

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 12:36 PM EDT

PDB ID : 1WLD

Title: Congerin II T88I single mutant

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Deposited on : 2004-06-22

Resolution : 1.60 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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)

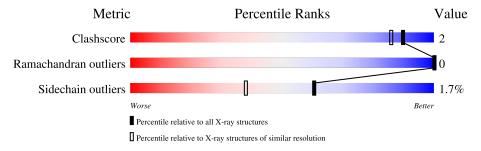
Validation Pipeline (wwPDB-VP) : 2.23.2

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 1.60 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
Clashscore	141614	3665 (1.60-1.60)		
Ramachandran outliers	138981	3564 (1.60-1.60)		
Sidechain outliers	138945	3563 (1.60-1.60)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	A	135	89%	9%				
2	В	2	100%					



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1262 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 CONGERIN II.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	134	Total	С	N	О	S	0	0	0
_	11	101	1079	683	190	203	3			O

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ILE	THR	engineered mutation	UNP Q9YIC2

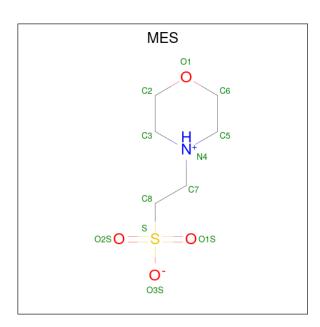
• Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	В	2	Total 23	C 12	O 11	0	0	0

• Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	Λ	1	Total	С	N	О	S	0	0
	Λ	1	12	6	1	4	1		U

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	148	Total O 148 148	0	0

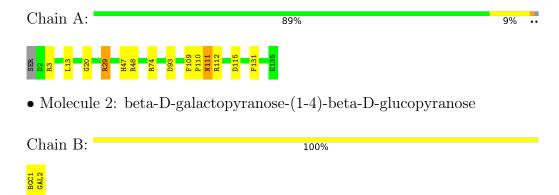


3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: CONGERIN II





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 42 21 2	Depositor	
Cell constants	60.97Å 60.97Å 79.91Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	8.00 - 1.60	Depositor	
% Data completeness	(Not available) (8.00-1.60)	Depositor	
(in resolution range)	(1101 available) (0.00 1.00)	Depositor	
R_{merge}	0.05	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC	Depositor	
R, R_{free}	0.187 , 0.224	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	1262	wwPDB-VP	
Average B, all atoms (Å ²)	20.0	wwPDB-VP	



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: BGC, GAL, MES

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		
IVIOI	vioi Chain RMSZ		# Z > 5	RMSZ	# Z > 5	
1	A	0.48	0/1103	1.24	9/1491 (0.6%)	

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	29	ARG	NE-CZ-NH1	13.63	127.11	120.30
1	A	74	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	A	3	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	3	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	48	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	112	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	93	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	29	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	3	ARG	CD-NE-CZ	5.46	131.24	123.60

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	1079	0	1039	4	0
2	В	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	12	0	0
4	A	148	0	0	0	0
All	All	1262	0	1072	4	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 2.

All (4) 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:111:ASN:HD21	1:A:115:ASP:H	1.60	0.49	
1:A:29:ARG:HA	1:A:47:HIS:O	2.19	0.43	
1:A:20:GLY:HA3	1:A:131:PHE:CE1	2.54	0.42	
1:A:109:PHE:CD1	1:A:110:PRO:HD2	2.57	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	A	132/135 (98%)	129 (98%)	3 (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	nalysed Rotameric		Percentiles	
1	A	117/118 (99%)	115 (98%)	2 (2%)	60 38	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	111	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	66	ASN
1	A	100	GLN
1	A	111	ASN
1	A	119	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)

2 monosaccharides 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	Dag	T inle	Link Bond lengths				Bond angles		
MIOI	туре	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	BGC	В	1	2	12,12,12	2.03	1 (8%)	17,17,17	1.52	3 (17%)	
2	GAL	В	2	2	11,11,12	3.16	3 (27%)	15,15,17	1.52	1 (6%)	

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
2	BGC	В	1	2	-	0/2/22/22	0/1/1/1
2	GAL	В	2	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(A)
2	В	2	GAL	C2-C3	-9.64	1.38	1.52
2	В	1	BGC	O1-C1	6.79	1.61	1.39
2	В	2	GAL	C4-C3	2.73	1.59	1.52
2	В	2	GAL	O3-C3	2.72	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	В	1	BGC	O1-C1-C2	-3.86	98.16	109.03
2	В	2	GAL	C3-C4-C5	-3.49	104.02	110.24
2	В	1	BGC	C1-O5-C5	-2.68	108.61	113.66
2	В	1	BGC	O1-C1-O5	-2.49	102.91	110.38

There are no chirality outliers.

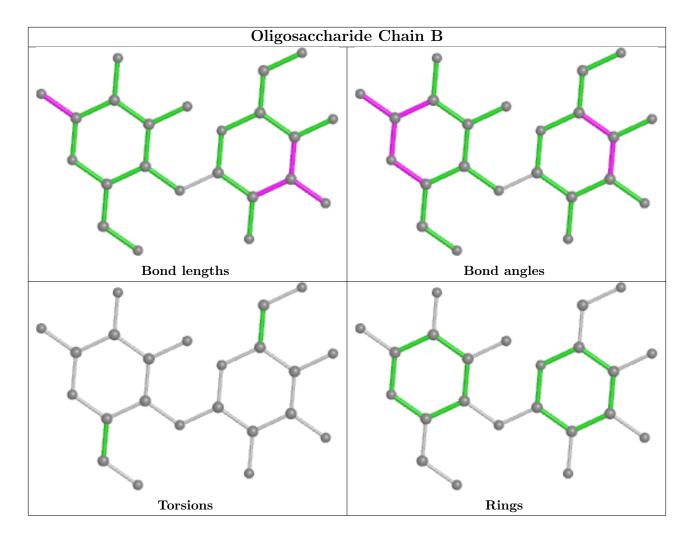
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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	Bo	Bond lengths			Bond angles		
MIOI	Type		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	MES	A	777	-	12,12,12	1.69	2 (16%)	14,16,16	3.42	10 (71%)	

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	MES	A	777	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
3	A	777	MES	C8-S	4.28	1.83	1.77
3	A	777	MES	C5-N4	-2.47	1.40	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	A	777	MES	C7-N4-C5	-5.84	96.31	111.23
3	A	777	MES	O3S-S-C8	5.25	114.26	105.77
3	A	777	MES	C2-C3-N4	-4.55	103.20	110.10
3	A	777	MES	O2S-S-C8	-4.54	101.45	106.92
3	A	777	MES	O3S-S-O1S	3.62	120.12	111.27
3	A	777	MES	C6-C5-N4	-3.33	105.06	110.10
3	A	777	MES	O1S-S-C8	-3.09	103.19	106.92
3	A	777	MES	C5-N4-C3	3.00	115.58	108.83
3	A	777	MES	O1-C2-C3	-2.30	106.73	111.80
3	A	777	MES	C6-O1-C2	-2.15	102.72	109.89

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 (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.

