



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4ECD / pdb_00004ecd
Title : 2.5 Angstrom Resolution Crystal Structure of Bifidobacterium longum Chorisynthase
Authors : Light, S.H.; Minasov, G.; Krishna, S.N.; Shuvalova, L.; Kwon, K.; Lavie, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-03-26
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

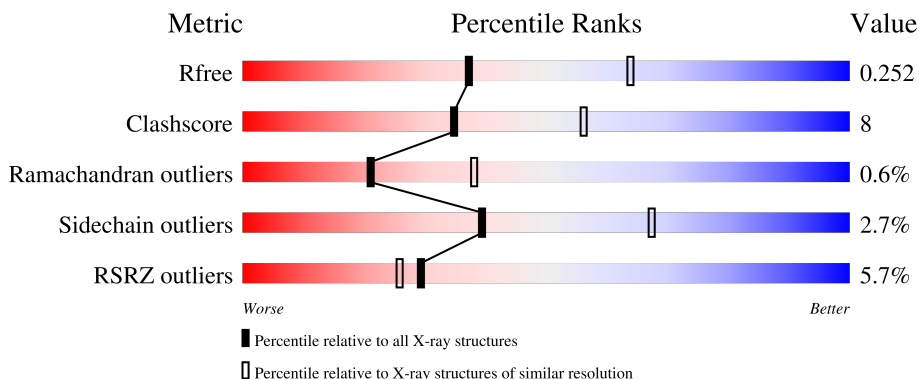
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	398	
1	B	398	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4151 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	Total	C	N	O	S	0	3	0
			2028	1264	366	391	7			
1	B	268	Total	C	N	O	S	0	1	0
			1983	1238	358	380	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B7GS97
A	-1	ASN	-	expression tag	UNP B7GS97
A	0	ALA	-	expression tag	UNP B7GS97
B	-2	SER	-	expression tag	UNP B7GS97
B	-1	ASN	-	expression tag	UNP B7GS97
B	0	ALA	-	expression tag	UNP B7GS97

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	68	Total	O	0	3
			71	71		
3	B	65	Total	O	0	0
			65	65		

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.94Å 123.94Å 97.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 2.50 29.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.54-2.50) 97.6 (29.54-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.253 0.197 , 0.252	Depositor DCC
R_{free} test set	1312 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.0	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	0.95	EDS
Total number of atoms	4151	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: CL

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	1.02	0/2056	1.09	9/2777 (0.3%)
1	B	1.01	4/2002 (0.2%)	1.03	3/2704 (0.1%)
All	All	1.01	4/4058 (0.1%)	1.06	12/5481 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	HIS	CG-CD2	6.36	1.42	1.35
1	B	165	HIS	CE1-NE2	5.91	1.38	1.32
1	B	65	HIS	CG-CD2	5.71	1.42	1.35
1	B	261	VAL	C-O	-5.53	1.17	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ALA	N-CA-C	6.77	118.32	111.07
1	A	192	SER	CA-C-N	5.84	125.52	119.56
1	A	192	SER	C-N-CA	5.84	125.52	119.56
1	B	252	ILE	CB-CA-C	-5.62	104.62	111.87
1	A	12	GLY	N-CA-C	-5.38	103.29	112.64
1	A	15	LEU	N-CA-C	-5.37	101.41	109.95
1	B	373	GLY	N-CA-C	-5.29	103.90	111.42
1	A	388	ALA	N-CA-C	-5.17	106.98	113.28
1	A	182[A]	THR	CA-C-N	-5.06	114.40	119.56
1	A	182[A]	THR	C-N-CA	-5.06	114.40	119.56
1	A	182[B]	THR	CA-C-N	-5.06	114.40	119.56
1	A	182[B]	THR	C-N-CA	-5.06	114.40	119.56

