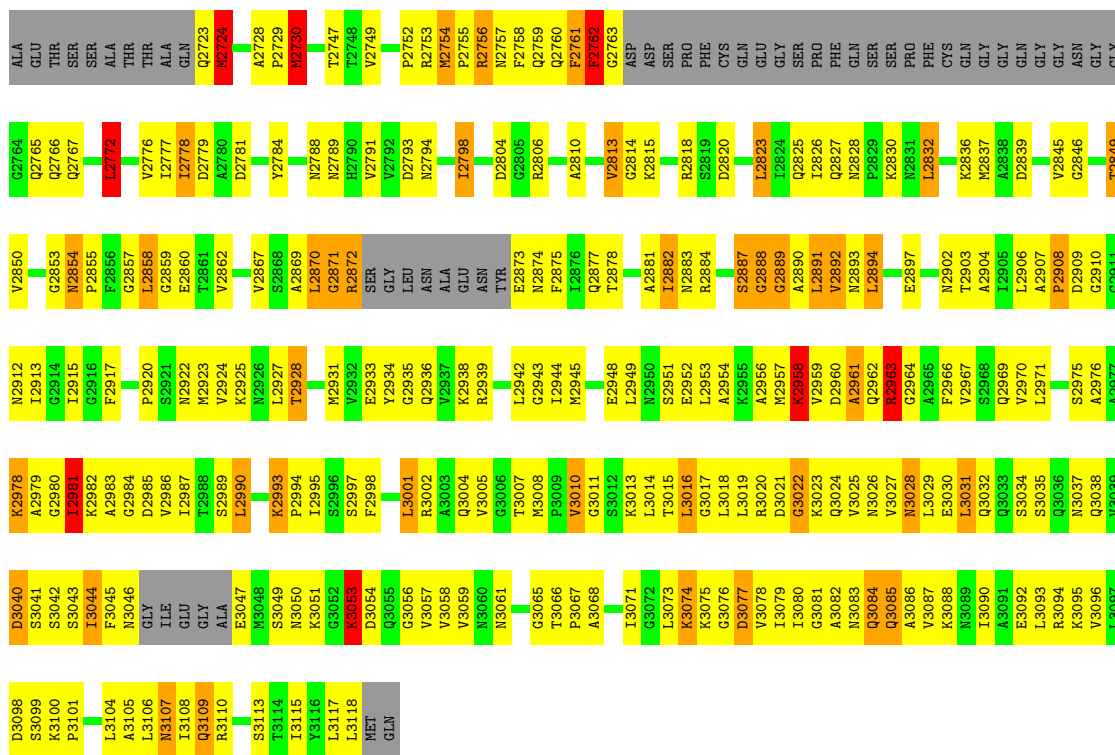


• Molecule 1: Protease do

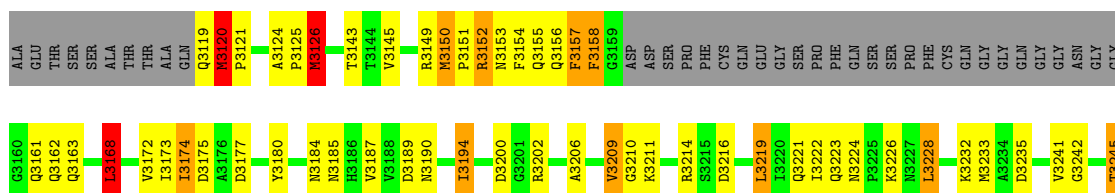




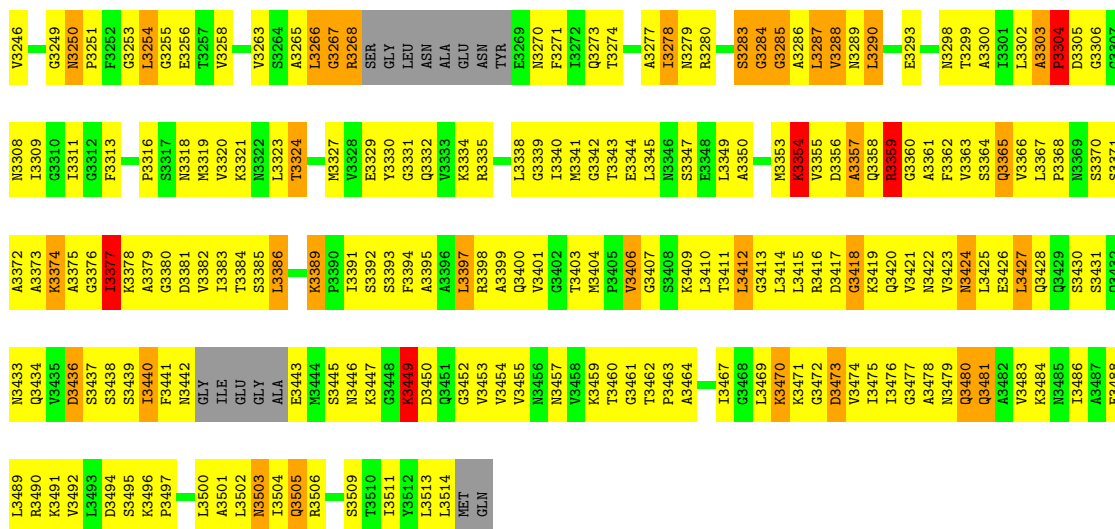
### • Molecule 1: Protease do



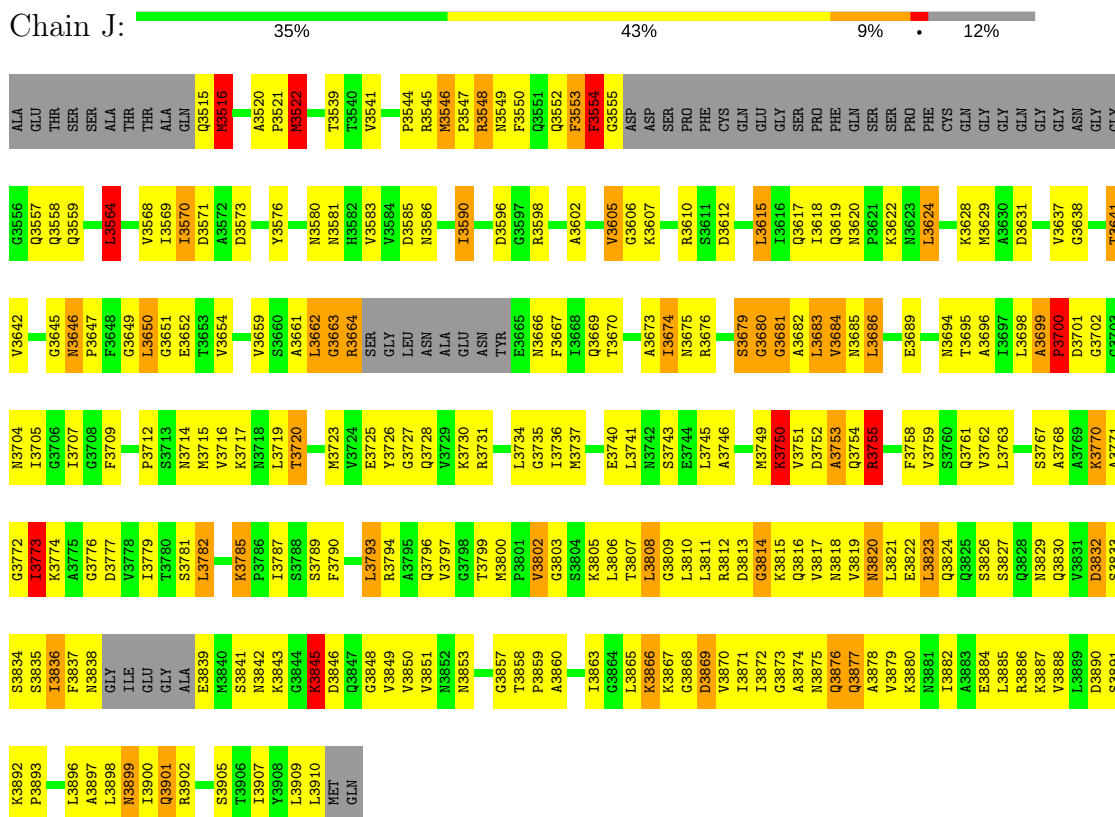
### • Molecule 1: Protease do



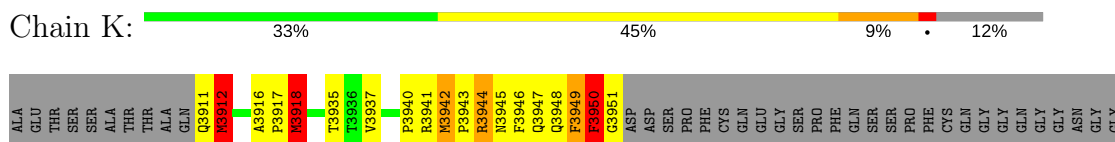


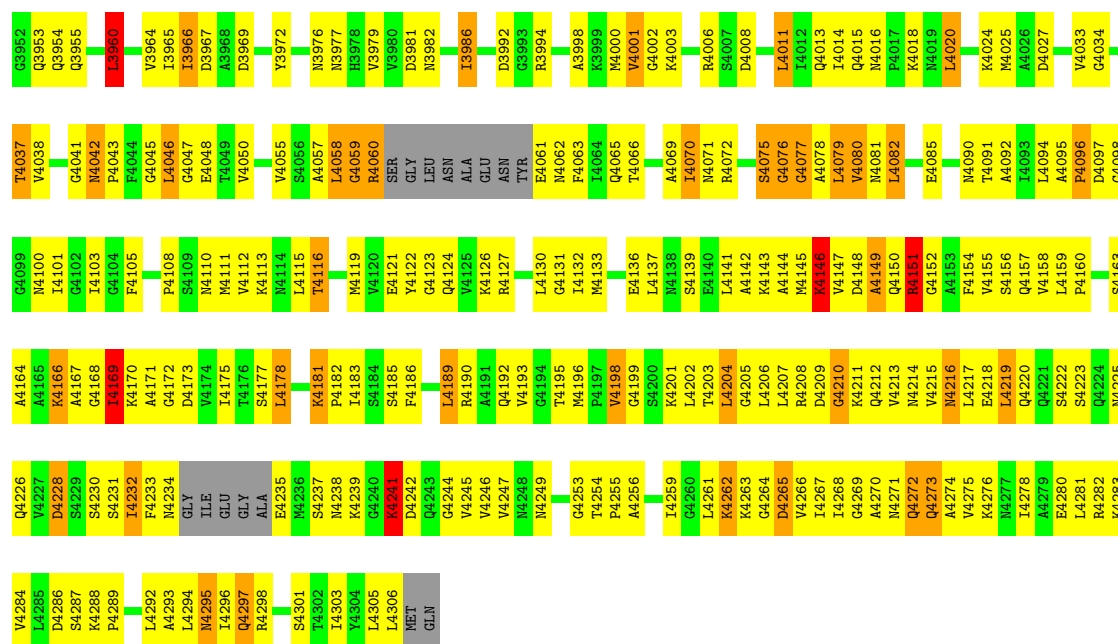


### • Molecule 1: Protease do



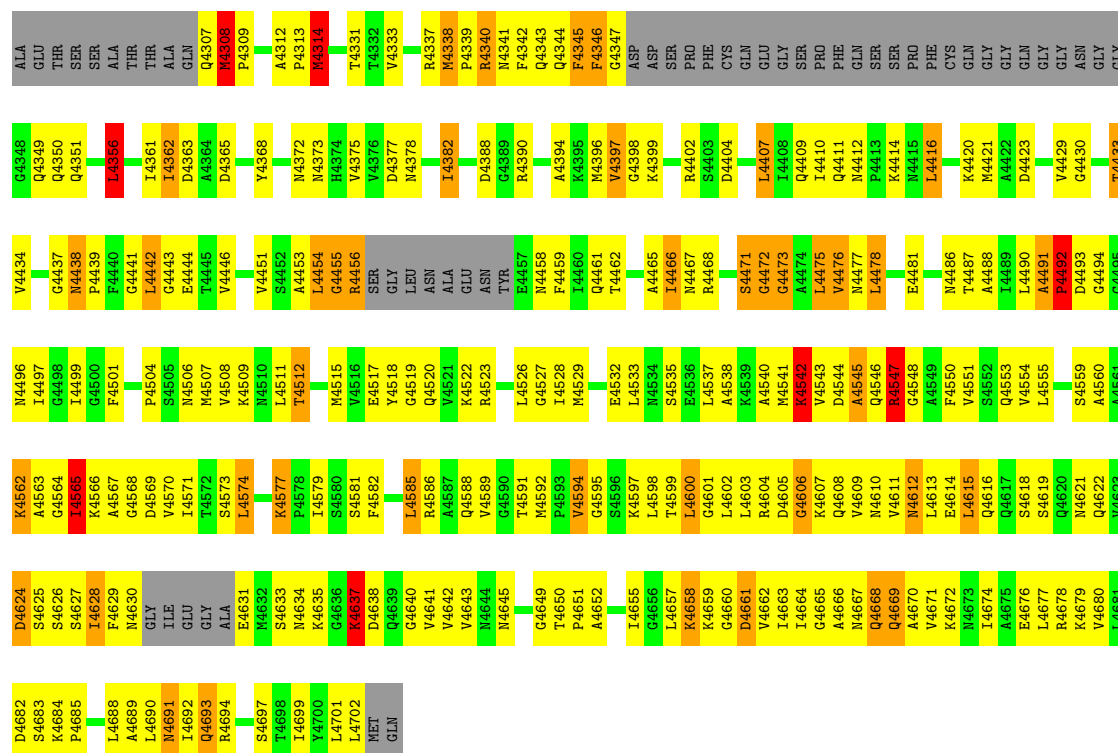
### • Molecule 1: Protease do





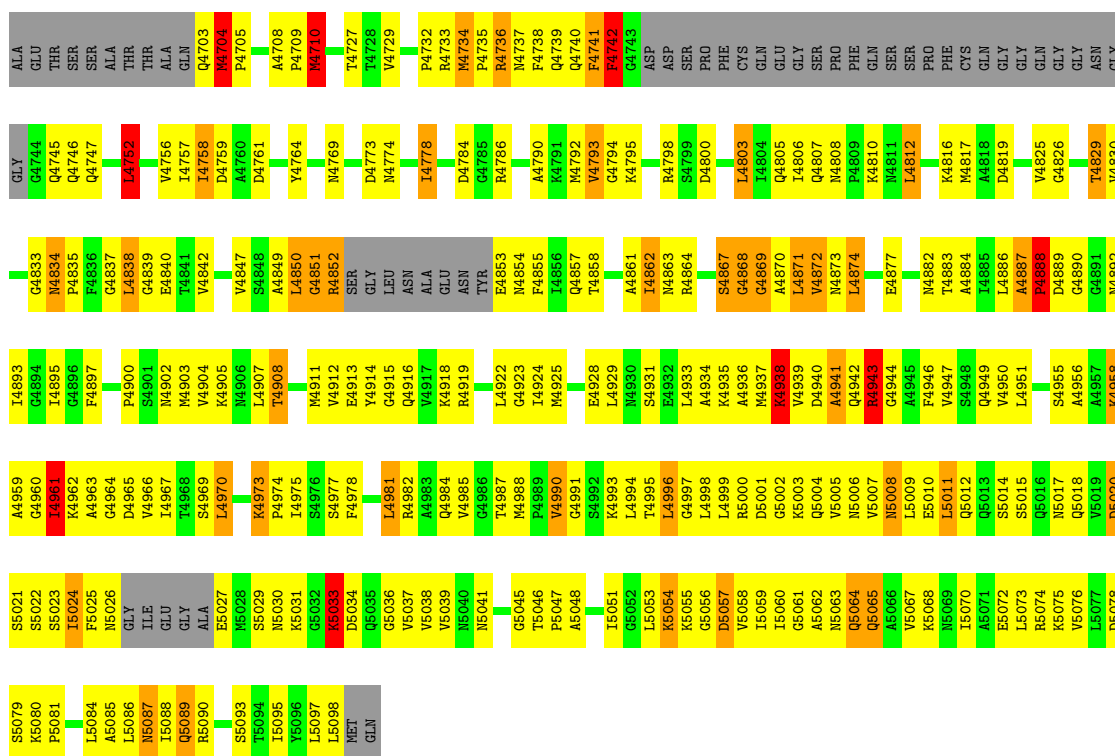
• Molecule 1: Protease do

Chain L: 34% 44% 9% 12%



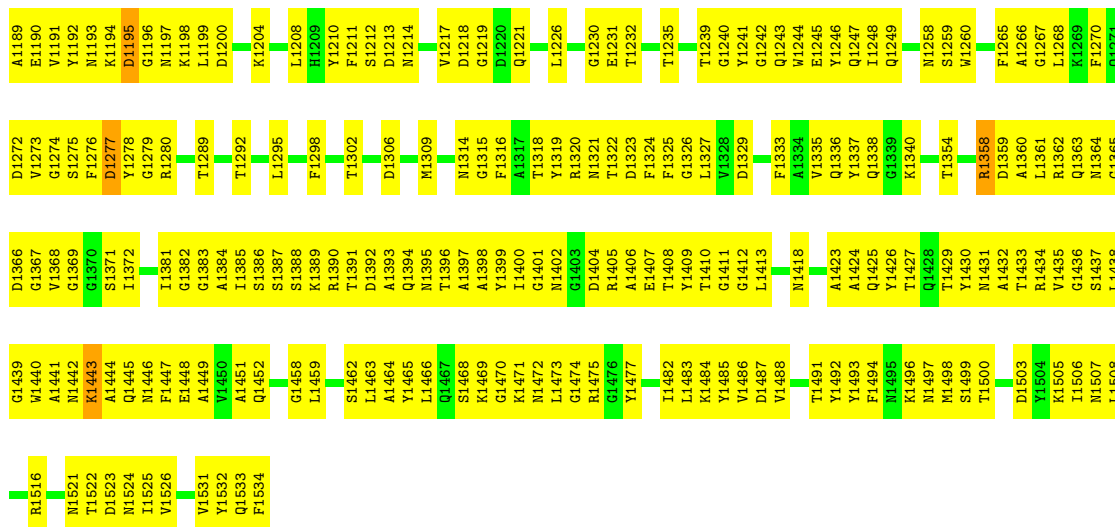
• Molecule 1: Protease do

Chain M: 33% 44% 9% 12%



- Molecule 2: Outer membrane protein C

Chain D:  40% 59%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	6285	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	68100	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	B	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	C	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	E	