



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:01 AM UTC

PDB ID : 2JET / pdb_00002jet
Title : Crystal structure of a trypsin-like mutant (S189D , A226G) chymotrypsin.
Authors : Jelinek, B.; Katona, G.; Fodor, K.; Venekei, I.; Graf, L.
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

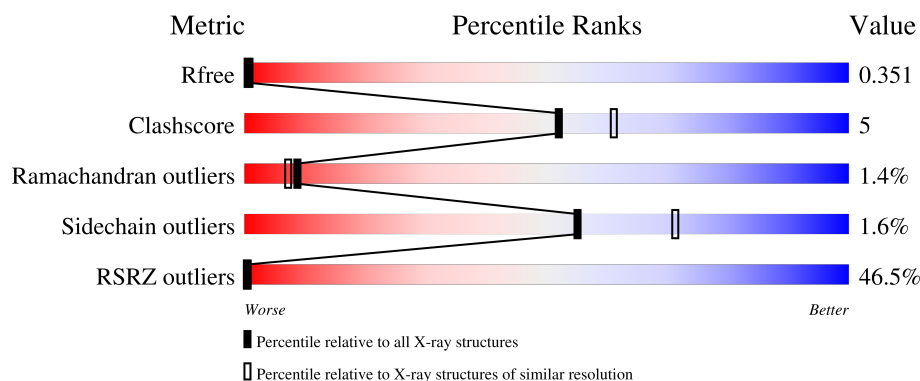
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of 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	15	67% 67% 7% 7% 20%
2	B	128	27% 87% 11% .
3	C	99	63% 81% 12% . 6%

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

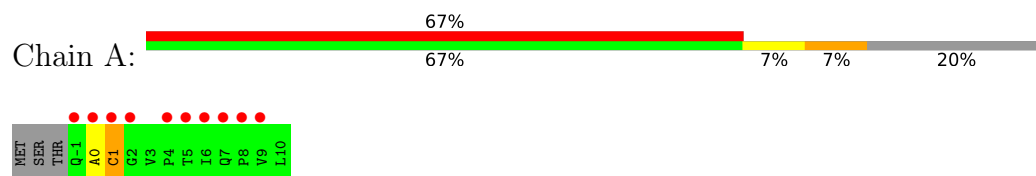
- Molecule 4 is water.

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		

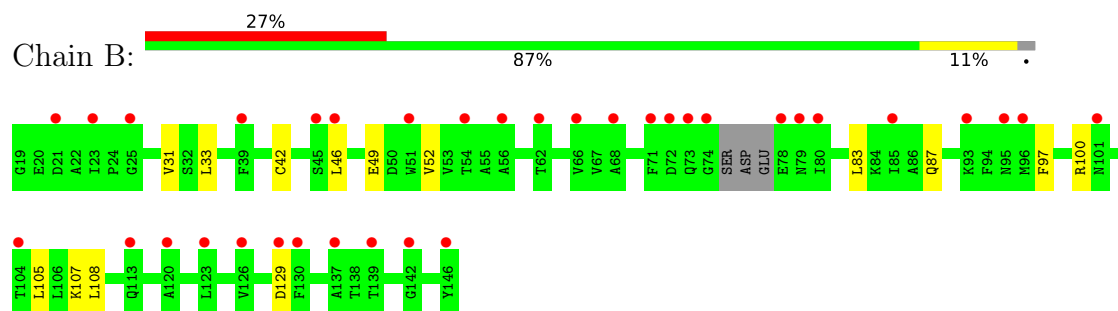
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

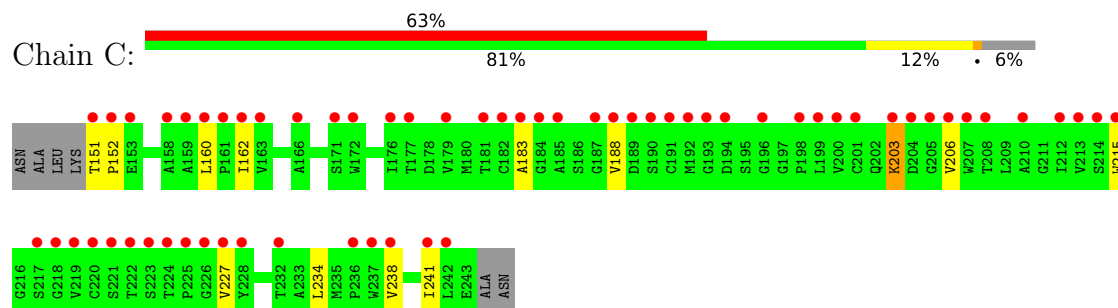
• Molecule 1: CHYMOTRYPSINOGEN B CHAIN A



• 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, α , β , γ	34.69Å 64.35Å 44.22Å 90.00° 102.09° 90.00°	Depositor
Resolution (Å)	43.23 – 2.20 43.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.23-2.20) 98.5 (43.23-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	1767	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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](#)

