



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

PDB ID : 1KXV
Title : Camelid VHH Domains in Complex with Porcine Pancreatic alpha-Amylase
Authors : Desmyter, A.; Spinelli, S.; Payan, F.; Lauwereys, M.; Wyns, L.; Muyldermans, S.; Cambillau, C.
Deposited on : 2002-02-01
Resolution : 1.60 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
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

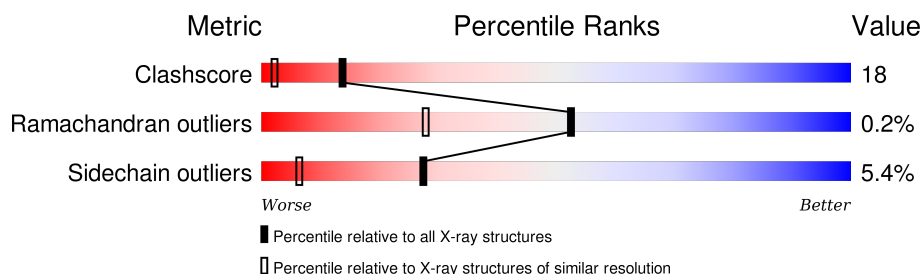
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	496	 77% 19% •
1	B	496	 76% 19% •
2	C	121	 82% 15% •••
2	D	121	 72% 18% 8% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10951 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 ALPHA-AMYLASE, PANCREATIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3900	2465	684	730	21			
1	B	496	Total	C	N	O	S	0	0	0
			3894	2459	685	729	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	LYS	GLN	SEE REMARK 999	UNP P00690
A	310	SER	ALA	SEE REMARK 999	UNP P00690
A	323	ILE	VAL	SEE REMARK 999	UNP P00690
A	404	GLN	GLU	SEE REMARK 999	UNP P00690
B	243	LYS	GLN	SEE REMARK 999	UNP P00690
B	310	SER	ALA	SEE REMARK 999	UNP P00690
B	323	ILE	VAL	SEE REMARK 999	UNP P00690
B	404	GLN	GLU	SEE REMARK 999	UNP P00690

- Molecule 2 is a protein called CAMELID VHH DOMAIN CAB10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	119	Total	C	N	O	S	0	0	0
			882	548	152	175	7			
2	D	121	Total	C	N	O	S	0	0	0
			898	556	155	180	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	590	Total	O	0	0
			590	590		
3	B	484	Total	O	0	0
			484	484		

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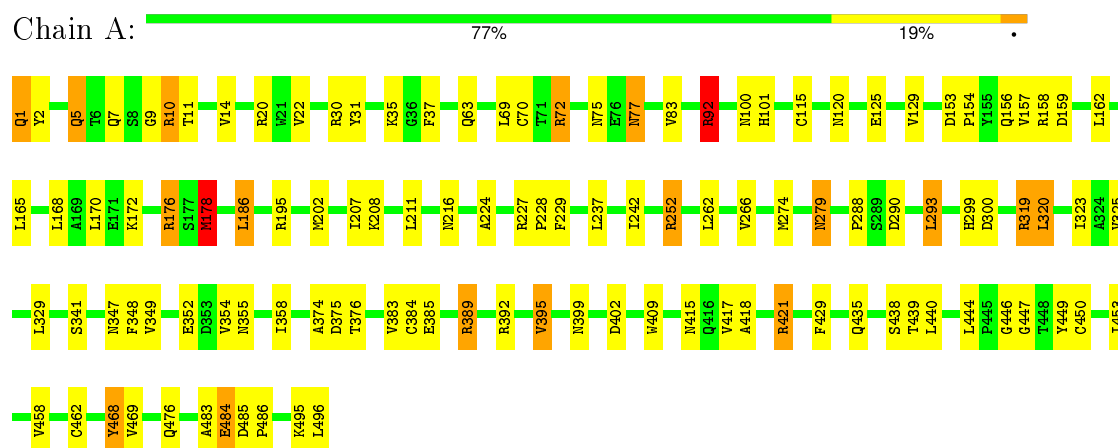
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	147	Total 147	O 147	0	0
3	D	156	Total 156	O 156	0	0

3 Residue-property plots

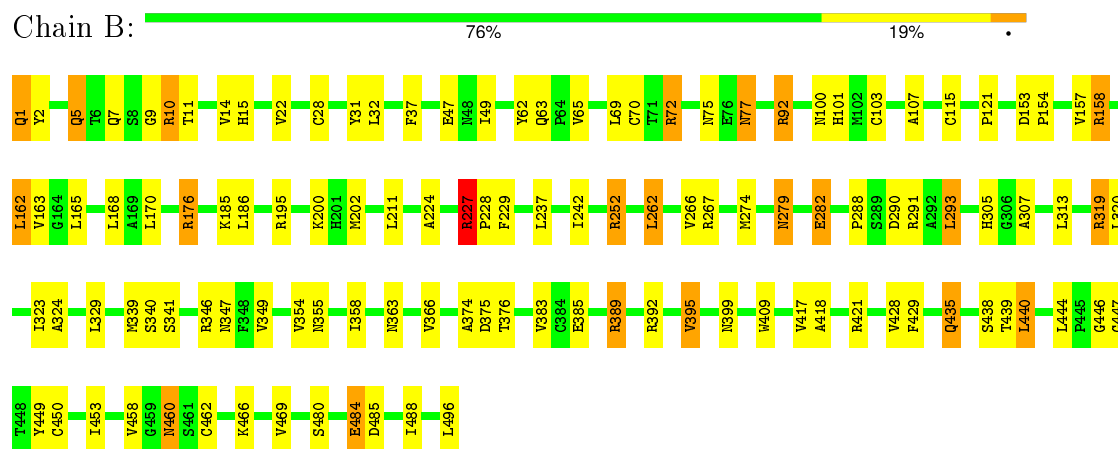
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