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	F	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	G	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	H	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	I	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	J	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	K	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	L	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
1	M	0.66	3/2945 (0.1%)	0.90	4/3973 (0.1%)
2	D	0.53	3/2773 (0.1%)	0.65	2/3753 (0.1%)
All	All	0.65	39/38113 (0.1%)	0.88	50/51429 (0.1%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1327	LEU	CB-CG	-13.69	1.12	1.52
2	D	1443	LYS	CB-CG	-6.20	1.35	1.52
1	F	1932	MET	CG-SD	5.89	1.96	1.81
1	A	2	MET	CG-SD	5.89	1.96	1.81
1	M	4704	MET	CG-SD	5.89	1.96	1.81

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	4887	ALA	C-N-CD	-20.89	74.64	120.60
1	I	3303	ALA	C-N-CD	-20.87	74.68	120.60
1	J	3699	ALA	C-N-CD	-20.87	74.69	120.60
1	C	977	ALA	C-N-CD	-20.87	74.69	120.60
1	G	2511	ALA	C-N-CD	-20.87	74.69	120.60

There are no chirality outliers.

There are no planarity outliers.

## 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	A	2918	0	2997	617	0
1	B	2918	0	2998	453	0
1	C	2918	0	2991	683	0
1	E	2918	0	2984	750	0
1	F	2918	0	2975	1462	0
1	G	2918	0	2987	694	0
1	H	2918	0	2990	619	0
1	I	2918	0	2974	1338	0
1	J	2918	0	2995	507	0
1	K	2918	0	2991	737	0
1	L	2918	0	2994	541	0
1	M	2918	0	2989	719	0
2	D	2714	0	2414	1585	0
All	All	37730	0	38279	7007	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 92.

The worst 5 of 7007 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1325:PHE:CD2	1:G:2357:ARG:HB2	1.18	1.68
2:D:1411:GLY:CA	1:L:4345:PHE:H	1.04	1.65
1:C:1036:PHE:CD2	1:E:1832:ARG:HA	1.25	1.64
2:D:1470:GLY:HA2	1:M:4738:PHE:CB	1.20	1.64
1:C:1088:LEU:HD22	1:E:1834:GLY:CA	1.17	1.64

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	B	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	C	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	E	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	F	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	G	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	H	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	I	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	J	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	K	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	L	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
1	M	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	25
2	D	344/346 (99%)	327 (95%)	17 (5%)	0	100	100
All	All	5000/5722 (87%)	4143 (83%)	605 (12%)	252 (5%)	5	27

5 of 252 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	PRO
1	A	236	LYS
1	A	259	ILE
1	A	288	VAL
1	A	322	ILE

### 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 PDB entries followed by that with respect to all EM

entries.

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	A	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	B	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	C	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	E	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	F	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	G	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	H	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	I	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	J	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	K	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	L	319/357 (89%)	273 (86%)	46 (14%)	4	22
1	M	319/357 (89%)	273 (86%)	46 (14%)	4	22
2	D	275/275 (100%)	271 (98%)	4 (2%)	70	85
All	All	4103/4559 (90%)	3547 (86%)	556 (14%)	8	23

5 of 556 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	2466	VAL
1	H	2978	LYS
1	M	4736	ARG
1	G	2512	PRO
1	H	2754	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 245 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	2429	GLN
1	H	3024	GLN
1	M	4745	GLN
1	G	2573	GLN
1	G	2687	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.