Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2024 – 12:19 pm GMT

PDB ID	:	8Q0R
Title	:	X-ray structure of MNEI mutant Mut9 (E23A, C41A, Y65R, S76Y)
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Deposited on	:	2023-07-29
Resolution	:	1.55 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 (1)) were used in the production of this report:

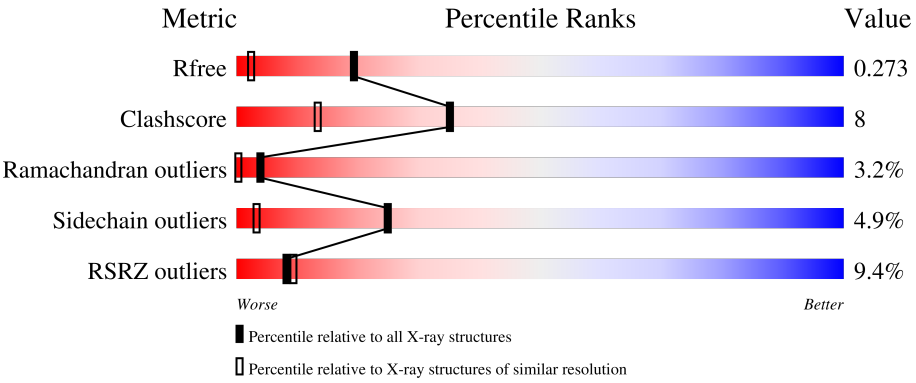
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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% 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	96	8% 82% 16%
1	BBB	96	10% 82% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	BBB	102	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1906 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.

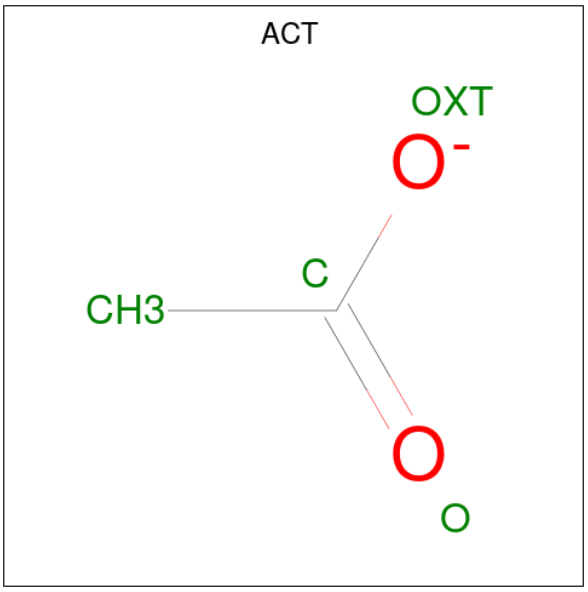
- Molecule 1 is a protein called Monellin chain B,Monellin chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	96	Total	C	N	O	S	0	5	0
			842	541	146	153	2			
1	BBB	96	Total	C	N	O	S	0	5	0
			844	546	149	148	1			

There are 14 discrepancies between the modelled and reference sequences:

