



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2023 – 09:46 AM EDT

PDB ID : 3UY9  
Title : Bovine trypsin variant X(tripleGlu217Phe227) in complex with small molecule inhibitor  
Authors : Tziridis, A.; Neumann, P.; Kolenko, P.; Stubbs, M.T.  
Deposited on : 2011-12-06  
Resolution : 3.22 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

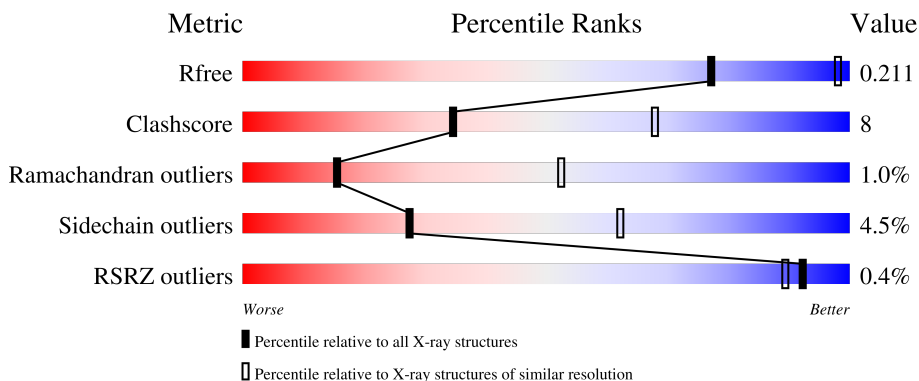
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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))
$R_{free}$	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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  $\geq 3$ , 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	223	86% 12% .
1	B	223	82% 17% .
1	C	223	81% 17% .
1	D	223	81% 17% .
1	E	223	86% 13% .

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Mol	Chain	Length	Quality of chain
1	F	223	 80% 18%
1	G	223	 81% 18%
1	H	223	 82% 17%
1	I	223	 78% 19%
1	J	223	 87% 12%
1	K	223	 80% 17%
1	L	223	 78% 20%
1	M	223	 79% 18%
1	N	223	 79% 19%
1	O	223	 74% 23%
1	P	223	 82% 16%

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
3	BEN	I	501	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26387 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 Cationic trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1639	1022	277	326	14	0	0	0
1	B	223	1639	1022	277	326	14	0	0	0
1	C	223	1639	1022	277	326	14	0	0	0
1	D	223	1639	1022	277	326	14	0	0	0
1	E	223	1639	1022	277	326	14	0	0	0
1	F	223	1639	1022	277	326	14	0	0	0
1	G	223	1639	1022	277	326	14	0	0	0
1	H	223	1639	1022	277	326	14	0	0	0
1	I	223	1639	1022	277	326	14	0	0	0
1	J	223	1639	1022	277	326	14	0	0	0
1	K	223	1639	1022	277	326	14	0	0	0
1	L	223	1639	1022	277	326	14	0	0	0
1	M	223	1639	1022	277	326	14	0	0	0
1	N	223	1639	1022	277	326	14	0	0	0
1	O	223	1639	1022	277	326	14	0	0	0
1	P	223	1639	1022	277	326	14	0	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLU	ASN	engineered mutation	UNP P00760
A	99	TYR	LEU	engineered mutation	UNP P00760
A	172	SER	TYR	engineered mutation	UNP P00760
A	173	SER	PRO	engineered mutation	UNP P00760
A	174	PHE	GLY	engineered mutation	UNP P00760
A	175	ILE	GLN	engineered mutation	UNP P00760
A	183	VAL	ALA	engineered mutation	UNP P00760
A	190	ALA	SER	engineered mutation	UNP P00760
A	217	GLU	SER	engineered mutation	UNP P00760
A	227	PHE	VAL	engineered mutation	UNP P00760
B	97	GLU	ASN	engineered mutation	UNP P00760
B	99	TYR	LEU	engineered mutation	UNP P00760
B	172	SER	TYR	engineered mutation	UNP P00760
B	173	SER	PRO	engineered mutation	UNP P00760
B	174	PHE	GLY	engineered mutation	UNP P00760
B	175	ILE	GLN	engineered mutation	UNP P00760
B	183	VAL	ALA	conflict	UNP P00760
B	190	ALA	SER	engineered mutation	UNP P00760
B	217	GLU	SER	engineered mutation	UNP P00760
B	227	PHE	VAL	engineered mutation	UNP P00760
C	97	GLU	ASN	engineered mutation	UNP P00760
C	99	TYR	LEU	engineered mutation	UNP P00760
C	172	SER	TYR	engineered mutation	UNP P00760
C	173	SER	PRO	engineered mutation	UNP P00760
C	174	PHE	GLY	engineered mutation	UNP P00760
C	175	ILE	GLN	engineered mutation	UNP P00760
C	183	VAL	ALA	engineered mutation	UNP P00760
C	190	ALA	SER	engineered mutation	UNP P00760
C	217	GLU	SER	engineered mutation	UNP P00760
C	227	PHE	VAL	engineered mutation	UNP P00760
D	97	GLU	ASN	engineered mutation	UNP P00760
D	99	TYR	LEU	engineered mutation	UNP P00760
D	172	SER	TYR	engineered mutation	UNP P00760
D	173	SER	PRO	engineered mutation	UNP P00760
D	174	PHE	GLY	engineered mutation	UNP P00760
D	175	ILE	GLN	engineered mutation	UNP P00760
D	183	VAL	ALA	conflict	UNP P00760
D	190	ALA	SER	engineered mutation	UNP P00760
D	217	GLU	SER	engineered mutation	UNP P00760
D	227	PHE	VAL	engineered mutation	UNP P00760
E	97	GLU	ASN	engineered mutation	UNP P00760
E	99	TYR	LEU	engineered mutation	UNP P00760

