



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:14 pm BST

PDB ID : 1N6E
Title : tricorn protease in complex with a tridecapeptide chloromethyl ketone derivative
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

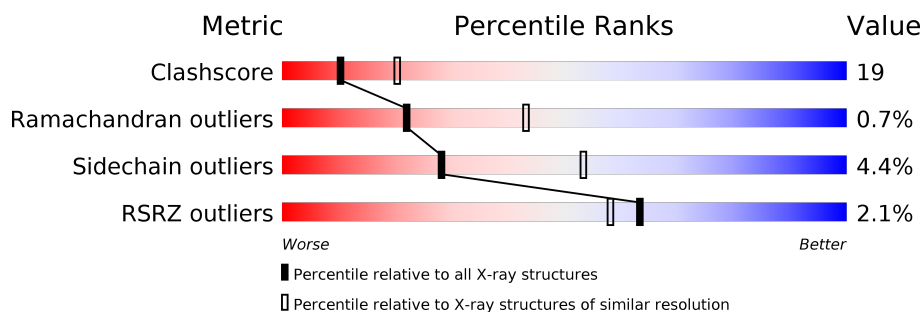
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	A	1071	<div> <div></div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div>
1	C	1071	<div> <div></div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div>
1	E	1071	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>35%</div> <div>• •</div> </div> </div>
1	G	1071	<div> <div></div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• •</div> </div> </div>
1	I	1071	<div> <div></div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div>
1	K	1071	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>• •</div> </div> </div>
2	B	13	<div> <div>46%</div> <div> <div></div> <div>54%</div> <div>23%</div> <div>8%</div> <div>15%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	13	<div><div></div><div>38%</div><div>54%</div><div>23%</div><div>8%</div><div>15%</div></div>
2	F	13	<div><div></div><div>46%</div><div>38%</div><div>31%</div><div>15%</div><div>15%</div></div>
2	H	13	<div><div></div><div>31%</div><div>54%</div><div>23%</div><div>8%</div><div>15%</div></div>
2	J	13	<div><div></div><div>54%</div><div>54%</div><div>23%</div><div>8%</div><div>15%</div></div>
2	L	13	<div><div></div><div>54%</div><div>46%</div><div>23%</div><div>15%</div><div>15%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50544 atoms, of which 0 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.

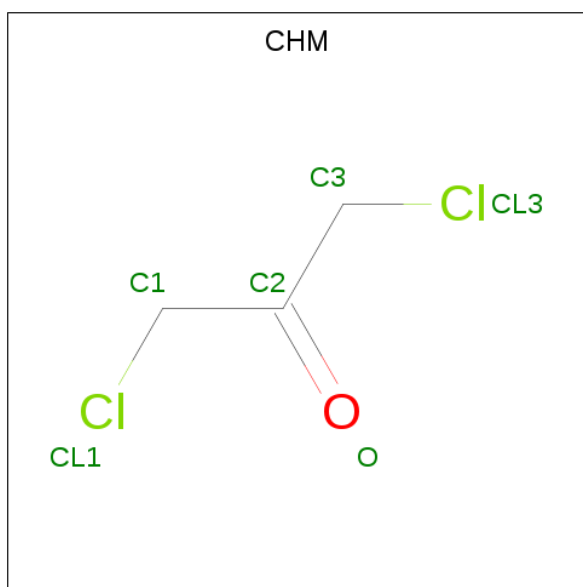
- Molecule 1 is a protein called tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	E	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	G	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	I	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	K	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			

- Molecule 2 is a protein called DQTQKAAAELTFF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	D	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	F	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	H	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	J	11	Total	C	N	O	0	0	0
			86	57	13	16			
2	L	11	Total	C	N	O	0	0	0
			86	57	13	16			

- Molecule 3 is 1,3-DICHLORO-PROPAN-2-ONE (three-letter code: CHM) (formula: C₃H₄Cl₂O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 1 1	0	0
3	D	1	Total C 1 1	0	0
3	F	1	Total C 1 1	0	0
3	H	1	Total C 1 1	0	0
3	J	1	Total C 1 1	0	0
3	L	1	Total C 1 1	0	0

