



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 31, 2017 – 10:46 AM EST

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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

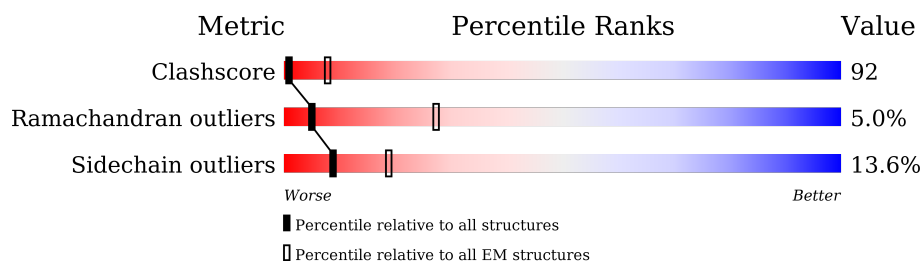
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	33% 44% 10% • 12%
1	B	448	34% 44% 9% • 12%
1	C	448	33% 44% 10% • 12%
1	E	448	33% 44% 9% • 12%
1	F	448	30% 47% 10% • 12%
1	G	448	33% 45% 9% • 12%
1	H	448	33% 45% 9% • 12%
1	I	448	31% 46% 10% • 12%
1	J	448	35% 43% 9% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	448	<div><div></div><div>33%45%9%•12%</div></div>
1	L	448	<div><div></div><div>34%44%9%•12%</div></div>
1	M	448	<div><div></div><div>33%44%9%•12%</div></div>
2	D	346	<div><div></div><div>40%59%•</div></div>

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		

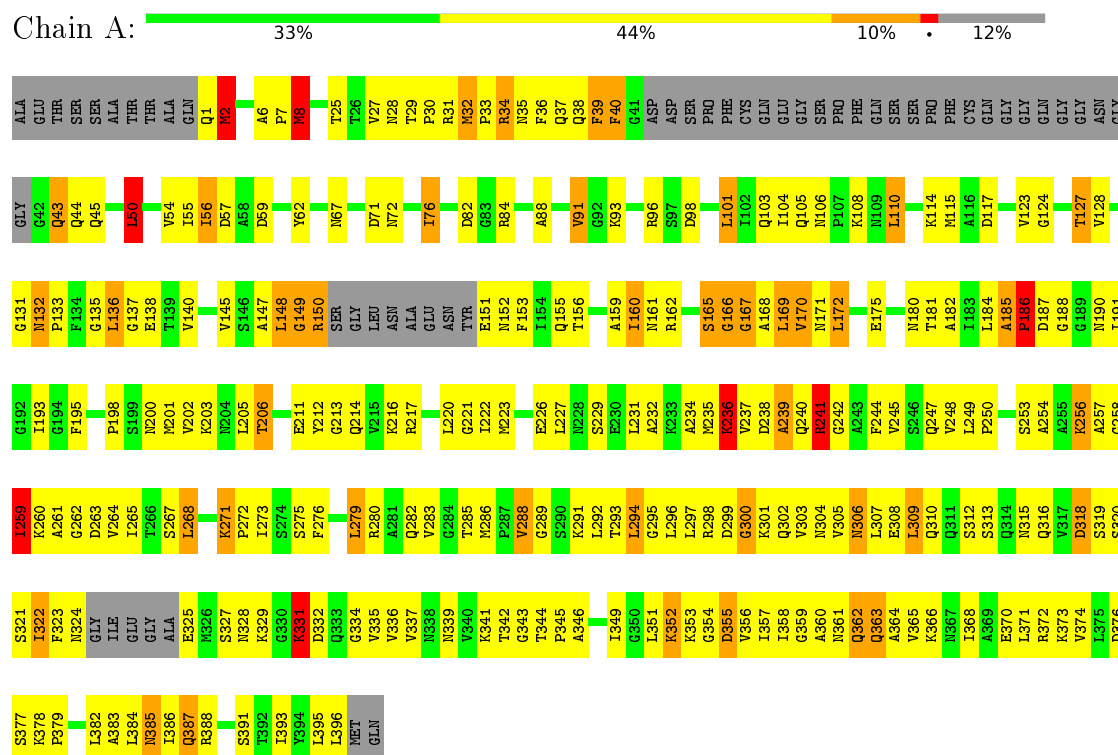
- Molecule 2 is a protein called Outer membrane protein C.