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Chain	Residue	Modelled	Actual	Comment	Reference
E	172	SER	TYR	engineered mutation	UNP P00760
E	173	SER	PRO	engineered mutation	UNP P00760
E	174	PHE	GLY	engineered mutation	UNP P00760
E	175	ILE	GLN	engineered mutation	UNP P00760
E	183	VAL	ALA	conflict	UNP P00760
E	190	ALA	SER	engineered mutation	UNP P00760
E	217	GLU	SER	engineered mutation	UNP P00760
E	227	PHE	VAL	engineered mutation	UNP P00760
F	97	GLU	ASN	engineered mutation	UNP P00760
F	99	TYR	LEU	engineered mutation	UNP P00760
F	172	SER	TYR	engineered mutation	UNP P00760
F	173	SER	PRO	engineered mutation	UNP P00760
F	174	PHE	GLY	engineered mutation	UNP P00760
F	175	ILE	GLN	engineered mutation	UNP P00760
F	183	VAL	ALA	conflict	UNP P00760
F	190	ALA	SER	engineered mutation	UNP P00760
F	217	GLU	SER	engineered mutation	UNP P00760
F	227	PHE	VAL	engineered mutation	UNP P00760
G	97	GLU	ASN	engineered mutation	UNP P00760
G	99	TYR	LEU	engineered mutation	UNP P00760
G	172	SER	TYR	engineered mutation	UNP P00760
G	173	SER	PRO	engineered mutation	UNP P00760
G	174	PHE	GLY	engineered mutation	UNP P00760
G	175	ILE	GLN	engineered mutation	UNP P00760
G	183	VAL	ALA	conflict	UNP P00760
G	190	ALA	SER	engineered mutation	UNP P00760
G	217	GLU	SER	engineered mutation	UNP P00760
G	227	PHE	VAL	engineered mutation	UNP P00760
H	97	GLU	ASN	engineered mutation	UNP P00760
H	99	TYR	LEU	engineered mutation	UNP P00760
H	172	SER	TYR	engineered mutation	UNP P00760
H	173	SER	PRO	engineered mutation	UNP P00760
H	174	PHE	GLY	engineered mutation	UNP P00760
H	175	ILE	GLN	engineered mutation	UNP P00760
H	183	VAL	ALA	conflict	UNP P00760
H	190	ALA	SER	engineered mutation	UNP P00760
H	217	GLU	SER	engineered mutation	UNP P00760
H	227	PHE	VAL	engineered mutation	UNP P00760
I	97	GLU	ASN	engineered mutation	UNP P00760
I	99	TYR	LEU	engineered mutation	UNP P00760
I	172	SER	TYR	engineered mutation	UNP P00760
I	173	SER	PRO	engineered mutation	UNP P00760

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Chain	Residue	Modelled	Actual	Comment	Reference
I	174	PHE	GLY	engineered mutation	UNP P00760
I	175	ILE	GLN	engineered mutation	UNP P00760
I	183	VAL	ALA	conflict	UNP P00760
I	190	ALA	SER	engineered mutation	UNP P00760
I	217	GLU	SER	engineered mutation	UNP P00760
I	227	PHE	VAL	engineered mutation	UNP P00760
J	97	GLU	ASN	engineered mutation	UNP P00760
J	99	TYR	LEU	engineered mutation	UNP P00760
J	172	SER	TYR	engineered mutation	UNP P00760
J	173	SER	PRO	engineered mutation	UNP P00760
J	174	PHE	GLY	engineered mutation	UNP P00760
J	175	ILE	GLN	engineered mutation	UNP P00760
J	183	VAL	ALA	conflict	UNP P00760
J	190	ALA	SER	engineered mutation	UNP P00760
J	217	GLU	SER	engineered mutation	UNP P00760
J	227	PHE	VAL	engineered mutation	UNP P00760
K	97	GLU	ASN	engineered mutation	UNP P00760
K	99	TYR	LEU	engineered mutation	UNP P00760
K	172	SER	TYR	engineered mutation	UNP P00760
K	173	SER	PRO	engineered mutation	UNP P00760
K	174	PHE	GLY	engineered mutation	UNP P00760
K	175	ILE	GLN	engineered mutation	UNP P00760
K	183	VAL	ALA	conflict	UNP P00760
K	190	ALA	SER	engineered mutation	UNP P00760
K	217	GLU	SER	engineered mutation	UNP P00760
K	227	PHE	VAL	engineered mutation	UNP P00760
L	97	GLU	ASN	engineered mutation	UNP P00760
L	99	TYR	LEU	engineered mutation	UNP P00760
L	172	SER	TYR	engineered mutation	UNP P00760
L	173	SER	PRO	engineered mutation	UNP P00760
L	174	PHE	GLY	engineered mutation	UNP P00760
L	175	ILE	GLN	engineered mutation	UNP P00760
L	183	VAL	ALA	conflict	UNP P00760
L	190	ALA	SER	engineered mutation	UNP P00760
L	217	GLU	SER	engineered mutation	UNP P00760
L	227	PHE	VAL	engineered mutation	UNP P00760
M	97	GLU	ASN	engineered mutation	UNP P00760
M	99	TYR	LEU	engineered mutation	UNP P00760
M	172	SER	TYR	engineered mutation	UNP P00760
M	173	SER	PRO	engineered mutation	UNP P00760
M	174	PHE	GLY	engineered mutation	UNP P00760
M	175	ILE	GLN	engineered mutation	UNP P00760