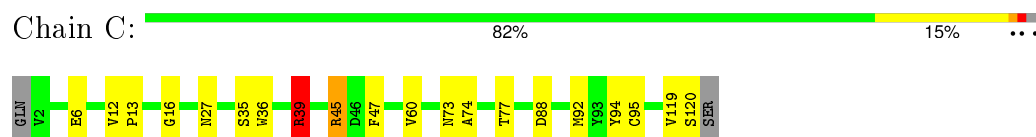
• Molecule 1: ALPHA-AMYLASE, PANCREATIC



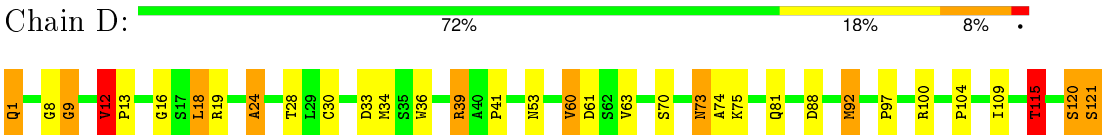
• Molecule 1: ALPHA-AMYLASE, PANCREATIC



• Molecule 2: CAMELID VHH DOMAIN CAB10



● Molecule 2: CAMELID VHH DOMAIN CAB10



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.57 Å 60.99 Å 107.33 Å 98.78° 100.88° 101.14°	Depositor
Resolution (Å)	29.34 – 1.60	Depositor
% Data completeness (in resolution range)	95.1 (29.34-1.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.205 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10951	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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	0.93	2/4010 (0.0%)	1.34	35/5450 (0.6%)
1	B	0.88	3/4003 (0.1%)	1.16	25/5439 (0.5%)
2	C	0.82	0/901	1.06	3/1225 (0.2%)
2	D	1.67	5/917 (0.5%)	1.56	18/1245 (1.4%)
All	All	0.99	10/9831 (0.1%)	1.27	81/13359 (0.6%)

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	C	0	2
All	All	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	121	SER	C-OXT	33.39	1.86	1.23
2	D	8	GLY	C-N	-23.54	0.90	1.33
2	D	1	GLN	C-N	-6.71	1.18	1.34
2	D	121	SER	N-CA	5.68	1.57	1.46
1	B	421	ARG	CD-NE	-5.67	1.36	1.46

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	60	VAL	CG1-CB-CG2	21.17	144.77	110.90
1	A	195	ARG	NE-CZ-NH1	-21.02	109.79	120.30
1	A	195	ARG	NE-CZ-NH2	20.61	130.61	120.30
2	D	121	SER	N-CA-CB	20.05	140.58	110.50
1	A	252	ARG	NE-CZ-NH2	19.88	130.24	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	TYR	Sidechain
2	C	39	ARG	Sidechain
2	C	45	ARG	Sidechain

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	3900	0	3671	143	0
1	B	3894	0	3666	164	0
2	C	882	0	848	16	0
2	D	898	0	862	21	0
3	A	590	0	0	27	0
3	B	484	0	0	24	0
3	C	147	0	0	4	0
3	D	156	0	0	8	0
All	All	10951	0	9047	344	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 18.

The worst 5 of 344 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:B:1:GLN:H1	1:B:1:GLN:NE2	1.19	1.40
1:B:1:GLN:NE2	1:B:1:GLN:N	1.90	1.19
1:B:282:GLU:OE1	3:B:626:HOH:O	1.66	1.14
1:A:1:GLN:OE1	1:A:1:GLN:CA	2.00	1.09
1:B:15:HIS:HB3	1:B:339:MET:HE3	1.31	1.08

There are no symmetry-related clashes.

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	494/496 (100%)	482 (98%)	12 (2%)	0	100	100
1	B	494/496 (100%)	480 (97%)	13 (3%)	1 (0%)	52	28
2	C	117/121 (97%)	112 (96%)	5 (4%)	0	100	100
2	D	119/121 (98%)	114 (96%)	4 (3%)	1 (1%)	24	6
All	All	1224/1234 (99%)	1188 (97%)	34 (3%)	2 (0%)	52	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	ALA
2	D	9	GLY

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	411/413 (100%)	391 (95%)	20 (5%)	31	8
1	B	410/413 (99%)	388 (95%)	22 (5%)	27	6
2	C	95/97 (98%)	91 (96%)	4 (4%)	36	11
2	D	97/97 (100%)	88 (91%)	9 (9%)	11	1
All	All	1013/1020 (99%)	958 (95%)	55 (5%)	27	6

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	115	CYS
1	B	262	LEU
2	D	41	PRO
1	B	162	LEU
1	B	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	HIS
1	B	161	GLN
2	D	53	ASN
1	B	75	ASN
1	B	101	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.