



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2024 – 12:15 pm GMT

PDB ID : 8Q0S
Title : X-ray structure of the single chain monellin derivative MNEI
Authors : Ferraro, G.; Merlino, A.; Lucignano, R.; Picone, D.
Deposited on : 2023-07-29
Resolution : 1.19 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

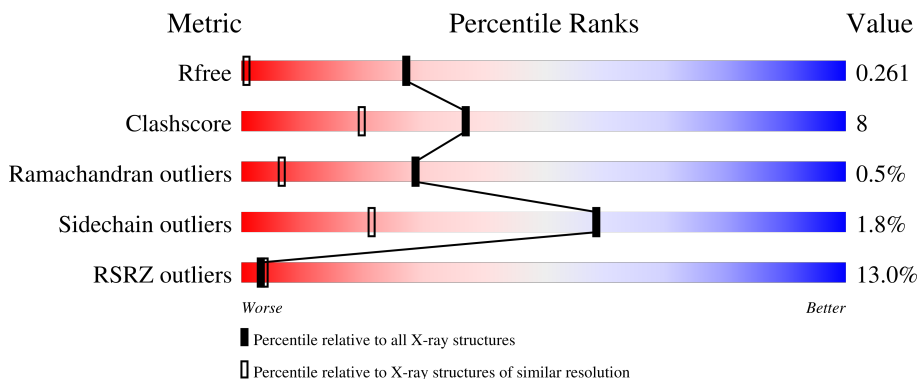
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	AAA	97	
1	BBB	97	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2103 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 chain B, Monellin chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	96	892	571	152	166	3	0	10	0
1	BBB	97	927	593	160	170	4	0	13	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP P02882
AAA	49	ASN	-	linker	UNP P02882
AAA	50	GLU	-	linker	UNP P02882
AAA	51	GLY	-	linker	UNP P02882
BBB	0	MET	-	initiating methionine	UNP P02882
BBB	49	ASN	-	linker	UNP P02882
BBB	50	GLU	-	linker	UNP P02882
BBB	51	GLY	-	linker	UNP P02882

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 6 3 3	0	0
3	AAA	1	Total C O 6 3 3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total 1	Na 1	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	132	Total 132	O 132	0	1
5	BBB	131	Total 131	O 131	0	2

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 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.

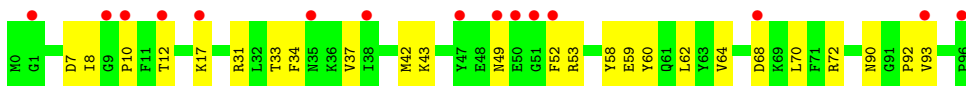
- Molecule 1: Monellin chain B, Monellin chain A

Chain AAA: 



- Molecule 1: Monellin chain B, Monellin chain A

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	31.65Å 38.97Å 44.13Å 106.00° 109.52° 103.36°	Depositor
Resolution (Å)	38.39 – 1.19 38.39 – 1.19	Depositor EDS
% Data completeness (in resolution range)	87.3 (38.39-1.19) 87.3 (38.39-1.19)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.256 0.224 , 0.261	Depositor DCC
R_{free} test set	2466 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2103	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ACT, NA, GOL

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	AAA	0.74	1/912 (0.1%)	0.93	2/1221 (0.2%)
1	BBB	0.72	0/947	0.91	0/1269
All	All	0.73	1/1859 (0.1%)	0.92	2/2490 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	23	GLU	CD-OE1	-5.42	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	84	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	AAA	84	ARG	CG-CD-NE	-5.21	100.85	111.80

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	AAA	892	0	879	11	0
1	BBB	927	0	921	20	0
2	AAA	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	12	0	16	0	0
4	AAA	1	0	0	0	0
5	AAA	132	0	0	1	0
5	BBB	131	0	0	6	0
All	All	2103	0	1822	29	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 8.