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Chain	Residue	Modelled	Actual	Comment	Reference
M	183	VAL	ALA	conflict	UNP P00760
M	190	ALA	SER	engineered mutation	UNP P00760
M	217	GLU	SER	engineered mutation	UNP P00760
M	227	PHE	VAL	engineered mutation	UNP P00760
N	97	GLU	ASN	engineered mutation	UNP P00760
N	99	TYR	LEU	engineered mutation	UNP P00760
N	172	SER	TYR	engineered mutation	UNP P00760
N	173	SER	PRO	engineered mutation	UNP P00760
N	174	PHE	GLY	engineered mutation	UNP P00760
N	175	ILE	GLN	engineered mutation	UNP P00760
N	183	VAL	ALA	conflict	UNP P00760
N	190	ALA	SER	engineered mutation	UNP P00760
N	217	GLU	SER	engineered mutation	UNP P00760
N	227	PHE	VAL	engineered mutation	UNP P00760
O	97	GLU	ASN	engineered mutation	UNP P00760
O	99	TYR	LEU	engineered mutation	UNP P00760
O	172	SER	TYR	engineered mutation	UNP P00760
O	173	SER	PRO	engineered mutation	UNP P00760
O	174	PHE	GLY	engineered mutation	UNP P00760
O	175	ILE	GLN	engineered mutation	UNP P00760
O	183	VAL	ALA	conflict	UNP P00760
O	190	ALA	SER	engineered mutation	UNP P00760
O	217	GLU	SER	engineered mutation	UNP P00760
O	227	PHE	VAL	engineered mutation	UNP P00760
P	97	GLU	ASN	engineered mutation	UNP P00760
P	99	TYR	LEU	engineered mutation	UNP P00760
P	172	SER	TYR	engineered mutation	UNP P00760
P	173	SER	PRO	engineered mutation	UNP P00760
P	174	PHE	GLY	engineered mutation	UNP P00760
P	175	ILE	GLN	engineered mutation	UNP P00760
P	183	VAL	ALA	conflict	UNP P00760
P	190	ALA	SER	engineered mutation	UNP P00760
P	217	GLU	SER	engineered mutation	UNP P00760
P	227	PHE	VAL	engineered mutation	UNP P00760

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

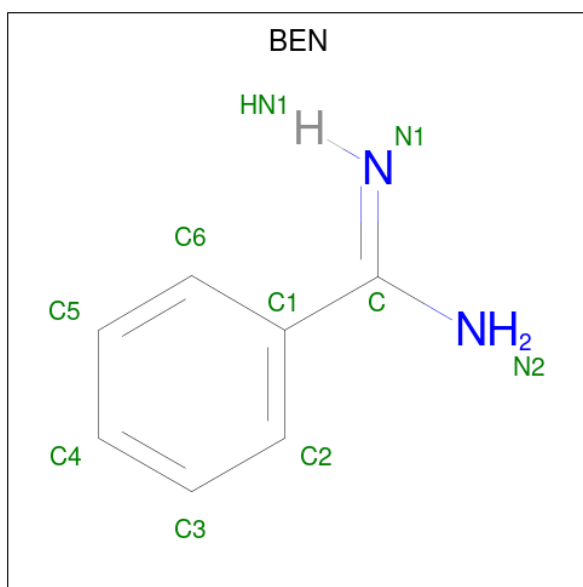
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0
2	M	1	Total Ca 1 1	0	0
2	N	1	Total Ca 1 1	0	0
2	O	1	Total Ca 1 1	0	0
2	P	1	Total Ca 1 1	0	0

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	C	1	Total	C	N	0	0
			9	7	2		
3	D	1	Total	C	N	0	0
			9	7	2		
3	E	1	Total	C	N	0	0
			9	7	2		
3	F	1	Total	C	N	0	0
			9	7	2		
3	G	1	Total	C	N	0	0
			9	7	2		
3	H	1	Total	C	N	0	0
			9	7	2		
3	I	1	Total	C	N	0	0
			9	7	2		
3	J	1	Total	C	N	0	0
			9	7	2		
3	K	1	Total	C	N	0	0
			9	7	2		
3	L	1	Total	C	N	0	0
			9	7	2		
3	M	1	Total	C	N	0	0
			9	7	2		
3	N	1	Total	C	N	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C N 9 7 2	0	0
3	P	1	Total C N 9 7 2	0	0


- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	P	1	Total Cl 1 1	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.