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

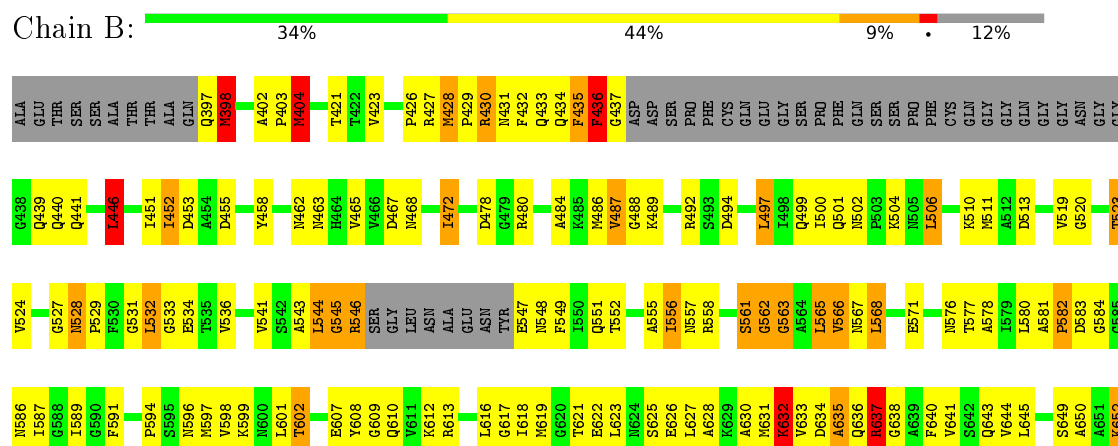
3 Residue-property plots

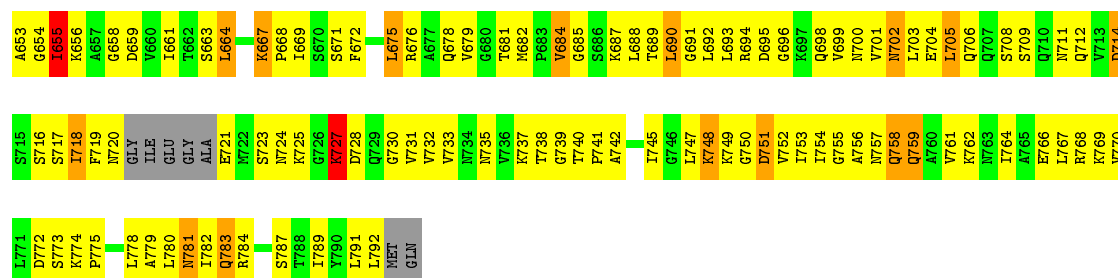
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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: Protease do