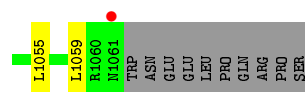
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	178	Total O 178 178	0	0
4	B	2	Total O 2 2	0	0
4	C	172	Total O 172 172	0	0
4	D	2	Total O 2 2	0	0
4	E	138	Total O 138 138	0	0
4	F	5	Total O 5 5	0	0

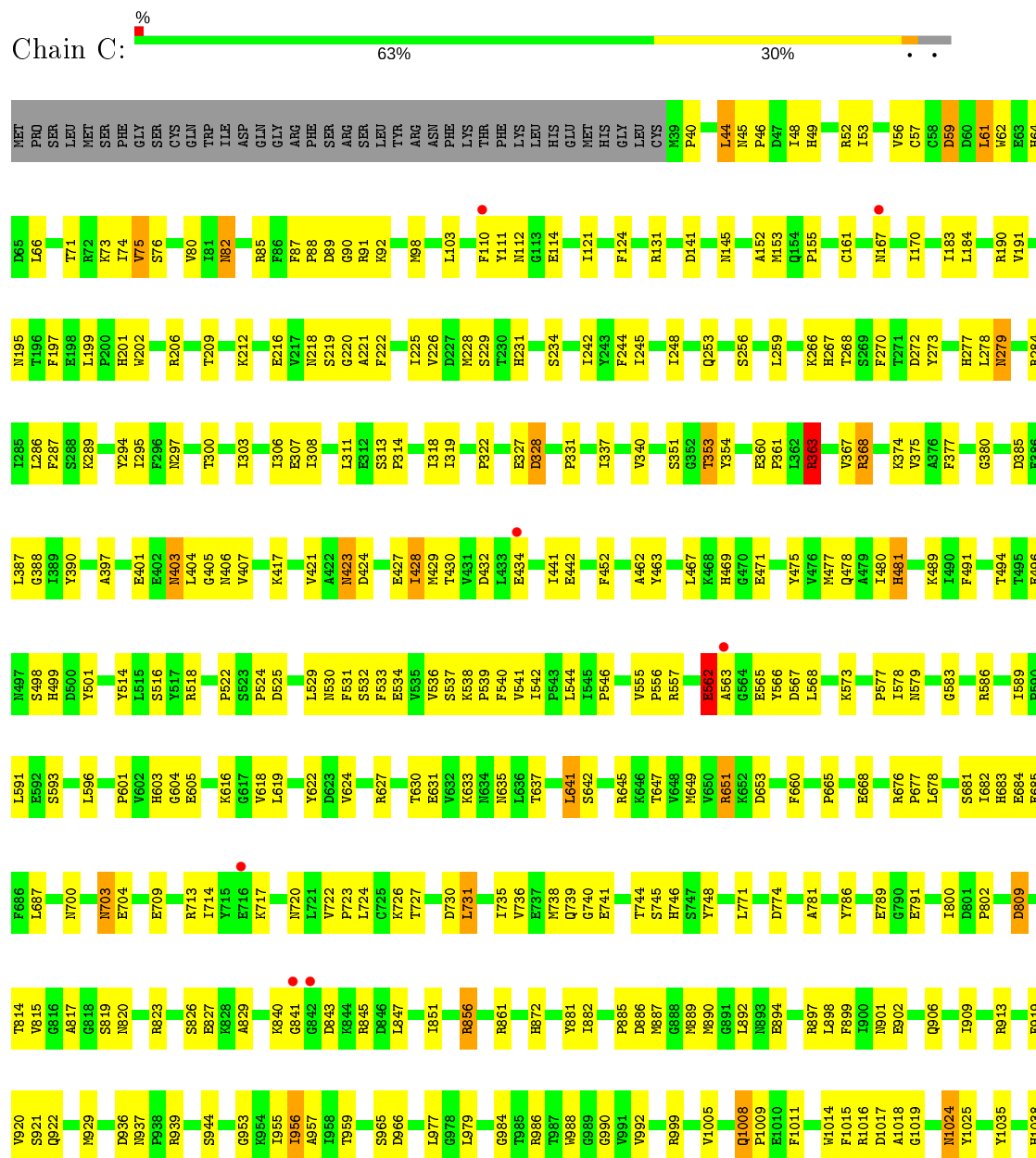
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	154	Total 154	O 154	0	0
4	H	2	Total 2	O 2	0	0
4	I	157	Total 157	O 157	0	0
4	J	2	Total 2	O 2	0	0
4	K	146	Total 146	O 146	0	0
4	L	2	Total 2	O 2	0	0

