Full wwPDB X-ray Structure Validation Report (i)

Aug 31, 2020 – 08:18 AM BST

PDB ID	:	1AH7
Title	:	PHOSPHOLIPASE C FROM BACILLUS CEREUS
Authors	:	Greaves, R.
Deposited on	:	1997-04-14
Resolution	:	1.50 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 following versions of software and data (see references (1)) were used in the production of this report:

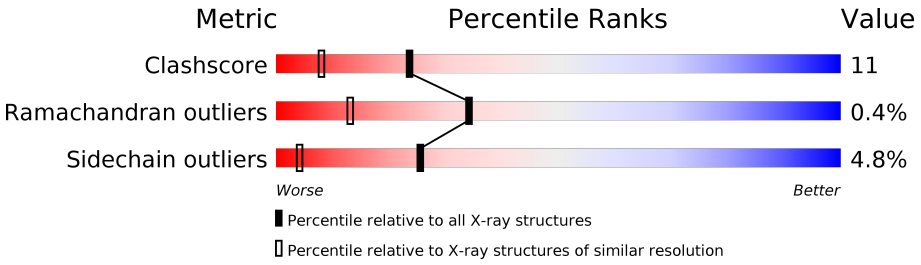
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 1.50 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	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 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	245	76% 19% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2267 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 PHOSPHOLIPASE C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	4	5	0
			2032	1296	343	388	5			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total	O	0	0
			232	232		

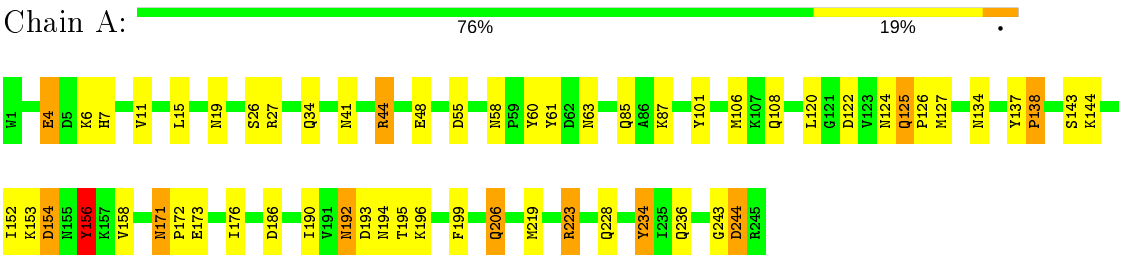
3 Residue-property plots (i)

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: PHOSPHOLIPASE C

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 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.76Å 89.76Å 74.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.45 – 1.50	Depositor
% Data completeness (in resolution range)	95.0 (12.45-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2267	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	1/2122 (0.0%)	1.43	18/2878 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	TYR	CE1-CZ	-6.96	1.29	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	TYR	CD1-CE1-CZ	25.68	142.92	119.80
1	A	156	TYR	CB-CG-CD2	20.92	133.55	121.00
1	A	156	TYR	CB-CG-CD1	-18.80	109.72	121.00
1	A	156	TYR	CG-CD1-CE1	-15.38	108.99	121.30
1	A	156	TYR	CE1-CZ-CE2	-10.92	102.33	119.80
1	A	156	TYR	CA-CB-CG	-8.45	97.34	113.40
1	A	156	TYR	CB-CA-C	-8.29	93.82	110.40
1	A	60	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	A	156	TYR	CZ-CE2-CD2	6.66	125.79	119.80
1	A	156	TYR	OH-CZ-CE2	6.53	137.72	120.10
1	A	122	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	44	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	154	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	223	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	138	PRO	N-CA-CB	5.68	110.11	103.30
1	A	55	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	137	TYR	CA-C-O	-5.26	109.05	120.10
1	A	234	TYR	CB-CG-CD2	-5.25	117.85	121.00

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	A	2032	0	1890	44	6
2	A	3	0	0	0	0
3	A	232	0	0	0	7
All	All	2267	0	1890	44	7

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 11.