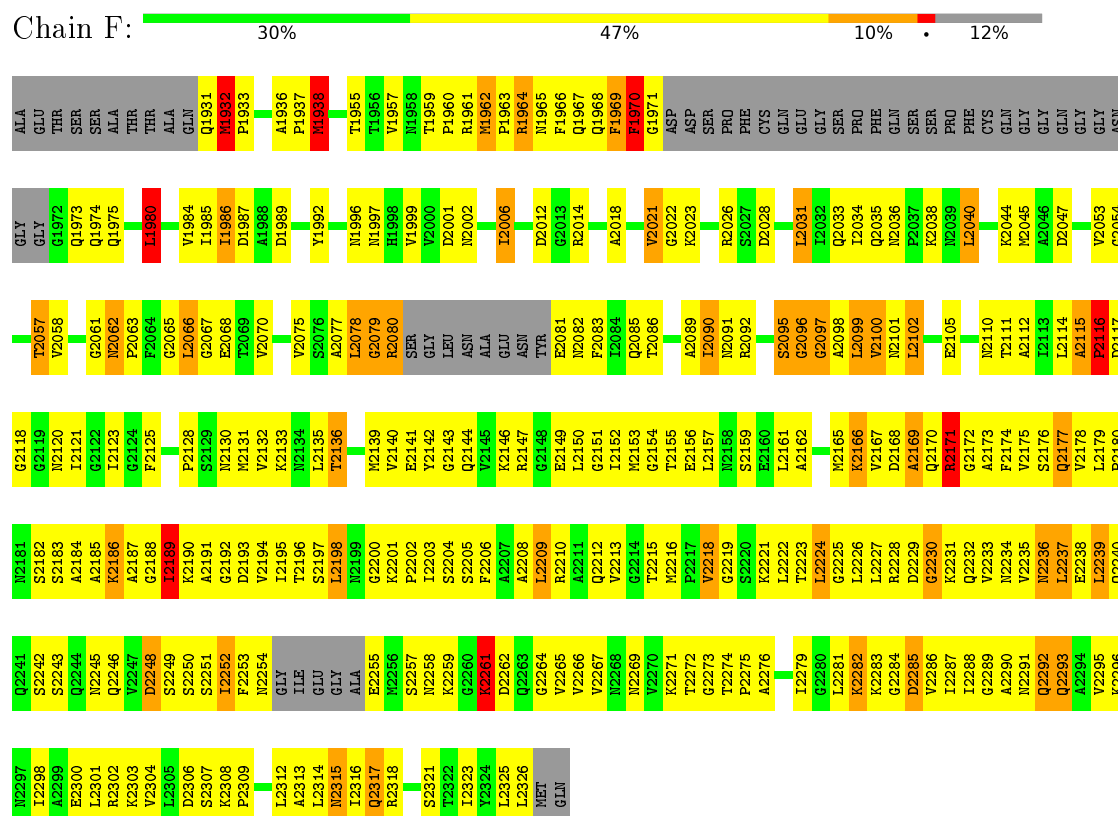
• Molecule 1: Protease do



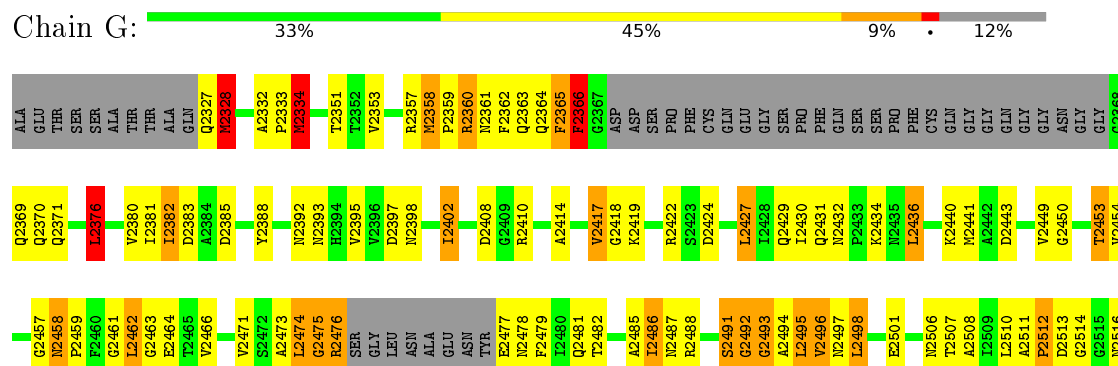


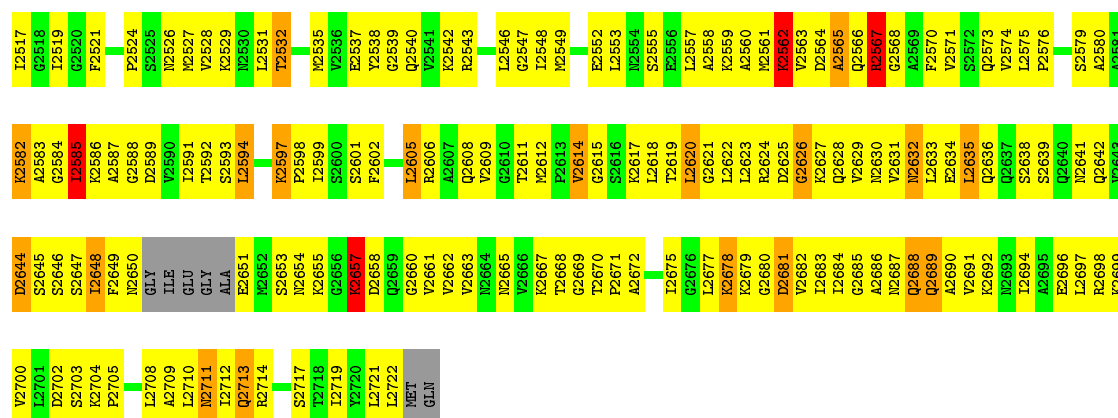


• Molecule 1: Protease do

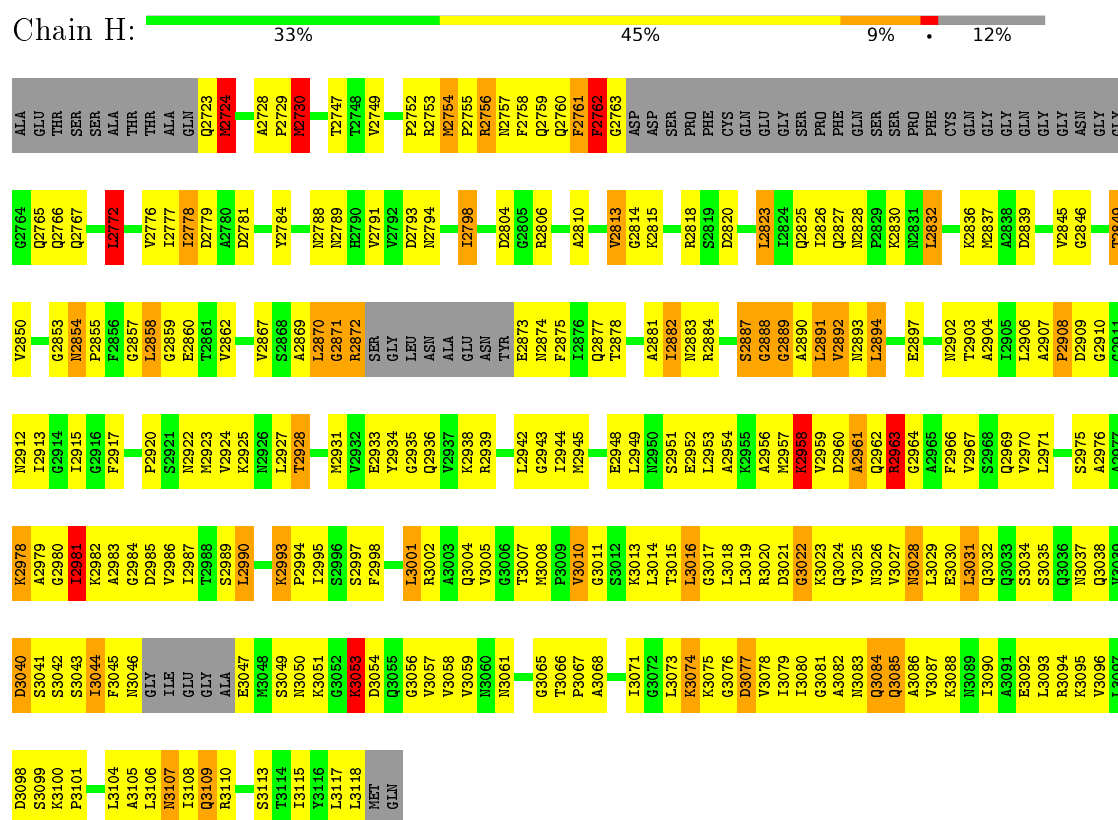


• Molecule 1: Protease do

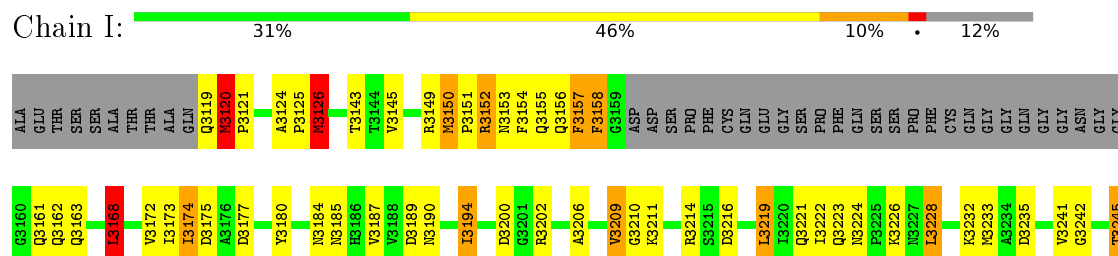


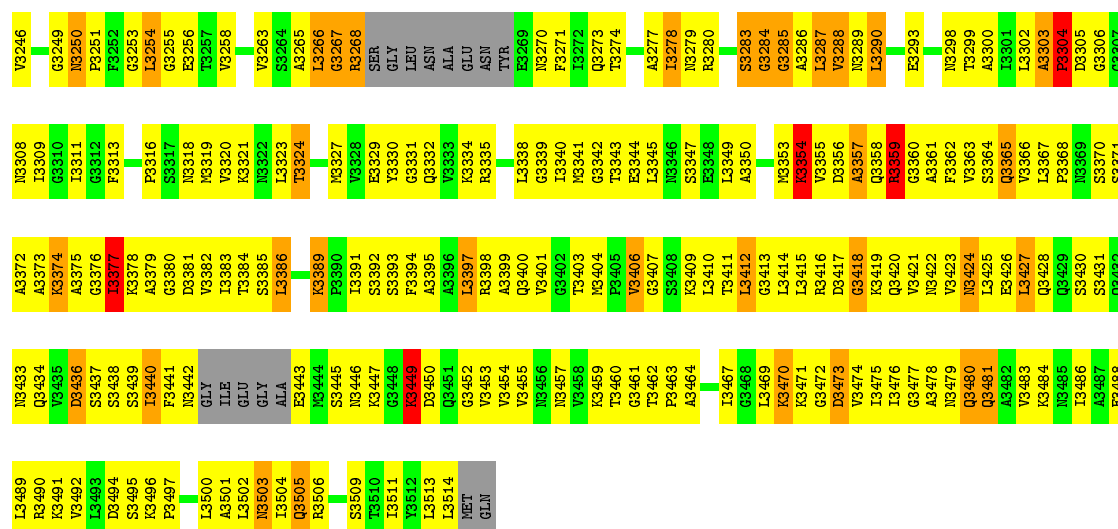


• Molecule 1: Protease do

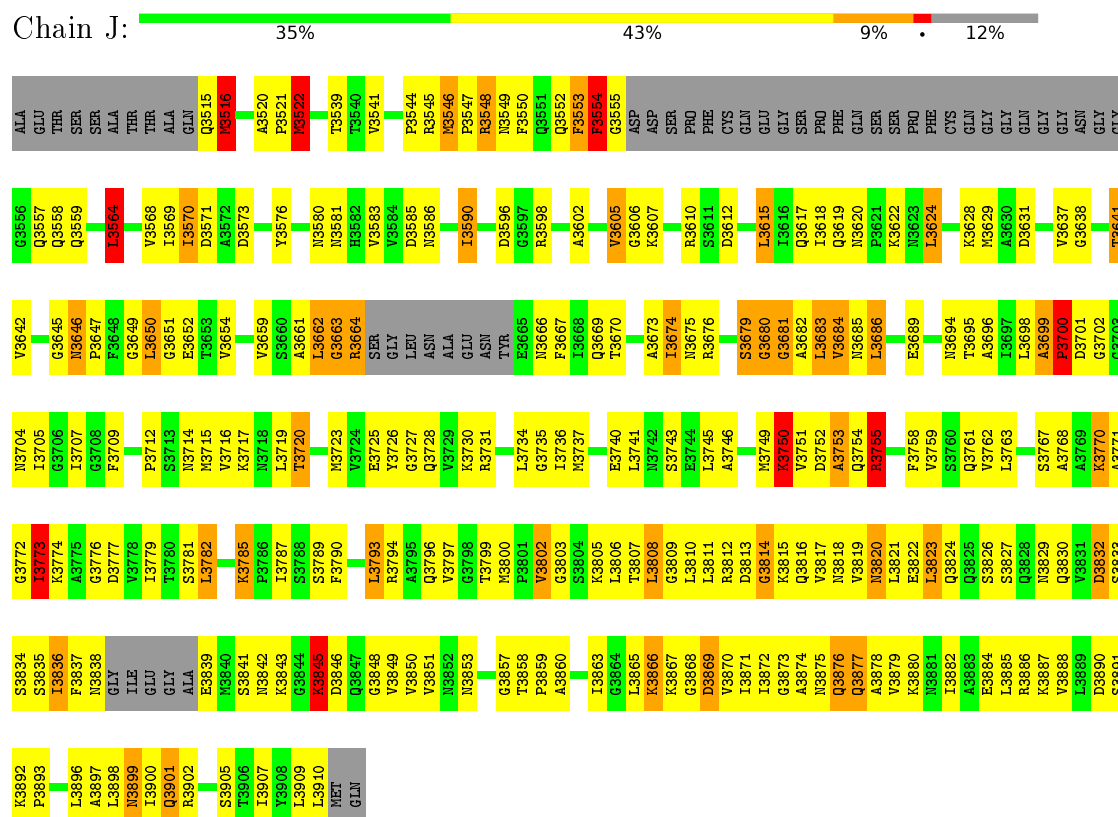


• Molecule 1: Protease do

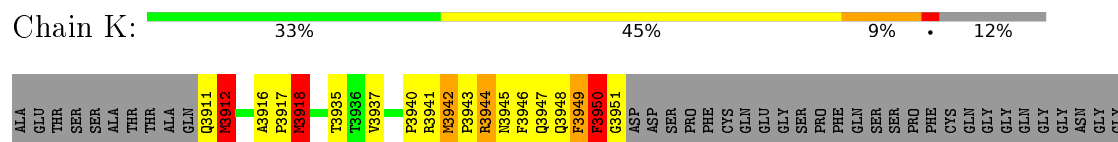


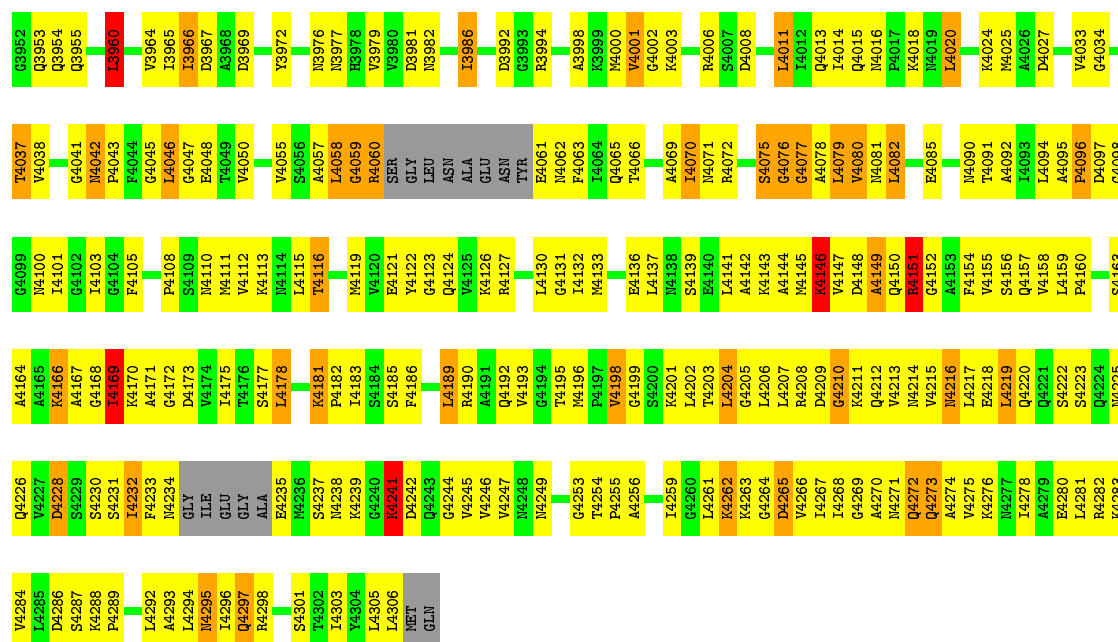


• Molecule 1: Protease do



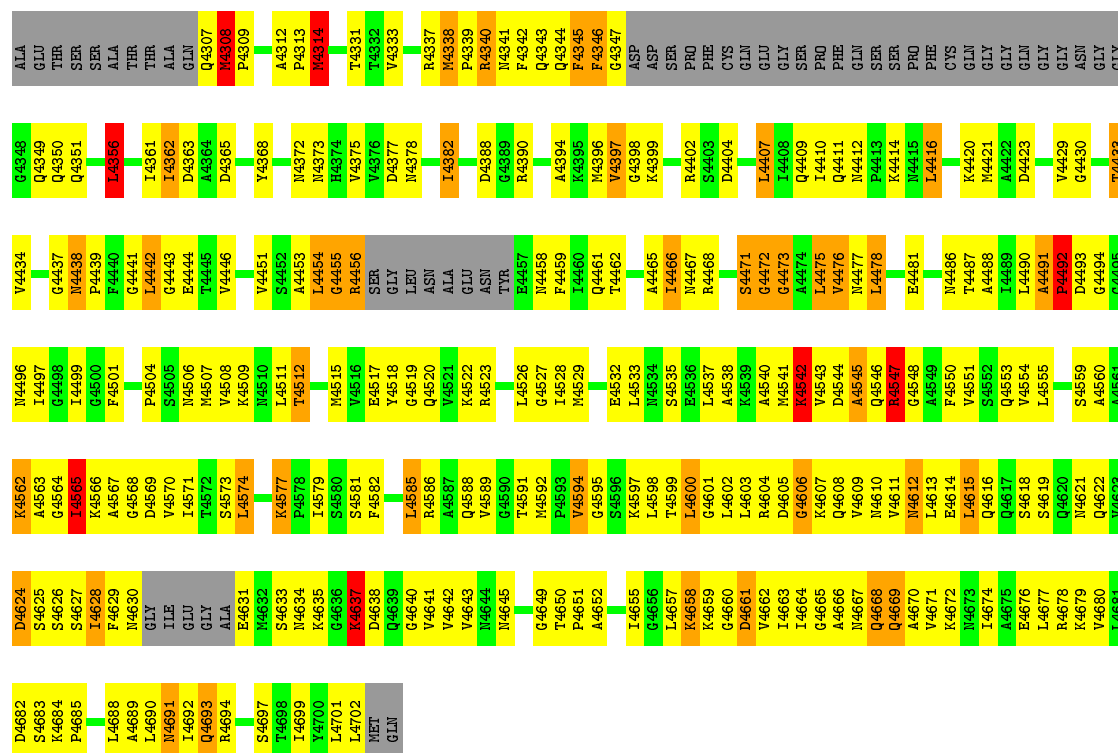
• Molecule 1: Protease do





Molecule 1: Protease do

Chain L: 34% 44% 9% 12%



Molecule 1: Protease do

