



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 10:47 PM EDT

PDB ID : 1LEH  
Title : LEUCINE DEHYDROGENASE FROM BACILLUS SPHAERICUS  
Authors : Baker, P.J.; Turnbull, A.P.; Sedelnikova, S.E.; Stillman, T.J.; Rice, D.W.  
Deposited on : 1995-06-09  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

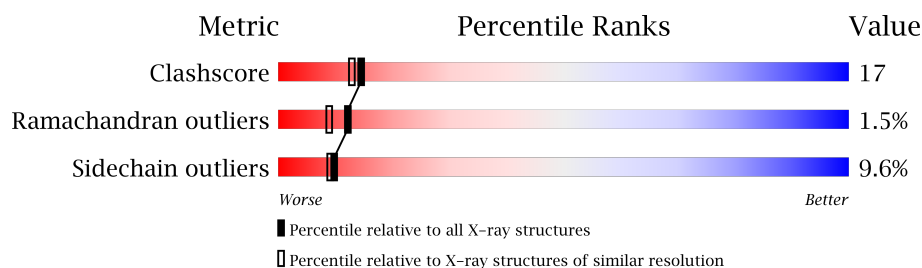
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	364	 66% 29% 5%
1	B	364	 61% 30% 8%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5604 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 LEUCINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2744	1725	473	533	13			
1	B	364	Total	C	N	O	S	0	0	0
			2744	1725	473	533	13			

