W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2017 – 02:47 AM EDT

PDB ID	:	1IV7
Title	:	Crystal Structure of Single Chain Monellin
Authors	:	Tamada, T.; Kato, Y.; Kuroki, R.
Deposited on	:	unknown
Resolution	:	1.82 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
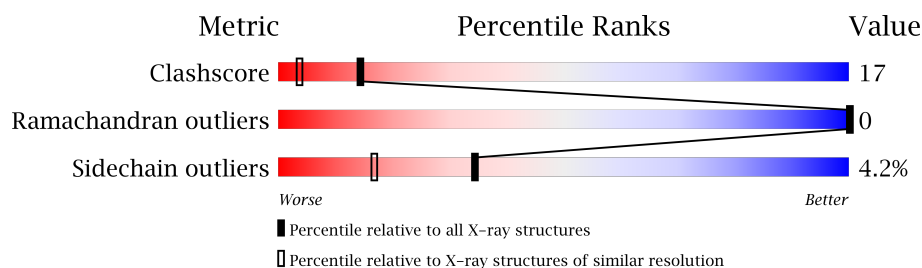with specific help available everywhere you see the (i) symbol.

---

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 1.82 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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		0
Sidechain outliers		4.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)

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 <=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	96	76% 20%
1	B	96	71% 23% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1702 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 Monellin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total 798	C 515	N 135	O 146	S 2	0	0	0
1	B	96	Total 798	C 515	N 135	O 146	S 2	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	ASN	GLU	ENGINEERED	UNP P02882
A	50	GLU	ASN	ENGINEERED	UNP P02882
A	51	GLY	-	LINKER	UNP P02881
B	149	ASN	GLU	ENGINEERED	UNP P02882
B	150	GLU	ASN	ENGINEERED	UNP P02882
B	151	GLY	-	LINKER	UNP P02881

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	52	Total 52	O 52	0	0
2	B	54	Total 54	O 54	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 the various outlier classes 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: Monellin

Chain A:

- Molecule 1: Monellin

Chain B:
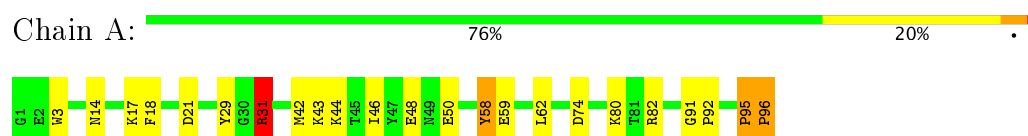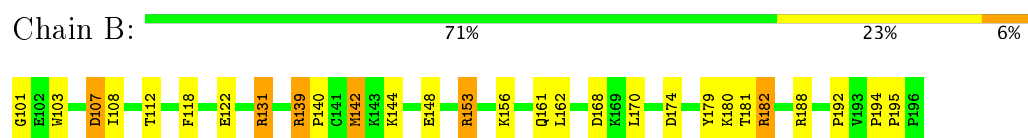
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	60.65Å 36.26Å 46.38Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	15.00 – 1.82	Depositor
% Data completeness (in resolution range)	93.2 (15.00-1.82)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.200 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1702	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.26	2/818 (0.2%)	1.20	5/1099 (0.5%)
1	B	1.26	0/818	1.15	4/1099 (0.4%)
All	All	1.26	2/1636 (0.1%)	1.18	9/2198 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	TYR	CD1-CE1	-5.63	1.30	1.39
1	A	58	TYR	CD1-CE1	-5.21	1.31	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	A	74	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	174	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	139	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	B	107	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	168	ASP	CB-CG-OD2	5.77	123.50	118.30

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	798	0	791	30	1

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	798	0	788	26	0
2	A	52	0	0	11	1
2	B	54	0	0	3	0
All	All	1702	0	1579	55	1

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 17.

The worst 5 of 55 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:101:GLY:HA3	2:B:240:HOH:O	1.08	1.20
1:A:31:ARG:CB	1:A:31:ARG:HH11	1.71	1.04
2:A:119:HOH:O	1:B:194:PRO:HG2	1.60	0.99
1:A:17:LYS:HE2	2:A:131:HOH:O	1.64	0.97
1:A:14:ASN:ND2	1:A:17:LYS:HE2	1.82	0.93

All (1) 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:50:GLU:OE1	2:A:112:HOH:O[1_565]	2.18	0.02

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	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
1	B	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
All	All	188/192 (98%)	183 (97%)	5 (3%)	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	84/84 (100%)	82 (98%)	2 (2%)	54	39
1	B	84/84 (100%)	79 (94%)	5 (6%)	22	8
All	All	168/168 (100%)	161 (96%)	7 (4%)	34	17

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142	MET
1	B	188	ARG
1	B	153	ARG
1	A	48	GLU
1	B	182	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	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 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 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.