Chain M: 33% 44% 9% 12%

S5079	S5080	P5081	L5084	A5085	L5086	M5087	I5088	Q5089	E5090	S5093	T5094	I5095	V5096	L5097	L5098	MET	GLN	ALA	GLU	THR	SER	SER	ALA	THR	THR	ALA	GLN	Q4703	R4704	P4705	A4708	P4709	R4710	T4727	T4728	V4729	P4732	R4733	M4734	P4735	R4736	M4737	F4738	Q4739	Q4740	F4741	R4742	G4743	ASP	ASP	SER	PRO	PHE	GLN	GLU	GLY	SER	PRO	PHE	GLN	GLY	GLY	GLN	GLY	GLY	ASN	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

• Molecule 2: Outer membrane protein C

Chain D:  40% 59%

	R1516	G1439	D1366	D1272	A1189
		W1440	G1367	V1273	E1190
	N1521	A1441	V1368	G1274	V1191
	T1522	N1442	G1369	S1275	Y1192
	D1523	K1443	G1370	F1276	N1193
		A1444	S1371	D1277	K1194
		Q1445	L1372	Y1278	D1195
		N1446		G1279	G1196
	V1526	F1447		R1280	N1197
		E1448			K1198
	V1531	A1449		T1289	L1199
	Y1532	V1450			D1200
	Q1533	A1451		T1292	
	F1534	Q1452		L1295	K1204
		G1458	S1388	F1298	L1208
		L1459	K1389		H1209
			R1390	T1302	Y1210
		S1462	D1391		F1211
		L1463	D1392		S1212
		A1464	A1393	D1306	D1213
		Y1465	Q1394		N1214
		L1466	N1395	M1309	
		G1467	T1396		
		S1468	A1397	N1314	V1217
		K1469	A1398	G1315	D1218
		G1470	Y1399	F1316	G1219
		K1471	T1400	A1317	D1220
		N1472	G1401	T1318	Q1221
		L1473	N1402	Y1319	
		G1474	G1403	R1320	L1226
		L1475	D1404	N1321	
		G1476	R1405	T1322	G1230
		Y1477	A1406	D1323	E1231
			E1407	F1324	T1232
			T1408	F1325	
		T1482	Y1409	G1326	T1235
		L1483	T1410	L1327	
		K1484	G1411	V1328	T1239
		Y1485	G1412	D1329	G1240