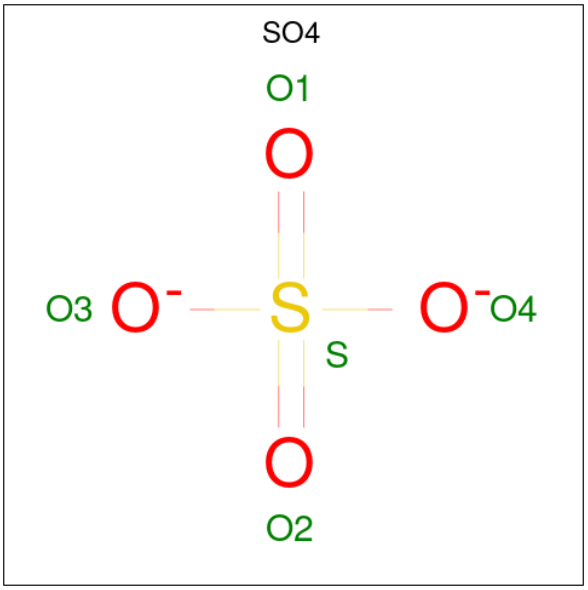
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	23	ALA	GLU	engineered mutation	UNP P02882
AAA	41	ALA	CYS	engineered mutation	UNP P02882
AAA	49	ASN	-	linker	UNP P02882
AAA	50	GLU	-	linker	UNP P02882
AAA	51	GLY	-	linker	UNP P02882
AAA	65	ARG	TYR	engineered mutation	UNP P02881
AAA	76	TYR	SER	engineered mutation	UNP P02881
BBB	23	ALA	GLU	engineered mutation	UNP P02882
BBB	41	ALA	CYS	engineered mutation	UNP P02882
BBB	49	ASN	-	linker	UNP P02882
BBB	50	GLU	-	linker	UNP P02882
BBB	51	GLY	-	linker	UNP P02882
BBB	65	ARG	TYR	engineered mutation	UNP P02881
BBB	76	TYR	SER	engineered mutation	UNP P02881

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	113	Total O 114 114	0	2
4	BBB	87	Total O 88 88	0	1

3 Residue-property plots (i)

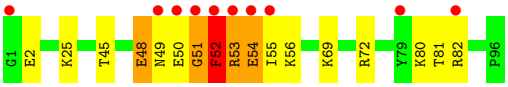
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.12Å 31.29Å 46.10Å 90.00° 108.65° 90.00°	Depositor
Resolution (Å)	35.58 – 1.55 43.68 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (35.58-1.55) 98.3 (43.68-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.221 , 0.275 0.228 , 0.273	Depositor DCC
R_{free} test set	1213 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.065 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	1906	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4

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	0.69	0/862	0.93	0/1158
1	BBB	0.70	0/864	0.91	0/1157
All	All	0.70	0/1726	0.92	0/2315

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AAA	842	0	832	13	0
1	BBB	844	0	856	16	0
2	AAA	4	0	3	0	0
2	BBB	4	0	3	0	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	2	0
4	AAA	114	0	0	3	0
4	BBB	88	0	0	4	0
All	All	1906	0	1694	28	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 (28) 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:AAA:39:ARG:NH2	4:AAA:201:HOH:O	2.14	0.80
1:AAA:82:ARG:HE	1:AAA:82:ARG:HA	1.55	0.72
1:AAA:93:VAL:HB	1:BBB:72[B]:ARG:HH12	1.56	0.69
1:BBB:69[B]:LYS:NZ	4:BBB:206:HOH:O	2.32	0.61
1:AAA:51:GLY:O	1:AAA:52:PHE:HB2	2.00	0.61
1:BBB:72[B]:ARG:HD2	4:BBB:244:HOH:O	2.01	0.60
1:BBB:51:GLY:O	1:BBB:52:PHE:HB2	2.00	0.59
1:BBB:48:GLU:CG	1:BBB:48:GLU:O	2.52	0.55
1:BBB:72[B]:ARG:CZ	3:BBB:102:SO4:O1	2.56	0.54
1:AAA:52:PHE:O	1:AAA:53:ARG:HB2	2.09	0.53
1:AAA:7:ASP:HB3	4:AAA:202:HOH:O	2.09	0.52
1:AAA:58:TYR:HE2	1:AAA:82:ARG:HH12	1.58	0.51
1:BBB:48:GLU:O	1:BBB:48:GLU:HG2	2.10	0.50
1:BBB:48:GLU:HB3	1:BBB:56:LYS:HD2	1.93	0.49
1:AAA:14:ASN:HB2	4:AAA:208:HOH:O	2.11	0.49
1:AAA:11:PHE:CZ	1:AAA:84[A]:ARG:NH2	2.82	0.48
1:BBB:53:ARG:O	1:BBB:54:GLU:HB3	2.14	0.47
1:BBB:80:LYS:HG3	1:BBB:81:THR:HG23	1.97	0.45
1:BBB:72[B]:ARG:NH2	3:BBB:102:SO4:O1	2.50	0.45
1:BBB:81:THR:O	1:BBB:82:ARG:HG2	2.17	0.44
1:AAA:52:PHE:HB3	1:AAA:54:GLU:HG3	2.00	0.44
1:BBB:45:THR:HG23	1:BBB:55:ILE:HG23	2.01	0.43
1:BBB:82:ARG:HB2	4:BBB:251:HOH:O	2.17	0.43
1:AAA:52:PHE:CB	1:AAA:54:GLU:HG3	2.50	0.41
1:AAA:77[A]:GLU:OE2	1:AAA:82:ARG:NH1	2.54	0.41
1:BBB:25:LYS:NZ	4:BBB:202:HOH:O	2.20	0.41
1:AAA:43:LYS:HE2	1:AAA:58:TYR:CD1	2.55	0.40
1:BBB:2:GLU:O	1:BBB:2:GLU:HG2	2.21	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	99/96 (103%)	93 (94%)	4 (4%)	2 (2%)	7 1
1	BBB	99/96 (103%)	92 (93%)	3 (3%)	4 (4%)	3 0
All	All	198/192 (103%)	185 (93%)	7 (4%)	6 (3%)	4 0