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	2028	0	2072	38	0
1	B	1983	0	2027	25	0
2	A	2	0	0	0	0
2	B	2	0	0	1	0
3	A	71	0	0	1	0
3	B	65	0	0	1	0
All	All	4151	0	4099	61	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 (61) 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:139[B]:GLU:OE2	1:A:139[B]:GLU:HA	1.72	0.86
1:A:237:TYR:CE2	1:A:303:MET:HE1	2.10	0.86
1:A:175:ASN:HD22	1:A:178:LEU:CD1	1.94	0.81
1:B:226:LEU:CD2	1:B:310:ARG:HG3	2.10	0.80
1:A:2:LEU:HD11	1:A:22:LEU:HD13	1.68	0.76
1:A:175:ASN:ND2	1:A:178:LEU:HD13	2.01	0.74
1:A:175:ASN:ND2	1:A:178:LEU:CD1	2.52	0.72
1:B:173:GLN:HE21	1:B:173:GLN:N	1.93	0.66
1:B:226:LEU:HD23	1:B:310:ARG:HG3	1.77	0.65
1:B:256:GLN:O	1:B:257:ALA:HB3	1.97	0.65
1:A:175:ASN:HD22	1:A:178:LEU:HD13	1.62	0.62
1:A:267:PHE:HB2	3:A:510:HOH:O	2.00	0.61
1:B:305:ASN:OD1	1:B:307:GLN:HB2	2.00	0.61
1:B:223:ILE:C	1:B:223:ILE:HD12	2.27	0.60
1:A:237:TYR:CZ	1:A:303:MET:HE1	2.38	0.58
1:A:226:LEU:CD2	1:A:310:ARG:HG2	2.35	0.57
1:A:256:GLN:O	1:A:257:ALA:HB3	2.04	0.57
1:A:226:LEU:HD23	1:A:310:ARG:HG2	1.87	0.57
1:B:236:THR:HA	1:B:303:MET:HE3	1.87	0.56
1:A:175:ASN:HD22	1:A:178:LEU:HD11	1.68	0.54
1:A:250:SER:OG	1:B:241:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:GLN:O	1:B:257:ALA:CB	2.58	0.52
1:B:253:MET:HE3	1:B:261:VAL:HG12	1.92	0.51
1:A:200:GLU:HG2	1:A:204:ARG:HH21	1.76	0.50
1:A:268:LEU:O	1:A:268:LEU:HD23	2.11	0.50
1:A:182[B]:THR:OG1	1:A:183:PRO:HD2	2.12	0.50
1:A:58:ARG:NH1	1:A:60:LEU:HD21	2.27	0.50
1:A:153:PHE:CZ	1:A:368:LEU:HD13	2.46	0.50
1:B:226:LEU:HA	1:B:309:ILE:O	2.12	0.49
1:A:182[B]:THR:HG23	1:A:184:ASP:H	1.77	0.48
1:B:138:ARG:NH1	1:B:256:GLN:HB3	2.28	0.48
1:A:262:GLU:HG3	1:B:267:PHE:CZ	2.49	0.48
1:B:383:LEU:O	1:B:387:LEU:HB2	2.14	0.48
2:B:402:CL:CL	3:B:501:HOH:O	2.57	0.47
1:B:172:VAL:HG13	1:B:204:ARG:NH1	2.29	0.47
1:A:230:VAL:HG21	1:A:309:ILE:HD12	1.96	0.46
1:B:245:ASP:N	1:B:245:ASP:OD1	2.48	0.46
1:A:253:MET:HE3	1:A:261:VAL:HG12	1.96	0.46
1:A:1[A]:MET:HE3	1:A:1[A]:MET:HB2	1.88	0.46
1:A:315:MET:HE3	1:A:317:PRO:HG3	1.99	0.45
1:B:199:LYS:HA	1:B:199:LYS:HD3	1.75	0.44
1:B:253:MET:CE	1:B:261:VAL:HG12	2.48	0.44
1:A:223:ILE:C	1:A:223:ILE:HD12	2.43	0.44
1:A:253:MET:HE1	1:A:260:GLY:C	2.42	0.44
1:A:54:GLN:HG2	1:A:55:ASP:N	2.32	0.44
1:A:194:VAL:HG12	1:A:194:VAL:O	2.18	0.44
1:B:253:MET:CA	1:B:253:MET:HE2	2.49	0.43
1:A:256:GLN:O	1:A:257:ALA:CB	2.66	0.42
1:B:21:GLY:O	1:B:368:LEU:HD21	2.20	0.42
1:A:182[B]:THR:HG22	1:A:185:ASP:OD2	2.20	0.42
1:A:194:VAL:O	1:A:194:VAL:CG1	2.68	0.42
1:B:163:VAL:HG11	1:B:181:PRO:HB2	2.02	0.42
1:A:36:ALA:HB2	1:A:148:GLU:OE1	2.20	0.41
1:A:177:ASP:N	1:A:177:ASP:OD1	2.53	0.41
1:A:21:GLY:O	1:A:368:LEU:HD21	2.20	0.41
1:B:169:LEU:C	1:B:169:LEU:HD23	2.46	0.41
1:B:249:ALA:HA	1:B:261:VAL:HG21	2.02	0.41
1:A:267:PHE:CZ	1:B:262:GLU:HG3	2.55	0.40
1:B:253:MET:HE1	1:B:260:GLY:C	2.45	0.40
1:A:182[B]:THR:HG23	1:A:184:ASP:N	2.35	0.40
1:A:237:TYR:CE2	1:A:303:MET:CE	2.95	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	265/398 (67%)	257 (97%)	6 (2%)	2 (1%)	16	31
1	B	256/398 (64%)	252 (98%)	3 (1%)	1 (0%)	30	49
All	All	521/796 (66%)	509 (98%)	9 (2%)	3 (1%)	21	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLY
1	A	372	GLY
1	B	257	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	206/307 (67%)	199 (97%)	7 (3%)	32	60
1	B	201/307 (66%)	197 (98%)	4 (2%)	48	75
All	All	407/614 (66%)	396 (97%)	11 (3%)	39	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	13	GLU
1	A	22	LEU