		V1486	L1412		Y1241
		D1487	L1413		G1242
		V1488		F1333	Q1243
			N1418	A1334	W1244
				V1335	E1245
		T1491		Q1336	Y1246
		Y1492	A1423	Y1337	Q1247
		Y1493	A1424	Q1338	I1248
		F1494	Q1425	G1339	Q1249
		H1495	Y1426	K1340	
		K1496	T1427		
		N1497	Q1428		N1258
		M1498	T1429	T1354	S1259
		S1499	Y1430		W1260
		T1500	N1431	R1358	
			A1432	D1359	F1265
		D1503	T1433	A1360	A1266
		Y1504	R1434	L1361	G1267
		K1505	V1435	R1362	L1268
		I1506	G1436	Q1363	K1269
		M1507	S1437	N1364	F1270
		L1508	L1438	G1365	G1271

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	29
1	B	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	C	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	E	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	F	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	G	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	H	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	I	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	J	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	K	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	L	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
1	M	388/448 (87%)	318 (82%)	49 (13%)	21 (5%)	2	29
2	D	344/346 (99%)	327 (95%)	17 (5%)	0	100	100
All	All	5000/5722 (87%)	4143 (83%)	605 (12%)	252 (5%)	5	31

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	25
1	B	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	C	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	E	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	F	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	G	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	H	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	I	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	J	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	K	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	L	319/357 (89%)	273 (86%)	46 (14%)	4	25
1	M	319/357 (89%)	273 (86%)	46 (14%)	4	25
2	D	275/275 (100%)	271 (98%)	4 (2%)	72	88
All	All	4103/4559 (90%)	3547 (86%)	556 (14%)	9	27

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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.