



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 03:39 PM EDT

PDB ID : 6CSJ
Title : Structure of a Bacillus coagulans polyol dehydrogenase double mutant with an acquired D-lactate dehydrogenase activity
Authors : Hurlbert, J.C.; St.John, F.J.
Deposited on : 2018-03-20
Resolution : 2.40 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
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

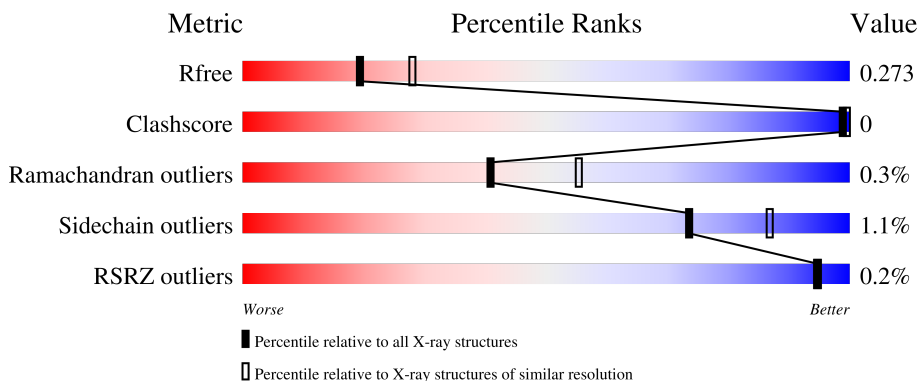
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	366	99%
1	B	366	98%
1	C	366	97%
1	D	366	99%
1	E	366	98%

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Mol	Chain	Length	Quality of chain
1	F	366	<p>% 98% .</p>
1	G	366	<p>98% ..</p>
1	H	366	<p>99% .</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22572 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 Glycerol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2760	1756	446	544	14	0	0	0
1	B	366	2759	1756	446	543	14	0	0	0
1	C	366	2759	1756	446	543	14	0	0	0
1	D	366	2759	1756	446	543	14	0	0	0
1	E	366	2759	1756	446	543	14	0	0	0
1	F	366	2756	1753	445	544	14	0	0	0
1	G	366	2759	1756	446	543	14	0	0	0
1	H	366	2759	1756	446	543	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
A	245	SER	PHE	engineered mutation	UNP A0A150JSL8
B	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
B	245	SER	PHE	engineered mutation	UNP A0A150JSL8
C	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
C	245	SER	PHE	engineered mutation	UNP A0A150JSL8
D	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
D	245	SER	PHE	engineered mutation	UNP A0A150JSL8
E	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
E	245	SER	PHE	engineered mutation	UNP A0A150JSL8
F	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
F	245	SER	PHE	engineered mutation	UNP A0A150JSL8
G	121	ASN	ASP	engineered mutation	UNP A0A150JSL8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	245	SER	PHE	engineered mutation	UNP A0A150JSL8
H	121	ASN	ASP	engineered mutation	UNP A0A150JSL8
H	245	SER	PHE	engineered mutation	UNP A0A150JSL8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	61	Total O 61 61	0	0
2	C	50	Total O 50 50	0	0
2	D	66	Total O 66 66	0	0
2	E	75	Total O 75 75	0	0
2	F	69	Total O 69 69	0	0
2	G	66	Total O 66 66	0	0
2	H	57	Total O 57 57	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 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.

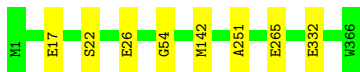
- Molecule 1: Glycerol dehydrogenase

Chain A:  99%



- Molecule 1: Glycerol dehydrogenase

Chain B:  98%



- Molecule 1: Glycerol dehydrogenase

Chain C:  97%



- Molecule 1: Glycerol dehydrogenase

Chain D:  99%



- Molecule 1: Glycerol dehydrogenase

Chain E:  98%



- Molecule 1: Glycerol dehydrogenase

Chain F:  98%



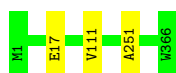
- Molecule 1: Glycerol dehydrogenase

Chain G:  98%  ..



- Molecule 1: Glycerol dehydrogenase

Chain H:  99%  .



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.67Å 211.77Å 149.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	149.71 – 2.40 49.90 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.1 (149.71-2.40) 96.1 (49.90-2.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0158 2016/10/03	Depositor
R, R_{free}	0.237 , 0.269 0.243 , 0.273	Depositor DCC
R_{free} test set	6235 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.914	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 7.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.209 for -k,-h,-l 0.000 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-l,1/2 *h-1/2*k 0.000 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+1,-1/ 2*h+1/2*k 0.000 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.000 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1 /2*h+1/2*k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22572	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7144e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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	0.45	0/2805	0.64	0/3798
1	B	0.47	0/2804	0.64	0/3798
1	C	0.45	0/2804	0.65	1/3798 (0.0%)
1	D	0.45	0/2804	0.63	0/3798
1	E	0.44	0/2804	0.62	0/3798
1	F	0.46	0/2801	0.64	0/3794
1	G	0.47	0/2804	0.65	0/3798
1	H	0.45	0/2804	0.63	0/3798
All	All	0.46	0/22430	0.64	1/30380 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	356	ASP	CB-CG-OD2	6.47	124.12	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	54	GLY	Peptide

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	A	2760	0	2793	1	0
1	B	2759	0	2793	1	0
1	C	2759	0	2793	7	0
1	D	2759	0	2793	2	0
1	E	2759	0	2793	2	0
1	F	2756	0	2782	1	0
1	G	2759	0	2793	2	0
1	H	2759	0	2793	0	0
2	A	58	0	0	0	0
2	B	61	0	0	1	0
2	C	50	0	0	1	0
2	D	66	0	0	1	0
2	E	75	0	0	0	0
2	F	69	0	0	0	0
2	G	66	0	0	1	0
2	H	57	0	0	0	0
All	All	22572	0	22333	16	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 0.