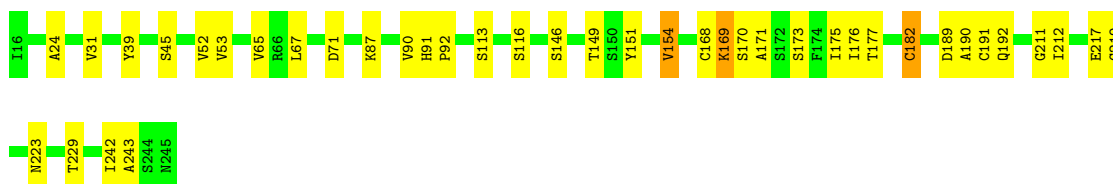
- Molecule 1: Cationic trypsin

Chain A:  86% 12%




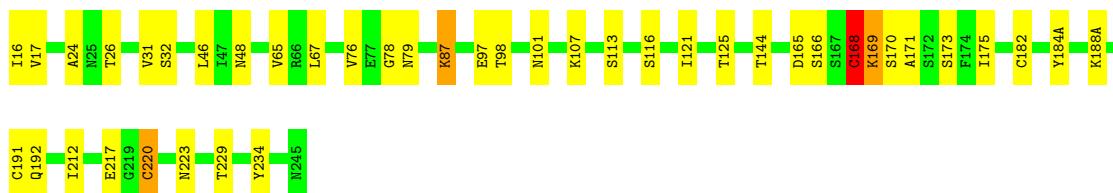
- Molecule 1: Cationic trypsin

Chain B:  82% 17%




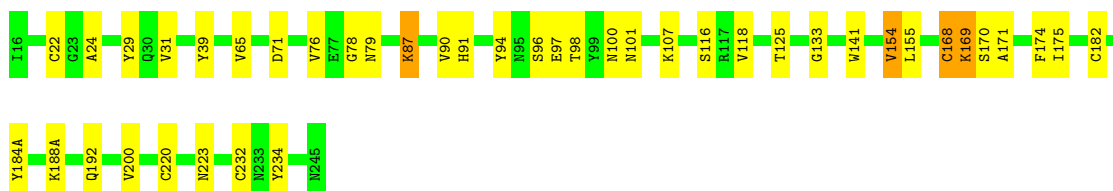
- Molecule 1: Cationic trypsin

Chain C:  81% 17%

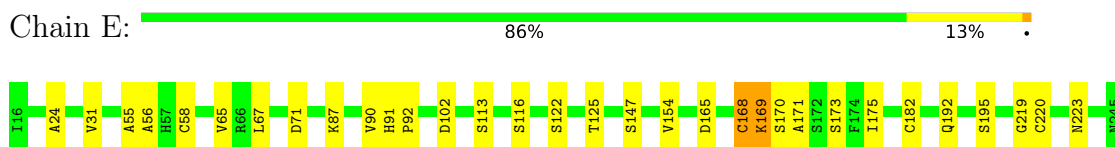


- Molecule 1: Cationic trypsin

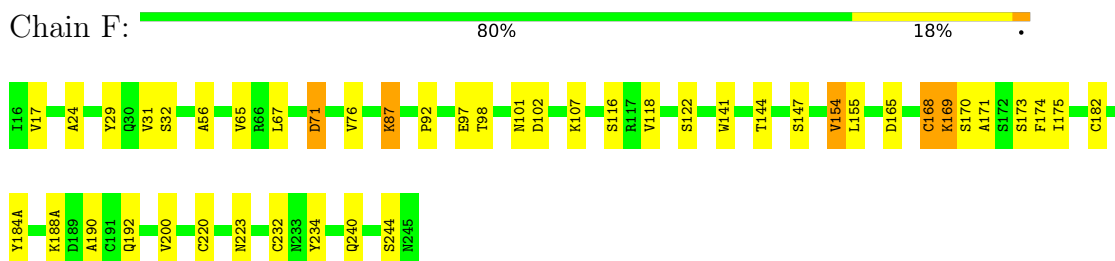
Chain D:  81% 17%



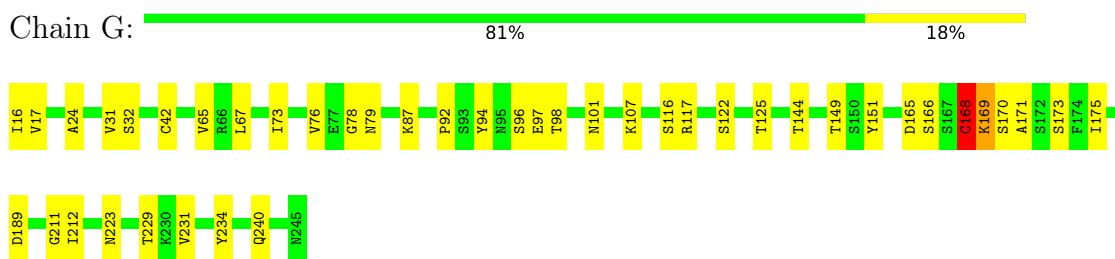
- Molecule 1: Cationic trypsin



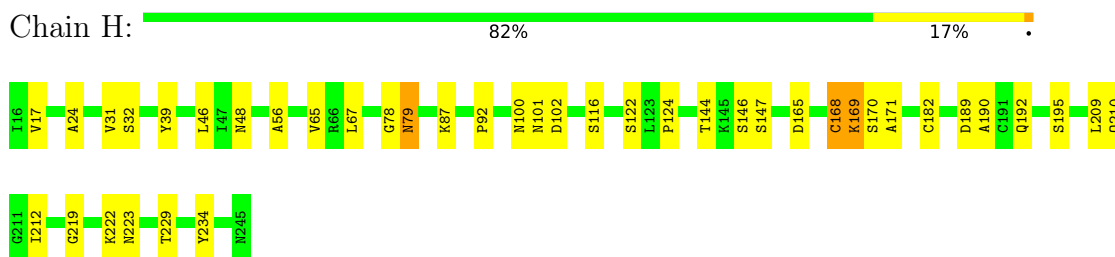
- Molecule 1: Cationic trypsin



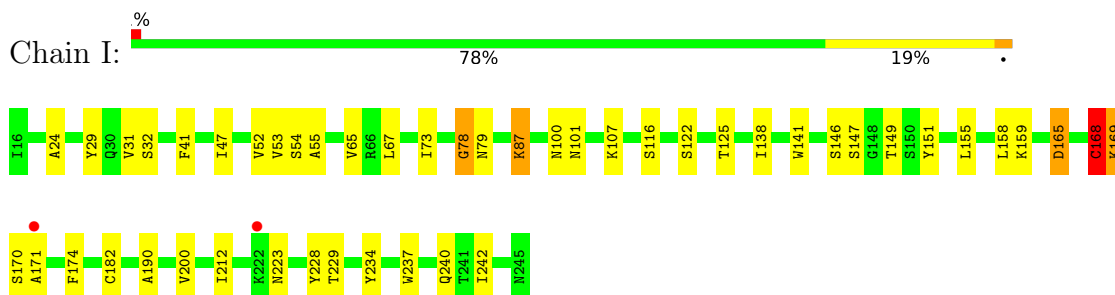
- Molecule 1: Cationic trypsin




- Molecule 1: Cationic trypsin



- Molecule 1: Cationic trypsin




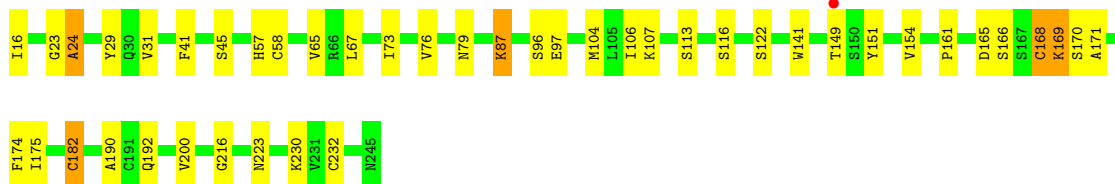
- Molecule 1: Cationic trypsin

Chain J:  87% 12%




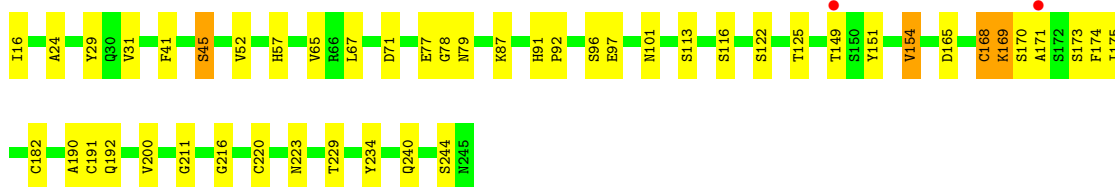
• Molecule 1: Cationic trypsin

Chain K:  80% 17%




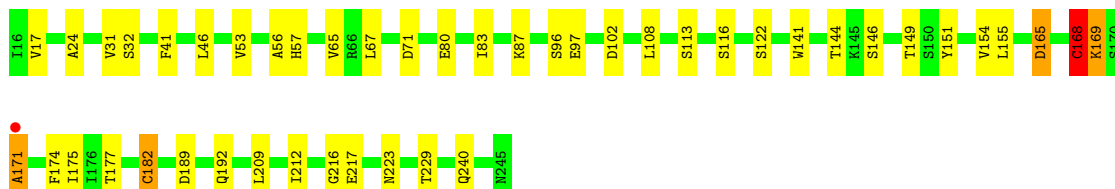
• Molecule 1: Cationic trypsin

Chain L:  78% 20%




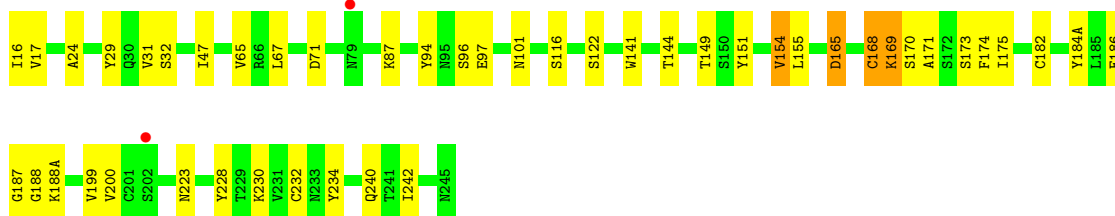
• Molecule 1: Cationic trypsin

Chain M:  79% 18%

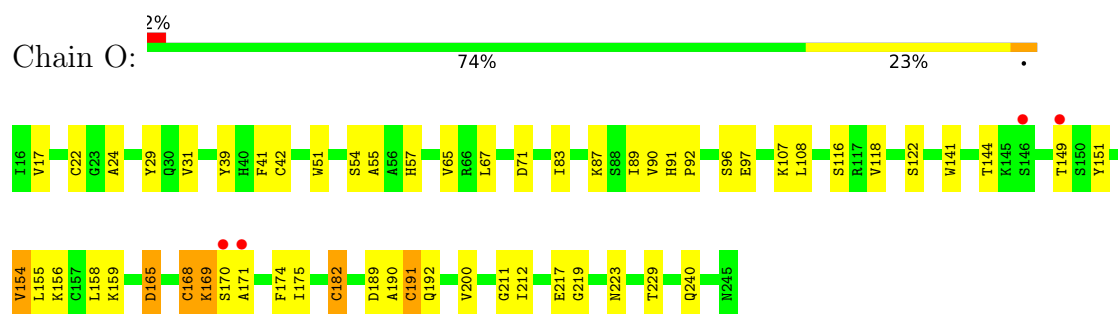


• Molecule 1: Cationic trypsin

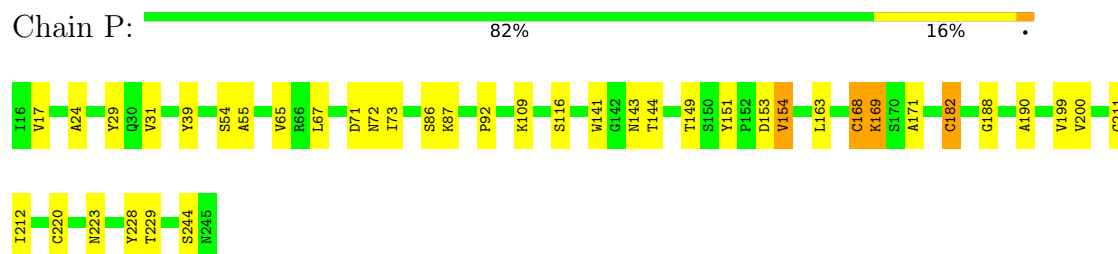
Chain N:  79% 19%



• Molecule 1: Cationic trypsin



• Molecule 1: Cationic trypsin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.07Å 98.57Å 120.78Å 89.62° 88.85° 103.99°	Depositor
Resolution (Å)	120.78 – 3.22 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	89.2 (120.78-3.22) 89.8 (20.00-3.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.205 , 0.261 0.213 , 0.211	Depositor DCC
$R_{free}$ test set	2867 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , -10.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.168 for -h,-k,l	Xtriage