There are 146 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ILE	LEU	CONFLICT	UNP Q7SIB4
A	9	LYS	THR	CONFLICT	UNP Q7SIB4
A	15	LEU	VAL	CONFLICT	UNP Q7SIB4
A	16	VAL	LEU	CONFLICT	UNP Q7SIB4
A	21	GLU	LYS	CONFLICT	UNP Q7SIB4
A	22	ALA	GLU	CONFLICT	UNP Q7SIB4
A	28	VAL	ILE	CONFLICT	UNP Q7SIB4
A	43	ALA	THR	CONFLICT	UNP Q7SIB4
A	47	THR	MET	CONFLICT	UNP Q7SIB4
A	50	ALA	SER	CONFLICT	UNP Q7SIB4
A	55	ILE	LEU	CONFLICT	UNP Q7SIB4
A	88	PHE	ARG	CONFLICT	UNP Q7SIB4
A	89	ALA	LYS	CONFLICT	UNP Q7SIB4
A	94	ASP	ALA	CONFLICT	UNP Q7SIB4
A	99	LEU	PHE	CONFLICT	UNP Q7SIB4
A	121	ASP	ALA	CONFLICT	UNP Q7SIB4
A	125	LEU	ILE	CONFLICT	UNP Q7SIB4
A	127	HIS	TYR	CONFLICT	UNP Q7SIB4
A	139	ALA	GLU	CONFLICT	UNP Q7SIB4
A	149	VAL	ALA	CONFLICT	UNP Q7SIB4
A	174	LEU	LYS	CONFLICT	UNP Q7SIB4
A	175	ALA	VAL	CONFLICT	UNP Q7SIB4
A	177	SER	ALA	CONFLICT	UNP Q7SIB4
A	181	LEU	VAL	CONFLICT	UNP Q7SIB4
A	186	LYS	TYR	CONFLICT	UNP Q7SIB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ALA	HIS	CONFLICT	UNP Q7SIB4
A	190	LYS	ARG	CONFLICT	UNP Q7SIB4
A	191	LYS	HIS	CONFLICT	UNP Q7SIB4
A	193	ASN	HIS	CONFLICT	UNP Q7SIB4
A	194	THR	GLU	CONFLICT	UNP Q7SIB4
A	200	VAL	ILE	CONFLICT	UNP Q7SIB4
A	204	VAL	ILE	CONFLICT	UNP Q7SIB4
A	207	ALA	GLU	CONFLICT	UNP Q7SIB4
A	208	ALA	VAL	CONFLICT	UNP Q7SIB4
A	210	SER	ALA	CONFLICT	UNP Q7SIB4
A	211	ALA	ARG	CONFLICT	UNP Q7SIB4
A	214	ALA	GLU	CONFLICT	UNP Q7SIB4
A	216	GLU	PHE	CONFLICT	UNP Q7SIB4
A	219	ASP	LYS	CONFLICT	UNP Q7SIB4
A	222	ALA	ASP	CONFLICT	UNP Q7SIB4
A	225	ALA	ASP	CONFLICT	UNP Q7SIB4
A	230	THR	GLU	CONFLICT	UNP Q7SIB4
A	241	ALA	GLY	CONFLICT	UNP Q7SIB4
A	242	VAL	ILE	CONFLICT	UNP Q7SIB4
A	243	LEU	ILE	CONFLICT	UNP Q7SIB4
A	246	PHE	GLN	CONFLICT	UNP Q7SIB4
A	266	ASP	GLU	CONFLICT	UNP Q7SIB4
A	271	LYS	ASP	CONFLICT	UNP Q7SIB4
A	272	TYR	ILE	CONFLICT	UNP Q7SIB4
A	273	LEU	ILE	CONFLICT	UNP Q7SIB4
A	276	LEU	MET	CONFLICT	UNP Q7SIB4
A	304	THR	GLU	CONFLICT	UNP Q7SIB4
A	309	ARG	LYS	CONFLICT	UNP Q7SIB4
A	310	VAL	ILE	CONFLICT	UNP Q7SIB4
A	311	ASP	GLU	CONFLICT	UNP Q7SIB4
A	312	GLY	GLN	CONFLICT	UNP Q7SIB4
A	316	SER	ASN	CONFLICT	UNP Q7SIB4
A	320	ILE	VAL	CONFLICT	UNP Q7SIB4
A	324	SER	ALA	CONFLICT	UNP Q7SIB4
A	328	GLY	ASN	CONFLICT	UNP Q7SIB4
A	329	VAL	ILE	CONFLICT	UNP Q7SIB4
A	331	SER	THR	CONFLICT	UNP Q7SIB4
A	344	ALA	GLU	CONFLICT	UNP Q7SIB4
A	345	LYS	THR	CONFLICT	UNP Q7SIB4
A	346	VAL	MET	CONFLICT	UNP Q7SIB4
A	347	ALA	ARG	CONFLICT	UNP Q7SIB4
A	350	ARG	ALA	CONFLICT	UNP Q7SIB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ASP	ASN	CONFLICT	UNP Q7SIB4
A	357	GLN	GLY	CONFLICT	UNP Q7SIB4
A	358	ARG	HIS	CONFLICT	UNP Q7SIB4
A	359	ASN	HIS	CONFLICT	UNP Q7SIB4
A	362	ASN	SER	CONFLICT	UNP Q7SIB4
A	363	GLY	ARG	CONFLICT	UNP Q7SIB4
