



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:28 pm GMT

PDB ID : 2JET  
Title : CRYSTAL STRUCTURE OF A TRYPSIN-LIKE MUTANT (S189D, A226G) CHYMOTRYPSIN.  
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Deposited on : 2007-01-22  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

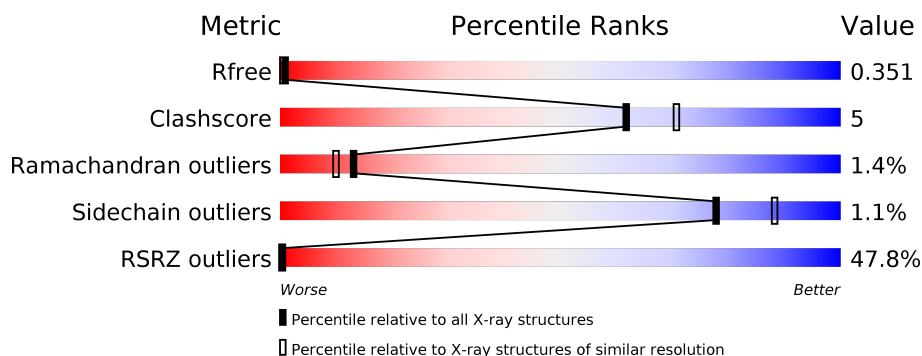
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 on the lower 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  $\leq 5\%$ . 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	15	
2	B	128	
3	C	99	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1767 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 CHYMOTRYPSINOGEN B CHAIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	12	Total	C	N	O	S	0	0	0
			85	54	14	16	1			

- Molecule 2 is a protein called CHYMOTRYPSINOGEN B CHAIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	19	0	0
			946	604	155	182	5			

- Molecule 3 is a protein called CHYMOTRYPSINOGEN B CHAIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	93	Total	C	N	O	S	2	0	0
			669	418	110	133	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	189	ASP	SER	ENGINEERED MUTATION	UNP P07338
C	226	GLY	ALA	ENGINEERED MUTATION	UNP P07338

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	37	Total	O	0	0
			37	37		
4	C	24	Total	O	0	0
			24	24		

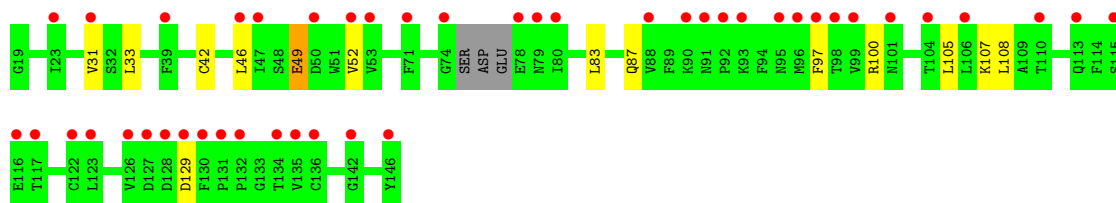
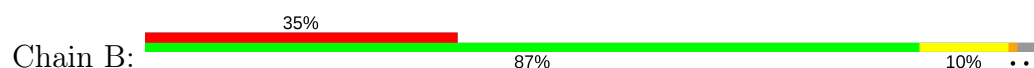
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

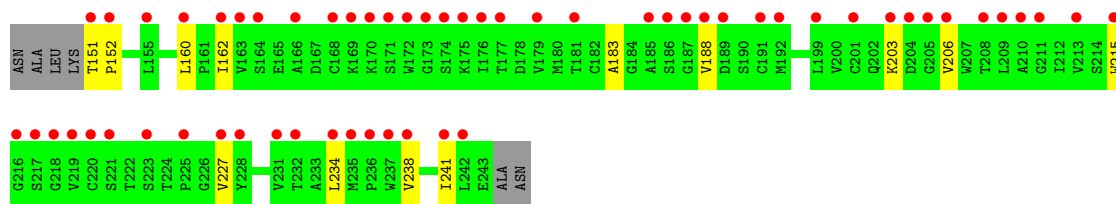
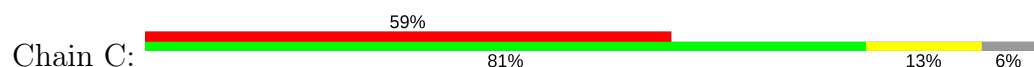
#### • Molecule 1: CHYMOTRYPSINOGEN B CHAIN A