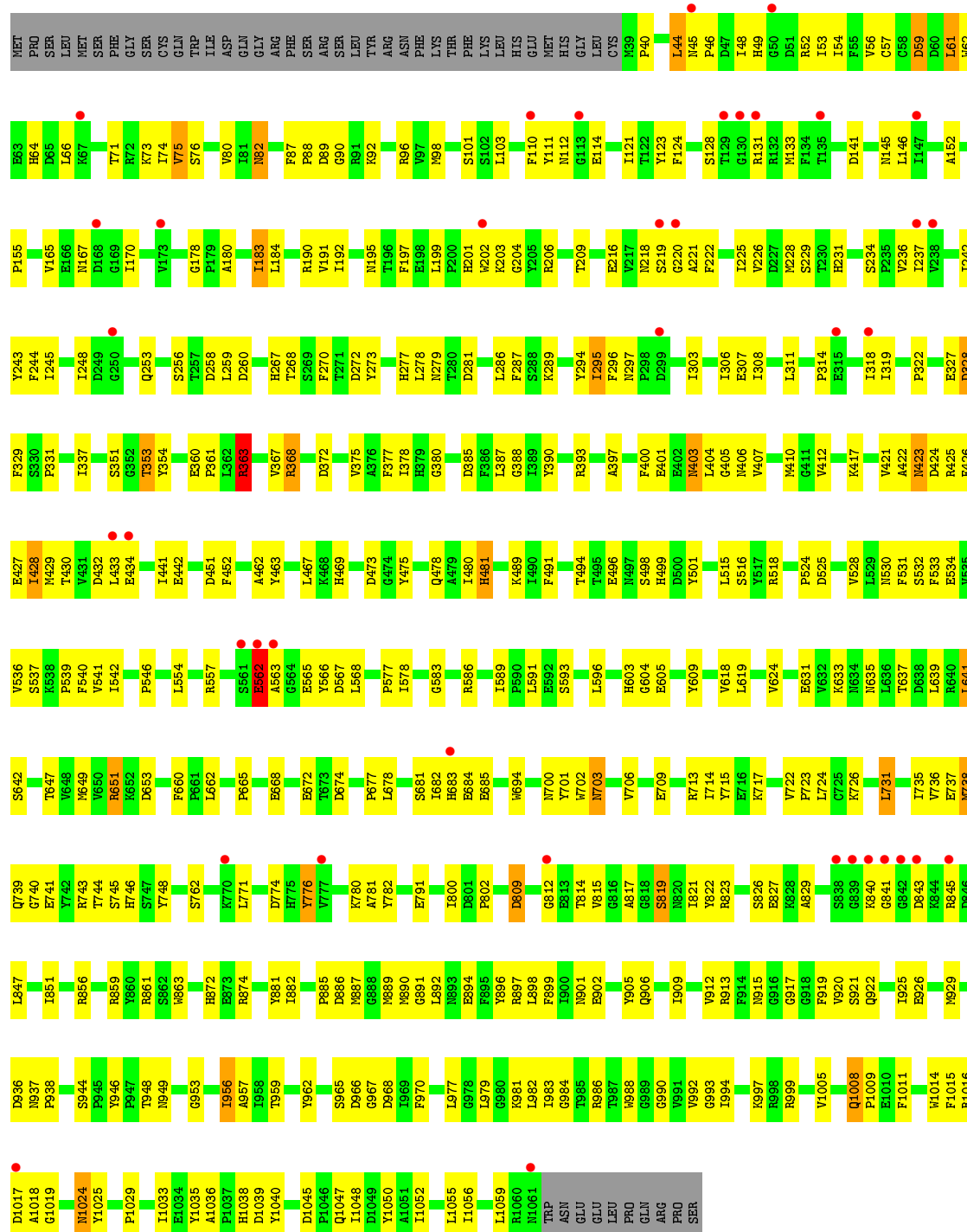


- Molecule 1: tricorn protease

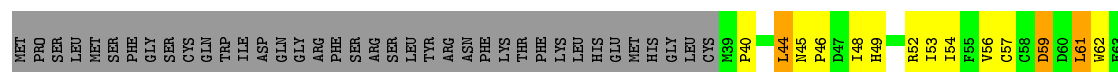


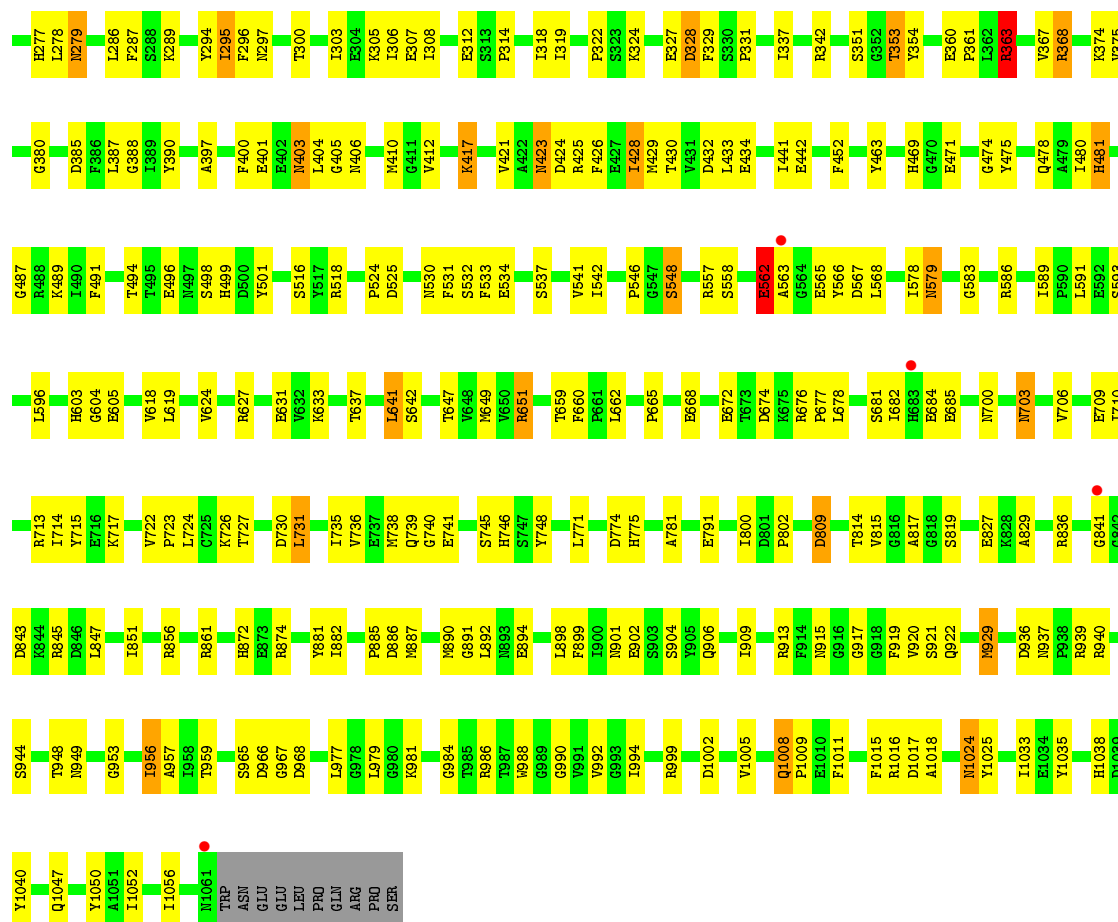
- Molecule 1: tricorn protease



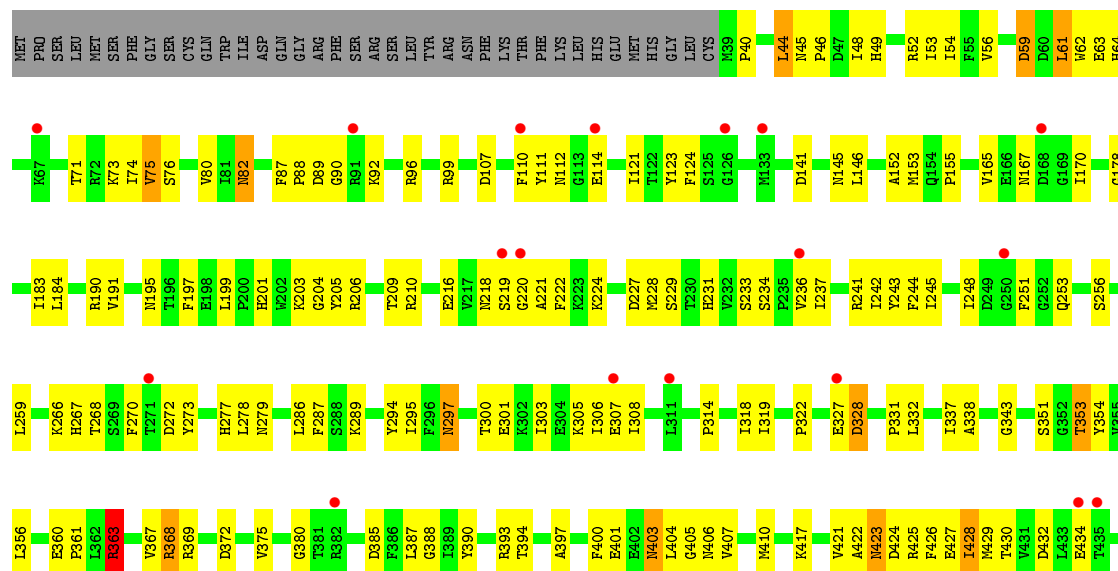


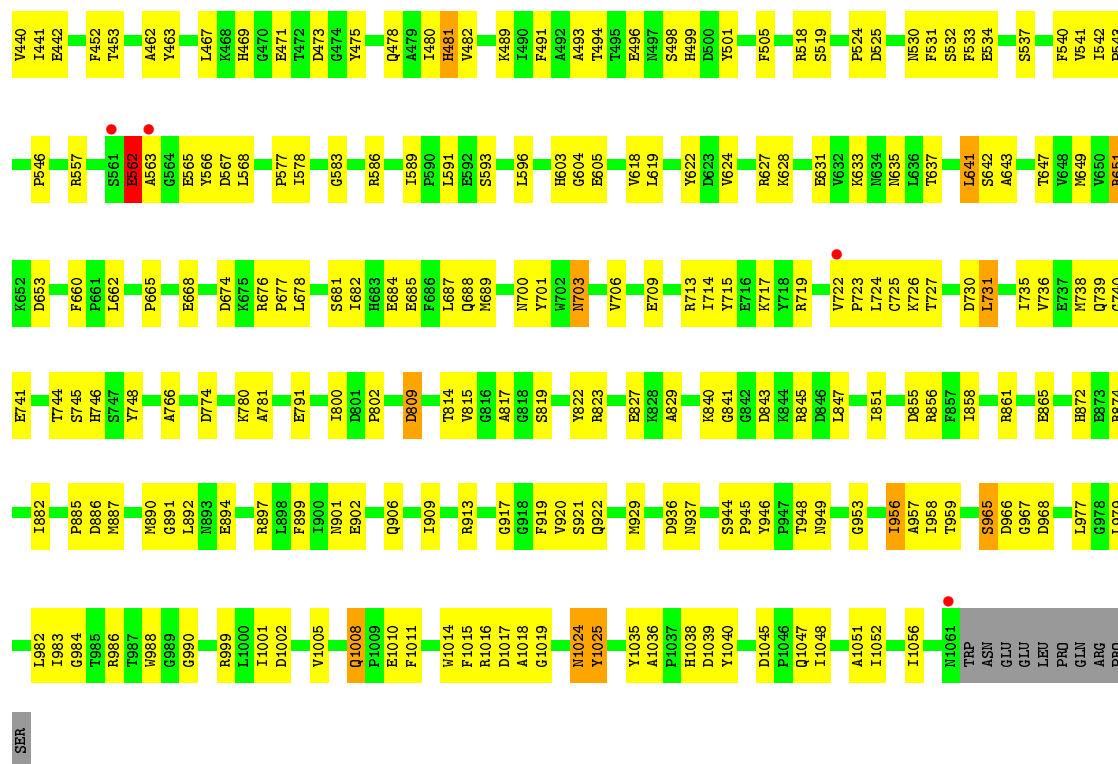
• Molecule 1: tricorn protease

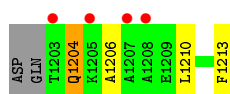




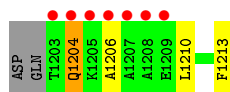
• Molecule 1: tricorn protease



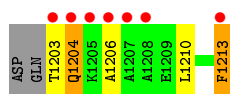




- Molecule 2: DQTQKAAAELTFF



- Molecule 2: DQTQKAAAELTFF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.47Å 245.10Å 157.89Å 90.00° 105.19° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 46.92 – 2.59	Depositor EDS
