



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 11:07 PM UTC

PDB ID : 1TO1 / pdb_00001to1
Title : crystal structure of the complex of subtilisin BPN' with chymotrypsin inhibitor 2 Y61A mutant
Authors : Radisky, E.S.; Kwan, G.; Karen Lu, C.J.; Koshland Jr., D.E.
Deposited on : 2004-06-11
Resolution : 1.68 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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

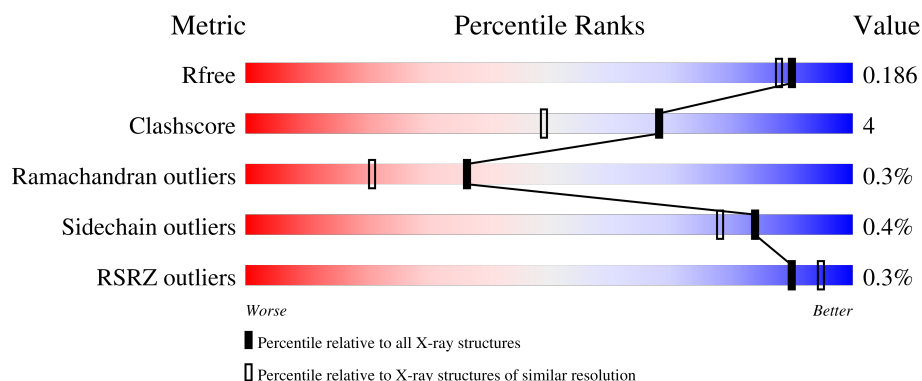
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

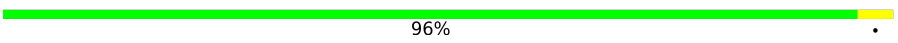
The reported resolution of this entry is 1.68 Å.

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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	E	281	 96%
2	I	64	 91% 8%

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
5	CIT	E	512	-	-	X	-
5	CIT	E	513	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3121 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 Subtilisin BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	281	Total	C	N	O	S	0	15	0
			2035	1254	360	416	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	276	HIS	-	expression tag	UNP P00782
E	277	HIS	-	expression tag	UNP P00782
E	278	HIS	-	expression tag	UNP P00782
E	279	HIS	-	expression tag	UNP P00782
E	280	HIS	-	expression tag	UNP P00782
E	281	HIS	-	expression tag	UNP P00782

- Molecule 2 is a protein called chymotrypsin inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	64	Total	C	N	O	S	0	3	1
			510	325	91	93	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	MET	-	initiating methionine	UNP Q40059
I	61	ALA	TYR	engineered mutation	UNP Q40059

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

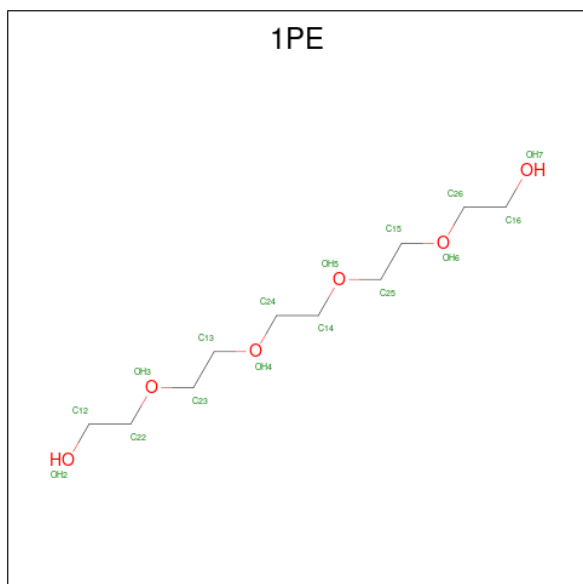
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			13	6	7		
5	E	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			11	7	4		
6	E	1	Total	C	O	0	0
			16	10	6		
6	E	1	Total	C	O	0	0
			13	9	4		
6	I	1	Total	C	O	0	0
			7	5	2		

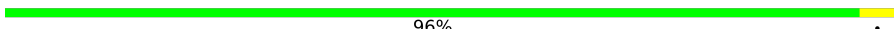
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	396	Total	O	0	0
			396	396		
7	I	105	Total	O	0	0
			105	105		

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: Subtilisin BPN'

Chain E:  96% .



- Molecule 2: chymotrypsin inhibitor 2

Chain I:  91% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.09Å 94.09Å 185.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.65 – 1.68 81.48 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (81.65-1.68) 99.3 (81.48-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.155 , 0.182 0.161 , 0.186	Depositor DCC
R_{free} test set	2786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3121	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: CIT, 1PE, NA, CA

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	E	0.99	1/2154 (0.0%)	0.98	1/2936 (0.0%)
2	I	1.01	1/531 (0.2%)	0.96	0/717
All	All	0.99	2/2685 (0.1%)	0.98	1/3653 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	59	MET	SD-CE	-6.19	1.64	1.79
1	E	85	ALA	CA-CB	5.54	1.59	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	186	ARG	CG-CD-NE	-5.04	100.90	112.00

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	E	2035	0	1968	6	0
2	I	510	0	549	4	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
5	E	26	0	10	8	0
6	E	40	0	48	3	1
6	I	7	0	6	2	0
7	E	396	0	0	1	0
7	I	105	0	0	2	0
All	All	3121	0	2581	19	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 4.

