



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:27 PM GMT

PDB ID : 1AVW
Title : COMPLEX PORCINE PANCREATIC TRYPSIN/SOYBEAN TRYPSIN INHIBITOR, ORTHORHOMBIC CRYSTAL FORM
Authors : Song, H.K.; Suh, S.W.
Deposited on : 1997-09-21
Resolution : 1.75 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

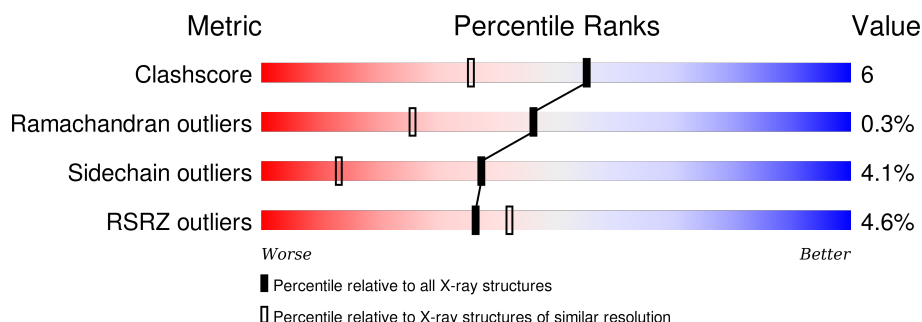
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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. 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	
2	B	177	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3042 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1631	1015	281	321	14			

- Molecule 2 is a protein called TRYPSIN INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1268	806	218	238	6			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	0
			99	99		
4	B	43	Total	O	0	0
			43	43		

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 errors 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.

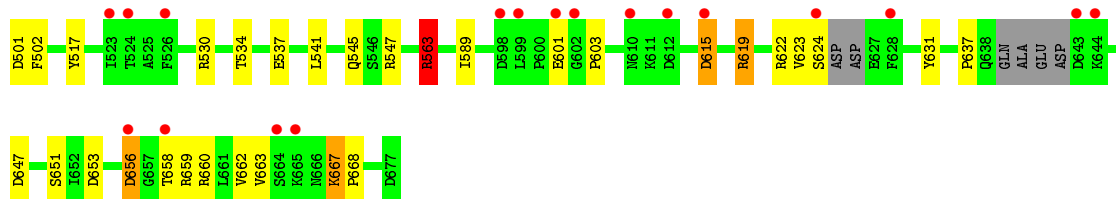
• Molecule 1: TRYPSIN

Chain A:  89% 9%



• Molecule 2: TRYPSIN INHIBITOR

Chain B:  10% 79% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.91Å 62.33Å 151.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.75 48.13 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.0 (8.00-1.75) 90.0 (48.13-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.75Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.189 , 0.214 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52626 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3042	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.43	0/1663	0.56	0/2260
2	B	0.44	0/1293	0.58	1/1748 (0.1%)
All	All	0.43	0/2956	0.57	1/4008 (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	A	0	1
2	B	0	5
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	563	ARG	NE-CZ-NH2	-8.19	116.21	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	ARG	Sidechain
2	B	517	TYR	Sidechain
2	B	530	ARG	Sidechain
2	B	563	ARG	Sidechain
2	B	631	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	667	LYS	Peptide

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	1631	0	1575	19	0
2	B	1268	0	1216	17	0
3	A	1	0	0	0	0
4	A	99	0	0	3	0
4	B	43	0	0	0	0
All	All	3042	0	2791	36	0

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 6.