% Data completeness (in resolution range)	86.6 (6.00-2.60) 85.7 (46.92-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.254 , 0.288 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50544	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.69	0/8367	0.76	1/11311 (0.0%)
1	C	0.69	1/8367 (0.0%)	0.76	1/11311 (0.0%)
1	E	0.68	0/8367	0.75	0/11311
1	G	0.66	0/8367	0.75	0/11311
1	I	0.67	1/8367 (0.0%)	0.75	0/11311
1	K	0.67	0/8367	0.75	0/11311
2	B	1.24	1/87 (1.1%)	0.61	0/116
2	D	1.29	1/87 (1.1%)	0.57	0/116
2	F	1.20	1/87 (1.1%)	0.60	0/116
2	H	1.34	1/87 (1.1%)	0.61	0/116
2	J	1.24	1/87 (1.1%)	0.60	0/116
2	L	1.07	1/87 (1.1%)	0.61	0/116
All	All	0.68	8/50724 (0.0%)	0.75	2/68562 (0.0%)

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	E	0	2
1	K	0	2
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1213	PHE	C-O	11.24	1.44	1.23
2	D	1213	PHE	C-O	10.99	1.44	1.23
2	B	1213	PHE	C-O	10.43	1.43	1.23
2	J	1213	PHE	C-O	10.35	1.43	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1213	PHE	C-O	9.64	1.41	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	861	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	C	886	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	776	TYR	Sidechain
1	E	822	TYR	Sidechain
1	K	1025	TYR	Sidechain
1	K	822	TYR	Sidechain

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	8177	0	8002	300	1
1	C	8177	0	8002	291	1
1	E	8177	0	8002	352	0
1	G	8177	0	8002	317	1
1	I	8177	0	8002	301	1
1	K	8177	0	8002	330	0
2	B	86	0	84	4	0
2	D	86	0	84	4	0
2	F	86	0	84	8	0
2	H	86	0	84	3	0
2	J	86	0	84	4	0
2	L	86	0	84	7	0
3	B	1	0	0	1	0
3	D	1	0	0	1	0
3	F	1	0	0	1	0
3	H	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	1	0
3	L	1	0	0	1	0
4	A	178	0	0	29	0
4	B	2	0	0	0	0
4	C	172	0	0	24	0
4	D	2	0	0	0	0
4	E	138	0	0	54	0
4	F	5	0	0	2	0
4	G	154	0	0	32	0
4	H	2	0	0	1	0
4	I	157	0	0	18	0
4	J	2	0	0	0	0
4	K	146	0	0	56	0
4	L	2	0	0	1	0
All	All	50544	0	48516	1807	2

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 19.

The worst 5 of 1807 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)
1:I:351:SER:OG	1:I:353:THR:HG22	1.41	1.17
1:C:351:SER:OG	1:C:353:THR:HG22	1.46	1.16
1:G:351:SER:OG	1:G:353:THR:HG22	1.47	1.15
1:A:351:SER:OG	1:A:353:THR:HG22	1.45	1.14
1:E:351:SER:OG	1:E:353:THR:HG22	1.46	1.13

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASN:N	1:I:143:ASP:OD2[2_545]	2.06	0.14
1:C:167:ASN:N	1:G:143:ASP:OD2[2_455]	2.12	0.08