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	0.46	0/86	0.75	0/117
2	B	0.49	2/969 (0.2%)	0.73	1/1321 (0.1%)
3	C	0.44	0/682	0.70	0/929
All	All	0.47	2/1737 (0.1%)	0.72	1/2367 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	ARG	CB-CG	-6.11	1.34	1.52
2	B	129	ASP	CB-CG	5.49	1.65	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	PHE	CA-CB-CG	13.41	127.21	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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 [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	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%)	11	10
All	All	222/242 (92%)	208 (94%)	11 (5%)	3 (1%)	9	7

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 [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	10/13 (77%)	9 (90%)	1 (10%)	7	7
2	B	104/108 (96%)	104 (100%)	0	100	100
3	C	75/79 (95%)	73 (97%)	2 (3%)	39	53
All	All	189/200 (94%)	186 (98%)	3 (2%)	55	71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
3	C	160	LEU
3	C	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	B	73	GLN
3	C	156	GLN
3	C	202	GLN
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 oligosaccharides 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, 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	12/15 (80%)	2.66	10 (83%)  	56, 56, 56, 57	0
2	B	125/128 (97%)	1.75	35 (28%)  	25, 55, 56, 57	4 (3%)
3	C	93/99 (93%)	2.39	62 (66%)  	43, 55, 56, 56	1 (1%)
All	All	230/242 (95%)	2.05	107 (46%)  	25, 55, 56, 57	5 (2%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	5.0
2	B	39	PHE	4.9
3	C	152	PRO	4.9
3	C	187	GLY	4.7
3	C	160	LEU	4.6
2	B	146	TYR	4.5
2	B	74	GLY	4.4
3	C	166	ALA	4.3
3	C	207	TRP	4.3
3	C	205	GLY	3.9
3	C	215	TRP	3.9
1	A	1	CYS	3.8
3	C	172	TRP	3.6
3	C	221	SER	3.6
3	C	204	ASP	3.5
3	C	181	THR	3.4
3	C	183	ALA	3.4
2	B	101	ASN	3.4
3	C	192	MET	3.3
3	C	196	GLY	3.3
2	B	71	PHE	3.3
3	C	188	VAL	3.3
3	C	200	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	227	VAL	3.3
3	C	194	ASP	3.2
3	C	185	ALA	3.2
3	C	228	TYR	3.2
3	C	163	VAL	3.2
3	C	199	LEU	3.1
1	A	6	ILE	3.1
2	B	23	ILE	3.1
3	C	158	ALA	2.9
3	C	206	VAL	2.9
3	C	214	SER	2.9
1	A	-1	GLN	2.9
3	C	241	ILE	2.9
2	B	96	MET	2.9
2	B	142	GLY	2.8
3	C	213	VAL	2.8
3	C	191	CYS	2.8
3	C	223	SER	2.8
3	C	225	PRO	2.8
3	C	159	ALA	2.8
2	B	126	VAL	2.7
2	B	46	LEU	2.6
2	B	68	ALA	2.6
2	B	139	THR	2.6
3	C	210	ALA	2.6
2	B	129	ASP	2.6
1	A	8	PRO	2.6
2	B	95	ASN	2.6
1	A	5	THR	2.6
2	B	62	THR	2.6
3	C	232	THR	2.6
3	C	220	CYS	2.5
2	B	78	GLU	2.5
3	C	219	VAL	2.5
3	C	222	THR	2.4
2	B	130	PHE	2.4
2	B	51	TRP	2.4
2	B	66	VAL	2.4
2	B	85	ILE	2.4
3	C	162	ILE	2.4
1	A	2	GLY	2.4
3	C	193	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	208	THR	2.4
3	C	176	ILE	2.4
3	C	212	ILE	2.4
3	C	226	GLY	2.3
1	A	9	VAL	2.3
1	A	7	GLN	2.3
2	B	137	ALA	2.3
3	C	242	LEU	2.3
3	C	184	GLY	2.3
3	C	190	SER	2.3
3	C	179	VAL	2.3
3	C	236	PRO	2.3
3	C	177	THR	2.3
2	B	123	LEU	2.2
3	C	201	CYS	2.2
2	B	73	GLN	2.2
3	C	153	GLU	2.2
3	C	198	PRO	2.2
3	C	218	GLY	2.2
2	B	54	THR	2.2
2	B	120	ALA	2.2
3	C	224	THR	2.2
2	B	25	GLY	2.2
3	C	151	THR	2.2
2	B	80	ILE	2.2
3	C	161	PRO	2.2
2	B	21	ASP	2.1
3	C	238	VAL	2.1
3	C	203	LYS	2.1
2	B	45	SER	2.1
3	C	217	SER	2.1
2	B	79	ASN	2.1
3	C	189	ASP	2.1
3	C	237	TRP	2.1
2	B	113	GLN	2.1
3	C	171	SER	2.1
2	B	56	ALA	2.1
2	B	93	LYS	2.1
3	C	182	CYS	2.0
2	B	72	ASP	2.0
1	A	4	PRO	2.0
2	B	104	THR	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 oligosaccharides 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.