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Mol	Chain	Res	Type
1	A	31	ASP
1	A	46	ARG
1	A	173	GLN
1	A	315	MET
1	B	27	ARG
1	B	40	ARG
1	B	79	ASN
1	B	173	GLN

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	173	GLN
1	A	175	ASN
1	B	65	HIS
1	B	173	GLN
1	B	382	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

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

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	A	274/398 (68%)	-0.02	19 (6%) 23 20	25, 42, 90, 138	3 (1%)
1	B	268/398 (67%)	-0.17	12 (4%) 38 33	25, 41, 80, 107	1 (0%)
All	All	542/796 (68%)	-0.09	31 (5%) 29 26	25, 41, 85, 138	4 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	6.1
1	A	0	ALA	3.9
1	B	268	LEU	3.9
1	A	268	LEU	3.9
1	A	171	GLY	3.7
1	A	295	ARG	3.7
1	A	237	TYR	3.7
1	A	266	GLY	3.6
1	B	1[A]	MET	3.4
1	B	212	ALA	3.0
1	A	172	VAL	2.9
1	B	345	SER	2.9
1	A	265	ASP	2.9
1	A	11	HIS	2.8
1	A	215	ALA	2.7
1	A	296	ALA	2.7
1	B	215	ALA	2.7
1	B	79	ASN	2.6
1	A	10	SER	2.6
1	B	389	SER	2.6
1	A	173	GLN	2.5
1	B	269	ALA	2.5
1	B	217	ASP	2.4
1	A	174	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	267	PHE	2.3
1	B	317	PRO	2.2
1	A	264	GLY	2.2
1	A	242	ARG	2.2
1	A	54	GLN	2.1
1	B	10	SER	2.1
1	B	218	THR	2.0

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 oligosaccharides 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
2	CL	A	402	1/1	0.91	0.09	55,55,55,55	0
2	CL	A	401	1/1	0.94	0.06	53,53,53,53	0
2	CL	B	402	1/1	0.94	0.08	46,46,46,46	0
2	CL	B	401	1/1	0.97	0.05	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.