Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 – 06:14 pm GMT

PDB ID	:	2JEW
Title	:	Crystal structure of ((2S)-5-amino-2-((1-n-propyl-1H-imidazol-4-yl) methyl)pentanoic acid) UK396,082 a TAFIa inhibitor, Bound to Activated Porcine Pancreatic carboxypeptidaseB
Authors	:	Brown, D.G.; Moore, R.S.
Deposited on	:	2007-01-24
Resolution	:	1.40 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 (i) 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 (i)) were used in the production of this report:

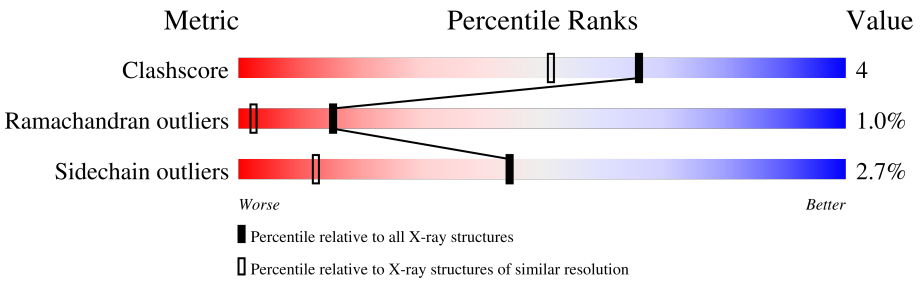
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.40 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	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	88% 8% • ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2759 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.

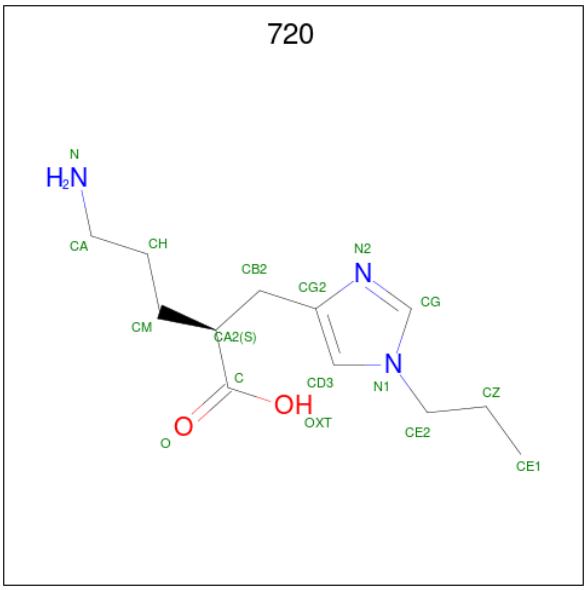
- Molecule 1 is a protein called CARBOXYPEPTIDASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2436	1560	397	467	12	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is (2S)-5-AMINO-2-[(1-PROPYL-1H-IMIDAZOL-4-YL)METHYL]PENTANOIC ACID (three-letter code: 720) (formula: $C_{12}H_{21}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	12	3	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	304	304	304	0	0

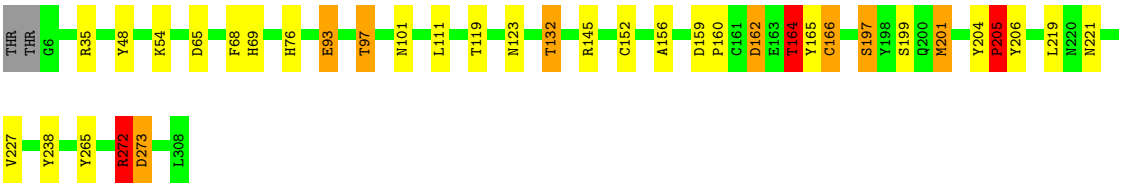
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

• Molecule 1: CARBOXYPEPTIDASE B

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.09Å 84.09Å 92.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 1.40	Depositor
% Data completeness (in resolution range)	99.8 (29.00-1.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 4.0.2	Depositor
R, R_{free}	0.190 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2759	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