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	52	PHE
1	BBB	52	PHE
1	BBB	54	GLU
1	AAA	48	GLU
1	BBB	49	ASN
1	BBB	51	GLY

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	87/82 (106%)	83 (95%)	4 (5%)	27 4
1	BBB	87/82 (106%)	83 (95%)	4 (5%)	27 4
All	All	174/164 (106%)	166 (95%)	8 (5%)	25 4

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	49	ASN
1	AAA	52	PHE
1	AAA	68	ASP
1	AAA	82	ARG
1	BBB	48	GLU
1	BBB	50	GLU
1	BBB	52	PHE

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Mol	Chain	Res	Type
1	BBB	53	ARG

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)

4 ligands 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	$\#\|Z\| > 2$
2	ACT	AAA	101	-	3,3,3	0.80	0	3,3,3	0.95	0
2	ACT	BBB	101	-	3,3,3	0.91	0	3,3,3	0.77	0
3	SO4	AAA	102	-	4,4,4	0.47	0	6,6,6	0.28	0
3	SO4	BBB	102	-	4,4,4	0.26	0	6,6,6	0.15	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	102	SO4	2	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

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, 95^{th} 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	96/96 (100%)	0.54	8 (8%) 11 12	14, 21, 53, 89	0
1	BBB	96/96 (100%)	0.76	10 (10%) 6 6	13, 23, 65, 81	0
All	All	192/192 (100%)	0.65	18 (9%) 8 9	13, 22, 65, 89	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	52	PHE	11.0
1	BBB	52	PHE	10.8
1	BBB	51	GLY	7.6
1	BBB	49	ASN	6.8
1	AAA	49	ASN	6.0
1	BBB	53	ARG	5.6
1	BBB	79	TYR	5.4
1	BBB	1	GLY	4.7
1	AAA	50	GLU	3.9
1	BBB	54	GLU	3.7
1	AAA	53	ARG	3.4
1	BBB	50	GLU	3.4
1	BBB	55	ILE	3.1
1	AAA	96	PRO	2.8
1	AAA	1	GLY	2.6
1	AAA	48	GLU	2.6
1	BBB	82	ARG	2.6
1	AAA	47	TYR	2.1

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

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, 95^{th} 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
2	ACT	AAA	101	4/4	0.65	0.23	46,46,47,47	0
2	ACT	BBB	101	4/4	0.86	0.24	38,40,42,44	0
3	SO4	BBB	102	5/5	0.94	0.13	27,27,29,30	5
3	SO4	AAA	102	5/5	0.98	0.06	28,30,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.