All (16) 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:C:130:ILE:CD1	1:C:141:LEU:HB2	2.35	0.56
1:C:130:ILE:HD13	1:C:141:LEU:HB2	1.92	0.52
1:E:22:SER:O	1:E:26:GLU:HG2	2.13	0.49
1:A:22:SER:O	1:A:26:GLU:HG2	2.13	0.48
1:C:22:SER:O	1:C:26:GLU:HG2	2.14	0.48
1:D:245:SER:HA	2:D:413:HOH:O	2.14	0.47
1:B:22:SER:O	1:B:26:GLU:HG2	2.15	0.47
1:C:130:ILE:CD1	1:C:141:LEU:CB	2.95	0.45
1:E:130:ILE:HD11	1:E:141:LEU:HD22	1.99	0.43
1:G:184:ARG:HD2	2:G:462:HOH:O	2.18	0.43
1:G:93:GLY:HA2	1:G:117:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:HOH:O	1:C:354:THR:HA	2.19	0.42
1:C:323:ARG:NH2	2:C:401:HOH:O	2.31	0.41
1:D:93:GLY:HA2	1:D:117:ILE:HD11	2.02	0.41
1:C:122:ALA:N	1:C:123:PRO:CD	2.85	0.40
1:F:111:VAL:HG13	1:F:147:PRO:HA	2.04	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	364/366 (100%)	358 (98%)	5 (1%)	1 (0%)	41	55
1	B	364/366 (100%)	359 (99%)	4 (1%)	1 (0%)	41	55
1	C	364/366 (100%)	358 (98%)	5 (1%)	1 (0%)	41	55
1	D	364/366 (100%)	358 (98%)	5 (1%)	1 (0%)	41	55
1	E	364/366 (100%)	358 (98%)	5 (1%)	1 (0%)	41	55
1	F	364/366 (100%)	359 (99%)	4 (1%)	1 (0%)	41	55
1	G	364/366 (100%)	359 (99%)	4 (1%)	1 (0%)	41	55
1	H	364/366 (100%)	358 (98%)	5 (1%)	1 (0%)	41	55
All	All	2912/2928 (100%)	2867 (98%)	37 (1%)	8 (0%)	41	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ALA
1	B	251	ALA
1	C	251	ALA
1	D	251	ALA
1	E	251	ALA

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Mol	Chain	Res	Type
1	F	251	ALA
1	G	251	ALA
1	H	251	ALA

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	292/292 (100%)	290 (99%)	2 (1%)	84	92
1	B	292/292 (100%)	288 (99%)	4 (1%)	67	82
1	C	292/292 (100%)	290 (99%)	2 (1%)	84	92
1	D	292/292 (100%)	290 (99%)	2 (1%)	84	92
1	E	292/292 (100%)	289 (99%)	3 (1%)	76	88
1	F	291/292 (100%)	287 (99%)	4 (1%)	67	82
1	G	292/292 (100%)	286 (98%)	6 (2%)	53	72
1	H	292/292 (100%)	290 (99%)	2 (1%)	84	92
All	All	2335/2336 (100%)	2310 (99%)	25 (1%)	73	87

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	317	LEU
1	B	17	GLU
1	B	142	MET
1	B	265	GLU
1	B	332	GLU
1	C	17	GLU
1	C	142	MET
1	D	17	GLU
1	D	117	ILE
1	E	17	GLU
1	E	265	GLU

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Mol	Chain	Res	Type
1	E	364	GLU
1	F	17	GLU
1	F	111	VAL
1	F	332	GLU
1	F	364	GLU
1	G	17	GLU
1	G	117	ILE
1	G	142	MET
1	G	184	ARG
1	G	265	GLU
1	G	332	GLU
1	H	17	GLU
1	H	111	VAL

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](#)

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	366/366 (100%)	-0.24	0 100 100	15, 25, 47, 63	0
1	B	366/366 (100%)	-0.20	0 100 100	14, 25, 46, 62	0
1	C	366/366 (100%)	-0.18	0 100 100	14, 25, 45, 63	0
1	D	366/366 (100%)	-0.22	2 (0%) 91 89	14, 25, 50, 74	0
1	E	366/366 (100%)	-0.22	0 100 100	14, 24, 45, 67	0
1	F	366/366 (100%)	-0.18	2 (0%) 91 89	14, 24, 50, 68	0
1	G	366/366 (100%)	-0.21	1 (0%) 94 93	13, 23, 47, 59	0
1	H	366/366 (100%)	-0.22	0 100 100	13, 24, 49, 63	0
All	All	2928/2928 (100%)	-0.21	5 (0%) 95 94	13, 24, 48, 74	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	317	LEU	4.0
1	D	317	LEU	2.5
1	G	317	LEU	2.5
1	F	56	GLU	2.3
1	D	316	GLU	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.