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: 720, ZN

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	0.59	1/2505 (0.0%)	1.07	16/3408 (0.5%)

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	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	ASN	C-N	9.18	1.55	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	PRO	O-C-N	-9.76	107.09	122.70
1	A	197	SER	O-C-N	-9.57	107.39	122.70
1	A	272	ARG	O-C-N	-9.25	107.90	122.70
1	A	162	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	164	THR	N-CA-CB	-7.76	95.55	110.30
1	A	201	MET	CA-CB-CG	7.40	125.88	113.30
1	A	159	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	132	THR	N-CA-CB	-6.91	97.18	110.30
1	A	69	HIS	CG-ND1-CE1	6.21	116.90	108.20
1	A	206	TYR	N-CA-CB	5.64	120.76	110.60
1	A	162	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	48	TYR	CB-CG-CD1	-5.42	117.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	SER	N-CA-CB	5.29	118.44	110.50
1	A	35	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	A	265	TYR	CB-CG-CD1	-5.26	117.85	121.00
1	A	273	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	SER	Mainchain,Peptide
1	A	205	PRO	Mainchain,Peptide
1	A	272	ARG	Mainchain,Peptide

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	2436	0	2319	18	0
2	A	2	0	0	0	0
3	A	17	0	20	0	0
4	A	304	0	0	4	0
All	All	2759	0	2339	18	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 4.

All (18) 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:156:ALA:HB1	1:A:166:CYS:SG	2.05	0.96
1:A:152:CYS:HG	1:A:166:CYS:HG	1.24	0.85
1:A:76:HIS:H	1:A:76:HIS:CD2	2.10	0.69
1:A:65:ASP:HB2	4:A:2085:HOH:O	2.05	0.56
1:A:93:GLU:O	1:A:97:THR:HG22	2.06	0.55
1:A:76:HIS:H	1:A:76:HIS:HD2	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG21	4:A:2165:HOH:O	2.07	0.54
1:A:54:LYS:HD3	1:A:101:ASN:ND2	2.24	0.52
1:A:156:ALA:CB	1:A:166:CYS:SG	2.89	0.50
1:A:76:HIS:CD2	1:A:76:HIS:N	2.79	0.49
1:A:145:ARG:O	1:A:166:CYS:HB3	2.13	0.49
1:A:227:VAL:HG13	1:A:238:TYR:HB2	1.96	0.47
1:A:160:PRO:HA	1:A:165:TYR:CG	2.52	0.43
1:A:68:PHE:CE1	1:A:111:LEU:HD22	2.55	0.42
1:A:162:ASP:HB3	4:A:2171:HOH:O	2.19	0.42
1:A:111:LEU:HB2	4:A:2085:HOH:O	2.20	0.40
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.51	0.40
1:A:119:THR:HA	1:A:123:ASN:O	2.22	0.40

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	302/306 (99%)	290 (96%)	9 (3%)	3 (1%)	15 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	A	272	ARG
1	A	273	ASP

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	257/259 (99%)	250 (97%)	7 (3%)	44 13

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	97	THR
1	A	132	THR
1	A	164	THR
1	A	166	CYS
1	A	201	MET
1	A	219	LEU

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

Mol	Chain	Res	Type
1	A	24	GLN
1	A	46	ASN
1	A	76	HIS
1	A	101	ASN
1	A	112	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	720	A	1310	2	15,17,17	2.12	2 (13%)	16,21,21	1.58	4 (25%)

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
3	720	A	1310	2	-	0/14/15/15	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1310	720	CG-N2	-6.17	1.24	1.35
3	A	1310	720	CD3-N1	-4.00	1.32	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1310	720	CD3-N1-CG	3.95	111.99	108.22
3	A	1310	720	CM-CA2-C	2.20	116.01	111.01
3	A	1310	720	CG2-CD3-N1	2.09	110.07	107.88
3	A	1310	720	CB2-CG2-CD3	2.03	132.12	127.95

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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.