The worst 5 of 19 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:E:99:ASP:HB2	2:I:49[A]:ILE:HD11	1.76	0.68
5:E:512:CIT:C6	5:E:513:CIT:O5	2.43	0.66
2:I:62[A]:ARG:NH2	2:I:64[A]:ASP:OD2	2.31	0.63
2:I:37:LYS:NZ	7:I:541:HOH:O	2.29	0.60
5:E:512:CIT:O6	5:E:513:CIT:O5	2.28	0.51

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)
6:E:514:1PE:C26	6:E:514:1PE:C26[9_765]	1.90	0.30

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	E	295/281 (105%)	286 (97%)	8 (3%)	1 (0%)	36 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	65/64 (102%)	64 (98%)	1 (2%)	0	100	100
All	All	360/345 (104%)	350 (97%)	9 (2%)	1 (0%)	36	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	63	SER

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	E	227/211 (108%)	227 (100%)	0	100	100
2	I	58/56 (104%)	56 (97%)	2 (3%)	32	8
All	All	285/267 (107%)	283 (99%)	2 (1%)	84	62

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

Mol	Chain	Res	Type
2	I	49[A]	ILE
2	I	49[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	252	ASN
1	E	275	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
6	1PE	E	514	-	10,10,15	0.63	0	9,9,14	0.61	0
6	1PE	I	516	-	6,6,15	0.63	0	5,5,14	0.47	0
6	1PE	E	517	-	12,12,15	0.62	0	11,11,14	0.41	0
5	CIT	E	513	-	12,12,12	1.48	3 (25%)	17,17,17	2.14	6 (35%)
6	1PE	E	515	-	15,15,15	0.45	0	14,14,14	0.41	0
5	CIT	E	512	-	12,12,12	3.86	4 (33%)	17,17,17	4.19	8 (47%)

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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	E	514	-	-	1/8/8/13	-
6	1PE	I	516	-	-	2/4/4/13	-
6	1PE	E	517	-	-	5/10/10/13	-
5	CIT	E	513	-	-	3/16/16/16	-
6	1PE	E	515	-	-	1/13/13/13	-
5	CIT	E	512	-	-	2/16/16/16	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	512	CIT	C3-C6	-10.96	1.42	1.53
5	E	512	CIT	O7-C3	5.66	1.54	1.43
5	E	512	CIT	O5-C6	3.27	1.32	1.22
5	E	512	CIT	C4-C3	2.77	1.57	1.54
5	E	513	CIT	C3-C6	-2.59	1.50	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	512	CIT	O7-C3-C6	-12.97	90.56	108.96
5	E	512	CIT	O7-C3-C4	6.09	123.27	109.38
5	E	512	CIT	O7-C3-C2	5.88	122.78	109.38
5	E	513	CIT	O6-C6-C3	4.92	122.57	113.14
5	E	513	CIT	O7-C3-C6	-3.95	103.35	108.96

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	513	CIT	C1-C2-C3-O7
5	E	513	CIT	C1-C2-C3-C6
6	E	517	1PE	OH5-C14-C24-OH4
5	E	513	CIT	C1-C2-C3-C4
6	I	516	1PE	OH6-C15-C25-OH5

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	514	1PE	0	1
6	I	516	1PE	2	0
6	E	517	1PE	2	0
5	E	513	CIT	6	0
6	E	515	1PE	1	0
5	E	512	CIT	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	E	281/281 (100%)	-0.75	1 (0%) 88 93	9, 14, 24, 31	14 (4%)
2	I	64/64 (100%)	-0.48	0 100 100	13, 17, 30, 37	3 (4%)
All	All	345/345 (100%)	-0.70	1 (0%) 90 95	9, 15, 26, 37	17 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	277	HIS	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](#)

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(Å ²)	Q<0.9
6	1PE	I	516	7/16	0.61	0.21	57,57,58,59	0
5	CIT	E	513	13/13	0.69	0.21	25,28,31,32	13
6	1PE	E	517	13/16	0.71	0.18	49,53,64,64	0
6	1PE	E	514	11/16	0.90	0.12	23,26,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	E	515	16/16	0.90	0.11	38,44,57,57	0
5	CIT	E	512	13/13	0.93	0.08	17,20,24,25	0
4	NA	E	511	1/1	0.98	0.04	18,18,18,18	0
3	CA	E	510	1/1	1.00	0.09	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.