#### • Molecule 2: CHYMOTRYPSINOGEN B CHAIN B



#### • Molecule 3: CHYMOTRYPSINOGEN B CHAIN C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	34.69Å 64.35Å 44.22Å 90.00° 102.09° 90.00°	Depositor
Resolution (Å)	43.23 – 2.20 35.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.23-2.20) 98.5 (35.89-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.276 , 0.334 0.284 , 0.351	Depositor DCC
$R_{free}$ test set	460 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	1767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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

### 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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/86	0.55	0/117
2	B	0.47	3/969 (0.3%)	0.65	5/1321 (0.4%)
3	C	0.31	0/682	0.49	0/929
All	All	0.40	3/1737 (0.2%)	0.59	5/2367 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	ARG	CB-CG	-6.83	1.34	1.52
2	B	129	ASP	CB-CG	6.68	1.65	1.51
2	B	49	GLU	CB-CG	-6.27	1.40	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	PHE	CB-CG-CD1	-10.30	113.59	120.80
2	B	97	PHE	CB-CG-CD2	8.98	127.09	120.80
2	B	129	ASP	CB-CG-OD2	-6.89	112.10	118.30
2	B	129	ASP	CB-CG-OD1	6.25	123.92	118.30
2	B	97	PHE	CA-CB-CG	5.55	127.21	113.90

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	85	0	91	0	0
2	B	946	0	909	12	1
3	C	669	0	658	9	1
4	A	6	0	0	0	0
4	B	37	0	0	0	0
4	C	24	0	0	0	0
All	All	1767	0	1658	17	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 5.

All (17) 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:B:46:LEU:HD12	2:B:52:VAL:HG22	1.62	0.80
2:B:105:LEU:CD1	3:C:241:ILE:HD11	2.24	0.68
2:B:105:LEU:HD12	3:C:241:ILE:HD11	1.80	0.63
2:B:31:VAL:HG11	2:B:46:LEU:HD13	1.81	0.63
2:B:31:VAL:CG1	2:B:46:LEU:HD13	2.31	0.61
2:B:105:LEU:HD11	3:C:238:VAL:HG13	1.83	0.60
2:B:31:VAL:HG11	2:B:46:LEU:CD1	2.35	0.56
2:B:87:GLN:HB2	2:B:107:LYS:HB3	1.92	0.52
2:B:83:LEU:HD13	2:B:108:LEU:HD13	1.98	0.44
3:C:151:THR:HA	3:C:152:PRO:HD2	1.92	0.43
3:C:215:TRP:CH2	3:C:227:VAL:HG21	2.54	0.42
3:C:162:ILE:HD13	3:C:183:ALA:HB2	2.02	0.42
2:B:105:LEU:HD13	3:C:241:ILE:HD11	2.01	0.41
2:B:33:LEU:HD12	2:B:42:CYS:HB3	2.01	0.41
3:C:234:LEU:O	3:C:238:VAL:HG23	2.21	0.41
3:C:203:LYS:O	3:C:206:VAL:HG12	2.21	0.40
2:B:31:VAL:HG13	2:B:46:LEU:HD13	2.03	0.40

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)
2:B:49:GLU:OE1	3:C:151:THR:N[1_455]	2.03	0.17

## 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 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	10/15 (67%)	8 (80%)	0	2 (20%)	0	0
2	B	121/128 (94%)	117 (97%)	4 (3%)	0	100	100
3	C	91/99 (92%)	83 (91%)	7 (8%)	1 (1%)	17	13
All	All	222/242 (92%)	208 (94%)	11 (5%)	3 (1%)	13	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	ALA
1	A	1	CYS
3	C	188	VAL

### 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	A	10/13 (77%)	9 (90%)	1 (10%)	9	8
2	B	104/108 (96%)	104 (100%)	0	100	100
3	C	75/79 (95%)	74 (99%)	1 (1%)	73	85
All	All	189/200 (94%)	187 (99%)	2 (1%)	78	88

All (2) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	1	CYS
3	C	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	B	101	ASN
3	C	239	GLN