All (36) 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:A:48:ASN:HD22	1:A:50:GLN:H	1.26	0.83
1:A:125:ARG:H	1:A:204:GLN:HE22	1.26	0.81
2:B:545:GLN:HE21	2:B:659:ARG:HE	1.30	0.76
1:A:125:ARG:H	1:A:204:GLN:NE2	1.86	0.74
2:B:545:GLN:NE2	2:B:659:ARG:HE	1.86	0.73
1:A:48:ASN:ND2	1:A:50:GLN:H	1.88	0.71
2:B:656:ASP:HB3	2:B:658:THR:H	1.68	0.59
1:A:87:LYS:NZ	4:A:871:HOH:O	2.31	0.59
2:B:647:ASP:HB3	2:B:668:PRO:HB3	1.84	0.58
2:B:619:ARG:CB	2:B:619:ARG:HH11	2.17	0.58
1:A:45:SER:OG	1:A:198:PRO:HB3	2.03	0.57
2:B:653:ASP:HA	2:B:660:ARG:NH2	2.20	0.56
4:A:804:HOH:O	2:B:563:ARG:HD3	2.06	0.56
2:B:619:ARG:HH11	2:B:619:ARG:HB2	1.72	0.55
1:A:115:ASN:HD22	1:A:117:ARG:H	1.56	0.53
1:A:66:ARG:HD2	1:A:82:PHE:CD1	2.44	0.52
2:B:501:ASP:CG	2:B:502:PHE:H	2.14	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:ASP:HA	2:B:660:ARG:HH21	1.78	0.48
2:B:615:ASP:O	2:B:637:PRO:HA	2.14	0.47
1:A:192:GLN:HB2	4:A:831:HOH:O	2.15	0.46
1:A:115:ASN:HD22	1:A:117:ARG:N	2.15	0.45
2:B:651:SER:HB2	2:B:662:VAL:HG21	1.98	0.45
1:A:124:PRO:HA	1:A:204:GLN:NE2	2.33	0.44
1:A:125:ARG:N	1:A:204:GLN:NE2	2.60	0.44
1:A:145:LYS:HD2	1:A:150:SER:HB2	2.00	0.44
1:A:115:ASN:ND2	1:A:118:VAL:H	2.16	0.44
2:B:501:ASP:CG	2:B:502:PHE:N	2.71	0.43
1:A:27:ILE:HD11	1:A:137:LEU:HD21	2.00	0.43
1:A:115:ASN:ND2	1:A:117:ARG:H	2.16	0.42
2:B:537:GLU:HG2	2:B:541:LEU:HD12	2.01	0.42
2:B:603:PRO:HG2	2:B:663:VAL:HB	2.02	0.42
1:A:67:LEU:HD12	1:A:67:LEU:N	2.34	0.42
2:B:622:ARG:HH11	2:B:624:SER:C	2.23	0.42
1:A:66:ARG:HD2	1:A:82:PHE:CE1	2.56	0.41
2:B:623:VAL:HG23	2:B:624:SER:N	2.36	0.41
1:A:158:LEU:HD11	1:A:188:LYS:HB3	2.03	0.41

There are no symmetry-related clashes.

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%)	216 (98%)	5 (2%)	0	100	100
2	B	165/177 (93%)	157 (95%)	7 (4%)	1 (1%)	30	12
All	All	386/400 (96%)	373 (97%)	12 (3%)	1 (0%)	46	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	667	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	181/183 (99%)	175 (97%)	6 (3%)	45	19
2	B	133/153 (87%)	126 (95%)	7 (5%)	28	7
All	All	314/336 (94%)	301 (96%)	13 (4%)	37	13

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	66	ARG
1	A	114	LEU
1	A	115	ASN
1	A	167	SER
1	A	195	SER
2	B	534	THR
2	B	547	ARG
2	B	589	ILE
2	B	601	GLU
2	B	615	ASP
2	B	619	ARG
2	B	656	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	ASN
1	A	84	ASN
1	A	101	ASN
1	A	115	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	175	GLN
1	A	204	GLN
1	A	210	GLN
1	A	223	ASN
1	A	239	GLN
2	B	545	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - 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	223/223 (100%)	-0.16	0 100 100	10, 19, 35, 60	0
2	B	171/177 (96%)	0.43	18 (10%) 8 11	12, 28, 82, 101	0
All	All	394/400 (98%)	0.10	18 (4%) 36 42	10, 23, 68, 101	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	628	PHE	6.4
2	B	602	GLY	4.4
2	B	598	ASP	3.7
2	B	599	LEU	3.6
2	B	643	ASP	3.3
2	B	601	GLU	3.3
2	B	524	THR	3.2
2	B	656	ASP	2.8
2	B	665	LYS	2.7
2	B	526	PHE	2.5
2	B	664	SER	2.4
2	B	615	ASP	2.4
2	B	644	LYS	2.3
2	B	610	ASN	2.3
2	B	612	ASP	2.2
2	B	624	SER	2.2
2	B	658	THR	2.2
2	B	523	ILE	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	A	700	1/1	0.99	0.07	-1.38	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.