Reported twinning fraction	0.878 for H, K, L 0.122 for -h,-k,l	Depositor
Outliers	0 of 56716 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	26387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, BEN, CL

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	1/1671 (0.1%)	0.64	0/2263
1	B	0.94	4/1671 (0.2%)	0.81	1/2263 (0.0%)
1	C	0.81	1/1671 (0.1%)	0.79	0/2263
1	D	0.89	4/1671 (0.2%)	0.80	0/2263
1	E	0.85	0/1671	0.79	0/2263
1	F	0.88	2/1671 (0.1%)	0.80	1/2263 (0.0%)
1	G	0.82	2/1671 (0.1%)	0.78	1/2263 (0.0%)
1	H	0.88	1/1671 (0.1%)	0.81	0/2263
1	I	0.87	2/1671 (0.1%)	0.78	0/2263
1	J	0.86	0/1671	0.78	0/2263
1	K	0.85	2/1671 (0.1%)	0.80	0/2263
1	L	0.88	0/1671	0.80	0/2263
1	M	0.98	3/1671 (0.2%)	0.83	1/2263 (0.0%)
1	N	0.91	0/1671	0.78	0/2263
1	O	1.00	5/1671 (0.3%)	0.82	0/2263
1	P	0.91	1/1671 (0.1%)	0.78	0/2263
All	All	0.88	28/26736 (0.1%)	0.79	4/36208 (0.0%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	CYS	CB-SG	-8.31	1.68	1.82
1	O	191	CYS	CB-SG	-7.67	1.69	1.82
1	M	171	ALA	CA-CB	6.55	1.66	1.52
1	D	232	CYS	CB-SG	-6.49	1.71	1.82
1	F	232	CYS	CB-SG	-6.49	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	CYS	CA-CB-SG	-6.43	102.42	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	ASP	CB-CG-OD1	6.27	123.94	118.30
1	F	71	ASP	CB-CG-OD1	5.26	123.03	118.30
1	M	168	CYS	CA-CB-SG	5.23	123.41	114.00

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	1639	0	1587	27	0
1	B	1639	0	1587	26	0
1	C	1639	0	1587	26	0
1	D	1639	0	1587	35	0
1	E	1639	0	1587	21	0
1	F	1639	0	1587	30	0
1	G	1639	0	1587	32	0
1	H	1639	0	1587	28	1
1	I	1639	0	1587	42	0
1	J	1639	0	1587	22	0
1	K	1639	0	1587	34	0
1	L	1639	0	1587	40	1
1	M	1639	0	1587	43	0
1	N	1639	0	1587	36	0
1	O	1639	0	1587	44	0