### 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.

## 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, 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	12/15 (80%)	2.52	7 (58%)  	56, 56, 56, 57	0
2	B	125/128 (97%)	1.81	45 (36%)  	54, 55, 56, 57	4 (3%)
3	C	93/99 (93%)	2.72	58 (62%)  	55, 55, 56, 56	1 (1%)
All	All	230/242 (95%)	2.22	110 (47%)  	54, 55, 56, 57	5 (2%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	166	ALA	11.9
3	C	187	GLY	11.0
3	C	218	GLY	7.1
3	C	204	ASP	7.0
3	C	170	LYS	6.0
3	C	152	PRO	5.9
3	C	172	TRP	5.7
2	B	74	GLY	5.7
1	A	-1	GLN	5.7
2	B	146	TYR	5.5
3	C	221	SER	5.1
3	C	188	VAL	5.1
3	C	201	CYS	5.0
3	C	171	SER	5.0
2	B	135	VAL	4.8
3	C	205	GLY	4.6
3	C	238	VAL	4.5
2	B	78	GLU	4.5
3	C	215	TRP	4.5
1	A	0	ALA	4.4
3	C	186	SER	4.4
2	B	39	PHE	4.3
3	C	163	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	185	ALA	4.2
2	B	96	MET	4.2
2	B	95	ASN	4.0
3	C	203	LYS	3.8
3	C	242	LEU	3.8
2	B	126	VAL	3.7
3	C	225	PRO	3.7
3	C	241	ILE	3.7
3	C	175	LYS	3.5
3	C	219	VAL	3.5
2	B	127	ASP	3.4
1	A	1	CYS	3.4
2	B	88	VAL	3.4
2	B	79	ASN	3.3
2	B	99	VAL	3.2
2	B	129	ASP	3.2
2	B	131	PRO	3.2
1	A	6	ILE	3.2
2	B	134	THR	3.2
2	B	101	ASN	3.2
2	B	53	VAL	3.1
3	C	151	THR	3.1
3	C	217	SER	3.1
2	B	97	PHE	3.0
2	B	92	PRO	2.9
3	C	174	SER	2.9
3	C	206	VAL	2.9
3	C	169	LYS	2.9
3	C	199	LEU	2.8
2	B	23	ILE	2.7
2	B	98	THR	2.7
3	C	155	LEU	2.6
2	B	113	GLN	2.6
2	B	128	ASP	2.6
3	C	176	ILE	2.6
3	C	192	MET	2.6
3	C	232	THR	2.6
2	B	132	PRO	2.5
3	C	173	GLY	2.5
3	C	181	THR	2.5
1	A	3	VAL	2.5
2	B	104	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	123	LEU	2.5
3	C	237	TRP	2.5
3	C	236	PRO	2.5
3	C	227	VAL	2.4
3	C	177	THR	2.4
2	B	80	ILE	2.4
3	C	160	LEU	2.4
3	C	191	CYS	2.4
2	B	130	PHE	2.4
3	C	168	CYS	2.4
3	C	211	GLY	2.4
3	C	179	VAL	2.4
1	A	2	GLY	2.3
3	C	209	LEU	2.3
2	B	93	LYS	2.3
3	C	223	SER	2.3
1	A	7	GLN	2.3
3	C	213	VAL	2.3
2	B	116	GLU	2.3
3	C	235	MET	2.2
2	B	122	CYS	2.2
3	C	162	ILE	2.2
2	B	91	ASN	2.2
3	C	234	LEU	2.2
2	B	71	PHE	2.2
3	C	220	CYS	2.2
2	B	90	LYS	2.2
2	B	115	SER	2.2
3	C	231	VAL	2.2
3	C	228	TYR	2.1
3	C	210	ALA	2.1
2	B	47	ILE	2.1
2	B	46	LEU	2.1
2	B	52	VAL	2.1
3	C	216	GLY	2.1
2	B	110	THR	2.1
3	C	164	SER	2.1
2	B	106	LEU	2.1
2	B	142	GLY	2.1
2	B	117	THR	2.1
2	B	31	VAL	2.1
3	C	208	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	189	ASP	2.1
2	B	136	CYS	2.1
2	B	50	ASP	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.