All (44) 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:19:ASN:HD21	1:A:44:ARG:HH12	1.16	0.94
1:A:158:VAL:H	1:A:228:GLN:HE22	1.27	0.82
1:A:153:LYS:HA	1:A:156:TYR:CE2	2.15	0.81
1:A:58:ASN:HD21	1:A:63:ASN:H	1.29	0.77
1:A:124:ASN:HD22	1:A:223:ARG:HH12	1.35	0.74
1:A:206:GLN:HE21	1:A:206:GLN:H	1.33	0.74
1:A:243:GLY:O	1:A:244:ASP:HB2	1.88	0.74
1:A:153:LYS:HA	1:A:156:TYR:CD2	2.24	0.71
1:A:4:GLU:HG3	1:A:11:VAL:HB	1.74	0.70
1:A:144:LYS:HD2	1:A:199:PHE:CE1	2.38	0.59
1:A:58:ASN:ND2	1:A:63:ASN:H	2.00	0.59
1:A:41:ASN:HD22	1:A:44:ARG:HE	1.52	0.58
1:A:144:LYS:HD2	1:A:199:PHE:HE1	1.68	0.58
1:A:192:ASN:ND2	1:A:195:THR:H	2.02	0.57
1:A:158:VAL:H	1:A:228:GLN:NE2	2.00	0.57
1:A:153:LYS:HA	1:A:156:TYR:HE2	1.63	0.57
1:A:153:LYS:O	1:A:156:TYR:CD2	2.59	0.55
1:A:134:ASN:ND2	1:A:143:SER:H	2.04	0.55
1:A:152:ILE:HB	1:A:156:TYR:OH	2.06	0.55
1:A:152:ILE:O	1:A:156:TYR:CE2	2.61	0.53
1:A:171:ASN:ND2	1:A:173:GLU:H	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:ND2	1:A:44:ARG:HH12	1.96	0.51
1:A:186:ASP:HB3	1:A:219:MET:SD	2.51	0.51
1:A:125:GLN:NE2	1:A:127:MET:H	2.10	0.50
1:A:26:SER:HA	1:A:34:GLN:HE22	1.76	0.50
1:A:206:GLN:H	1:A:206:GLN:NE2	2.06	0.50
1:A:4:GLU:HG2	1:A:11:VAL:O	2.12	0.49
1:A:58:ASN:HD21	1:A:63:ASN:N	2.06	0.48
1:A:41:ASN:ND2	1:A:44:ARG:HE	2.12	0.46
1:A:171:ASN:HD22	1:A:172:PRO:HD2	1.80	0.45
1:A:41:ASN:HD21	1:A:44:ARG:HH21	1.65	0.45
1:A:152:ILE:HD12	1:A:156:TYR:OH	2.17	0.44
1:A:243:GLY:O	1:A:244:ASP:CB	2.64	0.43
1:A:125:GLN:HE21	1:A:125:GLN:C	2.22	0.43
1:A:192:ASN:HD22	1:A:192:ASN:C	2.22	0.43
1:A:192:ASN:HD22	1:A:194:ASN:N	2.17	0.43
1:A:101:TYR:HA	1:A:106:MET:HE2	2.00	0.42
1:A:138:PRO:HD3	1:A:196:LYS:HG2	2.01	0.42
1:A:6:LYS:HG2	1:A:7:HIS:CE1	2.54	0.42
1:A:192:ASN:O	1:A:196:LYS:HG3	2.20	0.42
1:A:126:PRO:HG2	1:A:190:ILE:HD12	2.03	0.41
1:A:15:LEU:HD13	1:A:48:GLU:HG2	2.02	0.41
1:A:87:LYS:HA	1:A:176:ILE:HG21	2.03	0.40
1:A:120:LEU:HD22	1:A:234:TYR:CG	2.56	0.40

All (7) 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)
1:A:27[A]:ARG:NH2	3:A:361:HOH:O[4_555]	0.84	1.36
1:A:27[A]:ARG:CZ	3:A:361:HOH:O[4_555]	0.97	1.23
1:A:27[A]:ARG:NH1	3:A:361:HOH:O[4_555]	1.58	0.62
1:A:156:TYR:CE1	3:A:438:HOH:O[8_665]	2.06	0.14
1:A:154:ASP:OD1	3:A:396:HOH:O[4_555]	2.13	0.07
3:A:353:HOH:O	3:A:454:HOH:O[4_555]	2.14	0.06
1:A:193:ASP:OD1	3:A:366:HOH:O[7_555]	2.19	0.01

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	248/245 (101%)	242 (98%)	5 (2%)	1 (0%)	34 13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ASP

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	212/207 (102%)	202 (95%)	10 (5%)	26 4

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	61	TYR
1	A	85	GLN
1	A	108	GLN
1	A	125	GLN
1	A	156	TYR
1	A	171	ASN
1	A	192	ASN
1	A	206	GLN
1	A	236	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	34	GLN
1	A	41	ASN
1	A	49	ASN
1	A	58	ASN
1	A	63	ASN
1	A	124	ASN
1	A	125	GLN
1	A	131	ASN
1	A	134	ASN
1	A	147	ASN
1	A	155	ASN
1	A	166	ASN
1	A	171	ASN
1	A	192	ASN
1	A	194	ASN
1	A	206	GLN
1	A	228	GLN
1	A	236	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are 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

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.