1	P	1639	0	1587	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	9	0	7	3	0
3	B	9	0	7	0	0
3	C	9	0	7	0	0
3	D	9	0	7	2	0
3	E	9	0	7	0	0
3	F	9	0	7	1	0
3	G	9	0	8	0	0
3	H	9	0	7	1	0
3	I	9	0	7	4	0
3	J	9	0	7	0	0
3	K	9	0	7	3	0
3	L	9	0	7	3	0
3	M	9	0	8	2	0
3	N	9	0	7	2	0
3	O	9	0	7	3	0
3	P	9	0	7	1	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	P	1	0	0	0	0
All	All	26387	0	25506	430	1

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 8.

The worst 5 of 430 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:K:216:GLY:HA3	3:K:501:BEN:N1	1.70	1.05
1:J:79:ASN:ND2	1:O:240:GLN:HE21	1.55	1.04
1:G:31:VAL:HG11	1:G:65:VAL:HG13	1.41	0.99
1:F:31:VAL:HG11	1:F:65:VAL:HG13	1.41	0.98
1:I:79:ASN:ND2	1:M:240:GLN:HE21	1.65	0.94

All (1) 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:H:222:LYS:NZ	1:L:149:THR:O[1_655]	2.17	0.03

### 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	221/223 (99%)	209 (95%)	10 (4%)	2 (1%)	17	55
1	B	221/223 (99%)	203 (92%)	16 (7%)	2 (1%)	17	55
1	C	221/223 (99%)	206 (93%)	13 (6%)	2 (1%)	17	55
1	D	221/223 (99%)	207 (94%)	12 (5%)	2 (1%)	17	55
1	E	221/223 (99%)	205 (93%)	14 (6%)	2 (1%)	17	55
1	F	221/223 (99%)	205 (93%)	14 (6%)	2 (1%)	17	55
1	G	221/223 (99%)	207 (94%)	12 (5%)	2 (1%)	17	55
1	H	221/223 (99%)	205 (93%)	13 (6%)	3 (1%)	11	45
1	I	221/223 (99%)	205 (93%)	14 (6%)	2 (1%)	17	55
1	J	221/223 (99%)	204 (92%)	15 (7%)	2 (1%)	17	55
1	K	221/223 (99%)	205 (93%)	13 (6%)	3 (1%)	11	45
1	L	221/223 (99%)	207 (94%)	12 (5%)	2 (1%)	17	55
1	M	221/223 (99%)	207 (94%)	12 (5%)	2 (1%)	17	55
1	N	221/223 (99%)	205 (93%)	14 (6%)	2 (1%)	17	55
1	O	221/223 (99%)	203 (92%)	16 (7%)	2 (1%)	17	55
1	P	221/223 (99%)	203 (92%)	16 (7%)	2 (1%)	17	55
All	All	3536/3568 (99%)	3286 (93%)	216 (6%)	34 (1%)	15	52

