Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2024 – 04:13 pm BST

PDB ID	:	2UXY
Title	:	Aliphatic amidase
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Deposited on	:	2007-04-02
Resolution	:	1.25 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:

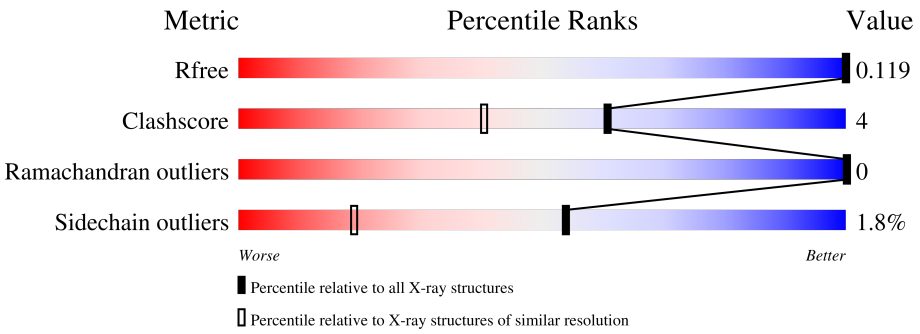
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 1.25 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}	164625	1447 (1.28-1.24)
Clashscore	180529	1571 (1.28-1.24)
Ramachandran outliers	177936	1538 (1.28-1.24)
Sidechain outliers	177891	1537 (1.28-1.24)

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%

Mol	Chain	Length	Quality of chain
1	A	341	91% 7% •

2 Entry composition (i)

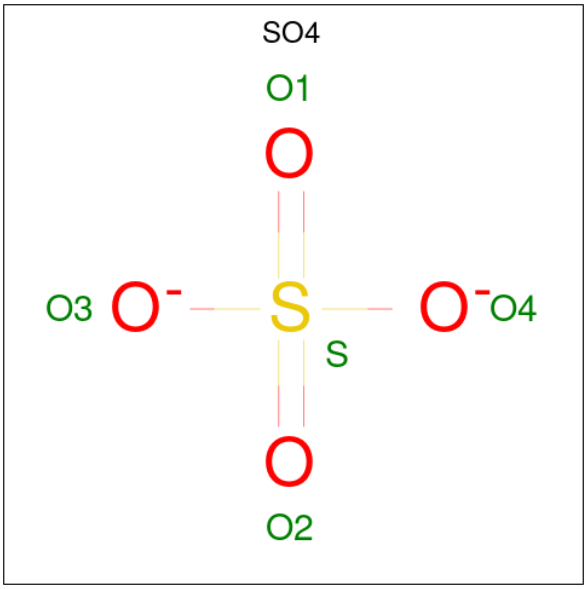
There are 3 unique types of molecules in this entry. The entry contains 3099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALIPHATIC AMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2789	1753	485	521	30	0	28	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	305	305	305	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.

- Molecule 1: ALIPHATIC AMIDASE

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	102.71Å 102.71Å 151.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	1.28 – 1.25 1.28 – 1.25	Depositor EDS
% Data completeness (in resolution range)	51.5 (1.28-1.25) 3.0 (1.28-1.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.25Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.111 , 0.136 0.119 , 0.119	Depositor DCC
R_{free} test set	62 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å^2)	8.0	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	44057.20 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3099	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, C3Y