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	A	1021/1071 (95%)	948 (93%)	67 (7%)	6 (1%)	25	47
1	C	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	19	39
1	E	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	19	39
1	G	1021/1071 (95%)	950 (93%)	63 (6%)	8 (1%)	19	39
1	I	1021/1071 (95%)	949 (93%)	64 (6%)	8 (1%)	19	39
1	K	1021/1071 (95%)	947 (93%)	66 (6%)	8 (1%)	19	39
2	B	9/13 (69%)	4 (44%)	5 (56%)	0	100	100
2	D	9/13 (69%)	4 (44%)	5 (56%)	0	100	100
2	F	9/13 (69%)	6 (67%)	3 (33%)	0	100	100
2	H	9/13 (69%)	5 (56%)	4 (44%)	0	100	100
2	J	9/13 (69%)	6 (67%)	3 (33%)	0	100	100
2	L	9/13 (69%)	5 (56%)	4 (44%)	0	100	100
All	All	6180/6504 (95%)	5721 (93%)	413 (7%)	46 (1%)	22	43

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	C	219	SER
1	E	219	SER
1	E	1018	ALA
1	G	219	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/928 (95%)	846 (96%)	37 (4%)	30	55
1	C	883/928 (95%)	846 (96%)	37 (4%)	30	55
1	E	883/928 (95%)	844 (96%)	39 (4%)	28	53
1	G	883/928 (95%)	845 (96%)	38 (4%)	29	54
1	I	883/928 (95%)	845 (96%)	38 (4%)	29	54
1	K	883/928 (95%)	848 (96%)	35 (4%)	31	57
2	B	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	D	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	F	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	H	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	J	8/10 (80%)	6 (75%)	2 (25%)	0	1
2	L	8/10 (80%)	6 (75%)	2 (25%)	0	1
All	All	5346/5628 (95%)	5110 (96%)	236 (4%)	28	53

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	819	SER
1	G	368	ARG
1	K	641	LEU
1	E	929	MET
1	G	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	733	ASN
1	G	297	ASN
1	K	611	GLN
1	E	867	ASN
1	E	1038	HIS

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 6 are modelled with single atom - 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	1023/1071 (95%)	-0.08	12 (1%) 79 76	16, 36, 58, 78	20 (1%)
1	C	1023/1071 (95%)	-0.08	7 (0%) 87 86	17, 36, 58, 78	20 (1%)
1	E	1023/1071 (95%)	0.19	39 (3%) 40 33	20, 39, 59, 80	20 (1%)
1	G	1023/1071 (95%)	-0.07	7 (0%) 87 86	20, 37, 58, 78	20 (1%)
1	I	1023/1071 (95%)	-0.05	8 (0%) 86 84	20, 37, 58, 78	20 (1%)
1	K	1023/1071 (95%)	0.14	22 (2%) 62 56	20, 39, 59, 79	20 (1%)
2	B	11/13 (84%)	2.53	6 (54%) 0 0	52, 84, 96, 99	0
2	D	11/13 (84%)	2.66	5 (45%) 0 0	52, 84, 96, 99	0
2	F	11/13 (84%)	2.65	6 (54%) 0 0	53, 85, 97, 98	0
2	H	11/13 (84%)	2.34	4 (36%) 0 0	52, 84, 96, 99	0
2	J	11/13 (84%)	3.19	7 (63%) 0 0	52, 84, 96, 99	0
2	L	11/13 (84%)	3.92	7 (63%) 0 0	54, 84, 96, 99	0
All	All	6204/6504 (95%)	0.04	130 (2%) 63 58	16, 38, 60, 99	120 (1%)

The worst 5 of 130 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	219	SER	12.1
1	G	219	SER	10.6
2	J	1203	THR	9.9
2	L	1203	THR	9.9
1	C	842	GLY	9.8

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 carbohydrates 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(\AA^2)	Q<0.9
3	CHM	F	2213	1/6	0.87	0.12	52,52,52,52	0
3	CHM	D	2213	1/6	0.88	0.11	52,52,52,52	0
3	CHM	L	2213	1/6	0.90	0.23	59,59,59,59	0
3	CHM	J	2213	1/6	0.94	0.09	56,56,56,56	0
3	CHM	H	2213	1/6	0.94	0.10	52,52,52,52	0
3	CHM	B	2213	1/6	0.94	0.12	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.