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	LYS

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Mol	Chain	Res	Type
1	D	169	LYS
1	K	169	LYS
1	A	169	LYS
1	C	169	LYS

### 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	184/185 (100%)	176 (96%)	8 (4%)	29	63
1	B	184/185 (100%)	177 (96%)	7 (4%)	33	66
1	C	184/185 (100%)	173 (94%)	11 (6%)	19	53
1	D	184/185 (100%)	177 (96%)	7 (4%)	33	66
1	E	184/185 (100%)	175 (95%)	9 (5%)	25	60
1	F	184/185 (100%)	175 (95%)	9 (5%)	25	60
1	G	184/185 (100%)	176 (96%)	8 (4%)	29	63
1	H	184/185 (100%)	177 (96%)	7 (4%)	33	66
1	I	184/185 (100%)	175 (95%)	9 (5%)	25	60
1	J	184/185 (100%)	178 (97%)	6 (3%)	38	70
1	K	184/185 (100%)	172 (94%)	12 (6%)	17	50
1	L	184/185 (100%)	172 (94%)	12 (6%)	17	50
1	M	184/185 (100%)	177 (96%)	7 (4%)	33	66
1	N	184/185 (100%)	176 (96%)	8 (4%)	29	63
1	O	184/185 (100%)	176 (96%)	8 (4%)	29	63
1	P	184/185 (100%)	179 (97%)	5 (3%)	44	74
All	All	2944/2960 (100%)	2811 (96%)	133 (4%)	27	62

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	154	VAL

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Mol	Chain	Res	Type
1	N	182	CYS
1	P	154	VAL
1	F	168	CYS
1	F	165	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	25	ASN
1	N	25	ASN
1	J	25	ASN
1	M	25	ASN
1	I	79	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 19 are monoatomic - leaving 16 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
3	BEN	A	481	-	9,9,9	1.39	1 (11%)	7,11,11	1.45	1 (14%)
3	BEN	J	501	-	9,9,9	1.47	1 (11%)	7,11,11	1.24	1 (14%)
3	BEN	H	501	-	9,9,9	1.38	2 (22%)	7,11,11	1.69	1 (14%)
3	BEN	B	481	-	9,9,9	1.53	1 (11%)	7,11,11	1.08	0
3	BEN	I	501	-	9,9,9	1.12	1 (11%)	7,11,11	0.99	1 (14%)
3	BEN	E	501	-	9,9,9	1.33	1 (11%)	7,11,11	1.50	1 (14%)
3	BEN	M	481	-	9,9,9	1.22	1 (11%)	7,11,11	1.05	0
3	BEN	N	501	-	9,9,9	1.21	1 (11%)	7,11,11	0.82	0
3	BEN	P	501	-	9,9,9	1.50	1 (11%)	7,11,11	0.77	0
3	BEN	C	481	-	9,9,9	1.54	1 (11%)	7,11,11	0.87	0
3	BEN	O	501	-	9,9,9	1.61	1 (11%)	7,11,11	1.05	0
3	BEN	K	501	-	9,9,9	1.70	1 (11%)	7,11,11	1.38	1 (14%)
3	BEN	F	501	-	9,9,9	1.06	1 (11%)	7,11,11	1.33	1 (14%)
3	BEN	D	501	-	9,9,9	1.54	1 (11%)	7,11,11	0.74	0
3	BEN	L	501	-	9,9,9	1.85	1 (11%)	7,11,11	1.33	1 (14%)
3	BEN	G	501	-	9,9,9	1.07	0	7,11,11	1.44	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	A	481	-	-	1/4/4/4	0/1/1/1
3	BEN	J	501	-	-	4/4/4/4	0/1/1/1
3	BEN	H	501	-	-	0/4/4/4	0/1/1/1
3	BEN	B	481	-	-	3/4/4/4	0/1/1/1
3	BEN	I	501	-	-	0/4/4/4	0/1/1/1
3	BEN	E	501	-	-	0/4/4/4	0/1/1/1
3	BEN	M	481	-	-	1/4/4/4	0/1/1/1
3	BEN	N	501	-	-	0/4/4/4	0/1/1/1
3	BEN	P	501	-	-	0/4/4/4	0/1/1/1
3	BEN	C	481	-	-	0/4/4/4	0/1/1/1
3	BEN	O	501	-	-	0/4/4/4	0/1/1/1
3	BEN	K	501	-	-	0/4/4/4	0/1/1/1
3	BEN	F	501	-	-	0/4/4/4	0/1/1/1
3	BEN	D	501	-	-	3/4/4/4	0/1/1/1
3	BEN	L	501	-	-	4/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	G	501	-	-	4/4/4/4	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	BEN	C1-C	-5.25	1.37	1.47
3	K	501	BEN	C1-C	-4.69	1.38	1.47
3	O	501	BEN	C1-C	-4.50	1.39	1.47
3	P	501	BEN	C1-C	-4.23	1.39	1.47
3	B	481	BEN	C1-C	-4.16	1.39	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	BEN	C1-C-N2	3.51	123.35	118.05
3	F	501	BEN	C1-C-N2	3.42	123.21	118.05
3	A	481	BEN	C1-C-N2	-3.11	113.35	118.05
3	J	501	BEN	C1-C-N2	3.04	122.63	118.05
3	H	501	BEN	C5-C6-C1	-3.00	116.79	120.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	501	BEN	N2-C-C1-C2
3	L	501	BEN	N2-C-C1-C6
3	B	481	BEN	N2-C-C1-C2
3	B	481	BEN	N2-C-C1-C6
3	D	501	BEN	N2-C-C1-C2