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	0.68	0/2949	1.36	30/3977 (0.8%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316[A]	ARG	CD-NE-CZ	25.92	159.88	123.60
1	A	316[B]	ARG	CD-NE-CZ	25.92	159.88	123.60
1	A	306	ARG	CD-NE-CZ	12.94	141.71	123.60
1	A	36[A]	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	A	36[B]	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	A	306	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	A	89	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	A	294	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	A	295[A]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	295[B]	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	241	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	282	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	202[A]	MET	CG-SD-CE	7.16	111.65	100.20
1	A	202[B]	MET	CG-SD-CE	7.16	111.65	100.20
1	A	112[A]	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	112[B]	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	89	ARG	NH1-CZ-NH2	6.76	126.84	119.40
1	A	198	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	321	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	321	ARG	CD-NE-CZ	6.29	132.41	123.60
1	A	295[A]	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	295[B]	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	284	TYR	CA-CB-CG	5.94	124.68	113.40
1	A	282	ARG	NE-CZ-NH2	-5.75	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317[A]	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	A	317[B]	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	A	194	TYR	CA-CB-CG	5.28	123.44	113.40
1	A	284	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	92	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	A	194	TYR	CB-CG-CD2	5.00	124.00	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	2789	0	2716	23	0
2	A	5	0	0	1	0
3	A	305	0	0	4	0
All	All	3099	0	2716	23	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 (23) 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:112[A]:ARG:HG3	3:A:2139:HOH:O	1.44	1.14
1:A:316[A]:ARG:HH21	1:A:316[A]:ARG:HB3	1.22	1.02
1:A:316[A]:ARG:HB3	1:A:316[A]:ARG:NH2	1.97	0.78
1:A:313:GLU:O	1:A:316[A]:ARG:NH2	2.16	0.78
1:A:85[A]:GLU:HG3	1:A:89:ARG:NH1	2.04	0.71
1:A:40[B]:GLU:OE2	3:A:2060:HOH:O	2.14	0.65
1:A:313:GLU:HA	1:A:316[A]:ARG:NH2	2.12	0.63
1:A:85[A]:GLU:CG	1:A:89:ARG:NH1	2.65	0.60
1:A:97:TRP:CG	1:A:156[B]:PRO:HG3	2.37	0.59
1:A:313:GLU:OE1	1:A:316[A]:ARG:NH1	2.37	0.58
1:A:89:ARG:NH2	2:A:1343:SO4:O2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASN:OD1	1:A:321:ARG:NH2	2.40	0.54
1:A:254:GLN:HE21	1:A:255:TYR:H	1.54	0.53
1:A:112[A]:ARG:CG	3:A:2139:HOH:O	2.23	0.50
1:A:112[A]:ARG:NH2	3:A:2138:HOH:O	2.44	0.50
1:A:313:GLU:CA	1:A:316[A]:ARG:NH2	2.77	0.48
1:A:85[A]:GLU:CG	1:A:89:ARG:HH12	2.27	0.48
1:A:138:TRP:CD1	1:A:166[B]:C3Y:H1C1	2.52	0.45
1:A:138:TRP:CD1	1:A:166[A]:C3Y:H1C1	2.52	0.44
1:A:188:ARG:CZ	1:A:190:GLN:HE22	2.29	0.44
1:A:85[A]:GLU:HG2	1:A:89:ARG:HH12	1.84	0.43
1:A:97:TRP:CD1	1:A:156[B]:PRO:HG3	2.54	0.43
1:A:19:ASN:HA	1:A:219:ASN:O	2.21	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	366/341 (107%)	357 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	303/275 (110%)	296 (98%)	7 (2%)	45 10

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

Mol	Chain	Res	Type
1	A	5	ASP
1	A	192	TYR
1	A	202[A]	MET
1	A	202[B]	MET
1	A	254	GLN
1	A	316[A]	ARG
1	A	316[B]	ARG

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

Mol	Chain	Res	Type
1	A	190	GLN
1	A	254	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	C3Y	A	166[B]	-	6,10,11	0.68	0	1,13,15	2.03	1 (100%)
1	C3Y	A	166[A]	-	6,10,11	0.70	0	1,13,15	2.03	1 (100%)

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
1	C3Y	A	166[B]	-	-	1/3/11/13	-
1	C3Y	A	166[A]	-	-	1/3/11/13	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166[A]	C3Y	O2-C2-C1	-2.03	103.53	107.83
1	A	166[B]	C3Y	O2-C2-C1	-2.03	103.53	107.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166[A]	C3Y	N-CA-CB-SG
1	A	166[B]	C3Y	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	166[B]	C3Y	1	0
1	A	166[A]	C3Y	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	A	1343	-	4,4,4	1.04	0	6,6,6	1.36	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1343	SO4	O4-S-O3	2.99	121.81	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1343	SO4	1	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.