All (29) 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:BBB:10:PRO:HD2	5:BBB:163:HOH:O	1.78	0.83
1:BBB:7:ASP:O	1:BBB:12[B]:THR:HG21	1.84	0.77
1:BBB:33[B]:THR:HG23	5:BBB:117:HOH:O	1.88	0.74
1:BBB:37:VAL:HG22	1:BBB:64[B]:VAL:HG12	1.69	0.73
1:BBB:17[A]:LYS:HG2	1:BBB:34:PHE:CE2	2.27	0.70
1:AAA:53:ARG:NH1	5:AAA:201:HOH:O	2.24	0.66
1:AAA:74[B]:ASP:OD2	1:AAA:87:LEU:HD12	1.96	0.66
1:AAA:96:PRO:OXT	1:BBB:59:GLU:OE1	2.15	0.64
1:BBB:43:LYS:HE3	1:BBB:58:TYR:CD1	2.34	0.62
1:AAA:35[B]:ASN:C	1:AAA:35[B]:ASN:HD22	2.04	0.60
1:AAA:47:TYR:CD1	1:AAA:53:ARG:HA	2.45	0.52
1:BBB:60:TYR:HB3	1:BBB:62:LEU:HD11	1.93	0.51
1:BBB:8:ILE:HA	1:BBB:12[B]:THR:OG1	2.12	0.50
1:AAA:17[A]:LYS:HG2	1:AAA:34:PHE:CD2	2.48	0.49
1:BBB:70[B]:LEU:O	1:BBB:92:PRO:HA	2.13	0.49
1:BBB:72[A]:ARG:NH1	5:BBB:103:HOH:O	2.41	0.49
1:BBB:60:TYR:HB3	1:BBB:62:LEU:CD1	2.43	0.48
1:BBB:17[C]:LYS:HG2	1:BBB:34:PHE:CD2	2.49	0.47
1:BBB:12[B]:THR:HG23	5:BBB:156:HOH:O	2.15	0.46
1:AAA:42[B]:MET:SD	1:BBB:42[B]:MET:SD	3.13	0.46
1:BBB:70[B]:LEU:HD23	1:BBB:93:VAL:O	2.15	0.46
1:BBB:17[C]:LYS:HG3	1:BBB:34:PHE:CE2	2.50	0.45
1:BBB:17[A]:LYS:HG2	1:BBB:34:PHE:CD2	2.52	0.44
1:BBB:53:ARG:NH2	5:BBB:106:HOH:O	2.50	0.44
1:AAA:5:ILE:HD13	1:AAA:42[A]:MET:SD	2.59	0.42
1:AAA:33[A]:THR:O	1:AAA:66:ALA:HA	2.20	0.41
1:AAA:18:PHE:CZ	1:AAA:22:GLU:HG3	2.56	0.41
1:AAA:35[B]:ASN:C	1:AAA:35[B]:ASN:ND2	2.73	0.41
1:BBB:31:ARG:NH1	5:BBB:113:HOH:O	2.55	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	AAA	105/97 (108%)	103 (98%)	2 (2%)	0	100	100
1	BBB	109/97 (112%)	105 (96%)	3 (3%)	1 (1%)	17	2
All	All	214/194 (110%)	208 (97%)	5 (2%)	1 (0%)	29	7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	52	PHE

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	AAA	95/85 (112%)	95 (100%)	0	100	100
1	BBB	99/85 (116%)	96 (97%)	3 (3%)	41	7
All	All	194/170 (114%)	191 (98%)	3 (2%)	59	29

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	49	ASN
1	BBB	68	ASP

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Mol	Chain	Res	Type
1	BBB	90	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	GOL	AAA	104	-	5,5,5	0.11	0	5,5,5	0.27	0
3	GOL	AAA	102	-	5,5,5	0.08	0	5,5,5	0.45	0
2	ACT	AAA	101	4	3,3,3	1.38	0	3,3,3	0.24	0
2	ACT	AAA	103	-	3,3,3	0.95	0	3,3,3	0.86	0

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	GOL	AAA	104	-	-	2/4/4/4	-
3	GOL	AAA	102	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	102	GOL	C1-C2-C3-O3
3	AAA	104	GOL	O1-C1-C2-C3
3	AAA	102	GOL	O2-C2-C3-O3
3	AAA	104	GOL	O1-C1-C2-O2
3	AAA	102	GOL	O1-C1-C2-O2

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	96/97 (98%)	0.88	10 (10%) 6 7	8, 14, 28, 40	0
1	BBB	97/97 (100%)	1.18	15 (15%) 2 2	8, 15, 27, 53	0
All	All	193/194 (99%)	1.03	25 (12%) 3 4	8, 15, 28, 53	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	51	GLY	11.6
1	AAA	53	ARG	5.4
1	BBB	50	GLU	4.7
1	BBB	49	ASN	4.4
1	AAA	52	PHE	4.2
1	BBB	10	PRO	4.0
1	BBB	68	ASP	3.3
1	BBB	52	PHE	3.2
1	BBB	9	GLY	3.1
1	AAA	1	GLY	3.0
1	BBB	1	GLY	2.7
1	AAA	2[A]	GLU	2.7
1	BBB	47	TYR	2.6
1	BBB	96	PRO	2.6
1	AAA	32	LEU	2.5
1	AAA	33[A]	THR	2.4
1	AAA	96	PRO	2.4
1	AAA	47	TYR	2.3
1	BBB	17[A]	LYS	2.3
1	AAA	55	ILE	2.3
1	AAA	54	GLU	2.2
1	BBB	38	ILE	2.2
1	BBB	12[A]	THR	2.2
1	BBB	35	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	93	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	AAA	104	6/6	0.65	0.29	49,50,50,51	0
2	ACT	AAA	103	4/4	0.71	0.14	41,41,42,43	0
2	ACT	AAA	101	4/4	0.77	0.16	13,14,21,27	0
4	NA	AAA	105	1/1	0.83	0.10	34,34,34,34	0
3	GOL	AAA	102	6/6	0.93	0.14	21,30,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.