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	481	BEN	3	0
3	H	501	BEN	1	0
3	I	501	BEN	4	0
3	M	481	BEN	2	0
3	N	501	BEN	2	0
3	P	501	BEN	1	0
3	O	501	BEN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	501	BEN	3	0
3	F	501	BEN	1	0
3	D	501	BEN	2	0
3	L	501	BEN	3	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/223 (100%)	-0.21	0 100 100	19, 36, 55, 68	0
1	B	223/223 (100%)	-0.26	0 100 100	17, 36, 55, 68	0
1	C	223/223 (100%)	-0.30	0 100 100	25, 36, 55, 68	0
1	D	223/223 (100%)	-0.29	0 100 100	18, 36, 55, 68	0
1	E	223/223 (100%)	-0.31	0 100 100	18, 36, 55, 68	0
1	F	223/223 (100%)	-0.32	0 100 100	20, 36, 55, 68	1 (0%)
1	G	223/223 (100%)	-0.32	0 100 100	25, 36, 55, 68	0
1	H	223/223 (100%)	-0.29	0 100 100	21, 36, 55, 68	0
1	I	223/223 (100%)	-0.27	2 (0%) 84 76	25, 36, 55, 68	0
1	J	223/223 (100%)	-0.32	1 (0%) 92 89	25, 36, 55, 68	0
1	K	223/223 (100%)	-0.26	1 (0%) 92 89	24, 36, 55, 68	0
1	L	223/223 (100%)	-0.19	2 (0%) 84 76	25, 36, 55, 68	0
1	M	223/223 (100%)	-0.19	1 (0%) 92 89	19, 36, 55, 68	0
1	N	223/223 (100%)	-0.07	2 (0%) 84 76	25, 36, 55, 68	0
1	O	223/223 (100%)	-0.14	4 (1%) 68 56	25, 36, 58, 68	0
1	P	223/223 (100%)	-0.20	0 100 100	25, 36, 55, 68	0
All	All	3568/3568 (100%)	-0.24	13 (0%) 92 89	17, 36, 55, 68	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	79	ASN	3.1
1	O	149	THR	3.1
1	L	171	ALA	3.1
1	O	171	ALA	2.9
1	J	170	SER	2.5

## 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CA	N	480	1/1	0.90	0.13	30,30,30,30	1
3	BEN	M	481	9/9	0.94	0.24	19,21,24,25	0
3	BEN	P	501	9/9	0.94	0.23	57,57,57,57	0
3	BEN	O	501	9/9	0.95	0.26	33,35,36,36	0
3	BEN	L	501	9/9	0.95	0.23	35,36,37,38	0
3	BEN	I	501	9/9	0.96	0.26	33,35,37,38	0
2	CA	G	480	1/1	0.96	0.11	30,30,30,30	0
2	CA	O	480	1/1	0.96	0.08	30,30,30,30	0
3	BEN	A	481	9/9	0.96	0.18	19,21,24,25	0
3	BEN	H	501	9/9	0.96	0.20	22,24,25,26	0
4	CL	P	502	1/1	0.96	0.10	30,30,30,30	0
3	BEN	F	501	9/9	0.97	0.29	19,20,21,21	0
3	BEN	G	501	9/9	0.97	0.21	14,15,16,17	0
2	CA	M	480	1/1	0.97	0.10	30,30,30,30	0
2	CA	D	480	1/1	0.97	0.07	30,30,30,30	0
3	BEN	J	501	9/9	0.97	0.24	25,27,28,29	0
3	BEN	K	501	9/9	0.97	0.25	36,37,37,38	0
2	CA	B	480	1/1	0.97	0.06	30,30,30,30	0
2	CA	P	480	1/1	0.97	0.04	30,30,30,30	0
3	BEN	N	501	9/9	0.97	0.21	23,25,27,28	0
2	CA	K	480	1/1	0.97	0.09	30,30,30,30	0
3	BEN	B	481	9/9	0.97	0.18	20,21,23,24	0
3	BEN	E	501	9/9	0.97	0.18	15,17,21,21	0
2	CA	F	480	1/1	0.98	0.08	30,30,30,30	0
2	CA	C	480	1/1	0.98	0.14	30,30,30,30	0
2	CA	I	480	1/1	0.98	0.10	30,30,30,30	0
3	BEN	C	481	9/9	0.98	0.20	15,15,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BEN	D	501	9/9	0.98	0.24	17,19,20,20	0
4	CL	H	481	1/1	0.98	0.11	30,30,30,30	0
2	CA	J	480	1/1	0.98	0.06	30,30,30,30	0
2	CA	H	480	1/1	0.99	0.09	30,30,30,30	0
2	CA	L	480	1/1	0.99	0.05	30,30,30,30	0
4	CL	E	502	1/1	0.99	0.15	30,30,30,30	0
2	CA	A	480	1/1	0.99	0.05	30,30,30,30	0
2	CA	E	480	1/1	0.99	0.10	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.