B	3	ILE	LEU	CONFLICT	UNP Q7SIB4
B	9	LYS	THR	CONFLICT	UNP Q7SIB4
B	15	LEU	VAL	CONFLICT	UNP Q7SIB4
B	16	VAL	LEU	CONFLICT	UNP Q7SIB4
B	21	GLU	LYS	CONFLICT	UNP Q7SIB4
B	22	ALA	GLU	CONFLICT	UNP Q7SIB4
B	28	VAL	ILE	CONFLICT	UNP Q7SIB4
B	43	ALA	THR	CONFLICT	UNP Q7SIB4
B	47	THR	MET	CONFLICT	UNP Q7SIB4
B	50	ALA	SER	CONFLICT	UNP Q7SIB4
B	55	ILE	LEU	CONFLICT	UNP Q7SIB4
B	88	PHE	ARG	CONFLICT	UNP Q7SIB4
B	89	ALA	LYS	CONFLICT	UNP Q7SIB4
B	94	ASP	ALA	CONFLICT	UNP Q7SIB4
B	99	LEU	PHE	CONFLICT	UNP Q7SIB4
B	121	ASP	ALA	CONFLICT	UNP Q7SIB4
B	125	LEU	ILE	CONFLICT	UNP Q7SIB4
B	127	HIS	TYR	CONFLICT	UNP Q7SIB4
B	139	ALA	GLU	CONFLICT	UNP Q7SIB4
B	149	VAL	ALA	CONFLICT	UNP Q7SIB4
B	174	LEU	LYS	CONFLICT	UNP Q7SIB4
B	175	ALA	VAL	CONFLICT	UNP Q7SIB4
B	177	SER	ALA	CONFLICT	UNP Q7SIB4
B	181	LEU	VAL	CONFLICT	UNP Q7SIB4
B	186	LYS	TYR	CONFLICT	UNP Q7SIB4
B	187	ALA	HIS	CONFLICT	UNP Q7SIB4
B	190	LYS	ARG	CONFLICT	UNP Q7SIB4
B	191	LYS	HIS	CONFLICT	UNP Q7SIB4
B	193	ASN	HIS	CONFLICT	UNP Q7SIB4
B	194	THR	GLU	CONFLICT	UNP Q7SIB4
B	200	VAL	ILE	CONFLICT	UNP Q7SIB4
B	204	VAL	ILE	CONFLICT	UNP Q7SIB4
B	207	ALA	GLU	CONFLICT	UNP Q7SIB4
B	208	ALA	VAL	CONFLICT	UNP Q7SIB4
B	210	SER	ALA	CONFLICT	UNP Q7SIB4
B	211	ALA	ARG	CONFLICT	UNP Q7SIB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	214	ALA	GLU	CONFLICT	UNP Q7SIB4
B	216	GLU	PHE	CONFLICT	UNP Q7SIB4
B	219	ASP	LYS	CONFLICT	UNP Q7SIB4
B	222	ALA	ASP	CONFLICT	UNP Q7SIB4
B	225	ALA	ASP	CONFLICT	UNP Q7SIB4
B	230	THR	GLU	CONFLICT	UNP Q7SIB4
B	241	ALA	GLY	CONFLICT	UNP Q7SIB4
B	242	VAL	ILE	CONFLICT	UNP Q7SIB4
B	243	LEU	ILE	CONFLICT	UNP Q7SIB4
B	246	PHE	GLN	CONFLICT	UNP Q7SIB4
B	266	ASP	GLU	CONFLICT	UNP Q7SIB4
B	271	LYS	ASP	CONFLICT	UNP Q7SIB4
B	272	TYR	ILE	CONFLICT	UNP Q7SIB4
B	273	LEU	ILE	CONFLICT	UNP Q7SIB4
B	276	LEU	MET	CONFLICT	UNP Q7SIB4
B	304	THR	GLU	CONFLICT	UNP Q7SIB4
B	309	ARG	LYS	CONFLICT	UNP Q7SIB4
B	310	VAL	ILE	CONFLICT	UNP Q7SIB4
B	311	ASP	GLU	CONFLICT	UNP Q7SIB4
B	312	GLY	GLN	CONFLICT	UNP Q7SIB4
B	316	SER	ASN	CONFLICT	UNP Q7SIB4
B	320	ILE	VAL	CONFLICT	UNP Q7SIB4
B	324	SER	ALA	CONFLICT	UNP Q7SIB4
B	328	GLY	ASN	CONFLICT	UNP Q7SIB4
B	329	VAL	ILE	CONFLICT	UNP Q7SIB4
B	331	SER	THR	CONFLICT	UNP Q7SIB4
B	344	ALA	GLU	CONFLICT	UNP Q7SIB4
B	345	LYS	THR	CONFLICT	UNP Q7SIB4
B	346	VAL	MET	CONFLICT	UNP Q7SIB4
B	347	ALA	ARG	CONFLICT	UNP Q7SIB4
B	350	ARG	ALA	CONFLICT	UNP Q7SIB4
B	356	ASP	ASN	CONFLICT	UNP Q7SIB4
B	357	GLN	GLY	CONFLICT	UNP Q7SIB4
B	358	ARG	HIS	CONFLICT	UNP Q7SIB4
B	359	ASN	HIS	CONFLICT	UNP Q7SIB4
B	362	ASN	SER	CONFLICT	UNP Q7SIB4
B	363	GLY	ARG	CONFLICT	UNP Q7SIB4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	70	Total O 70 70	0	0

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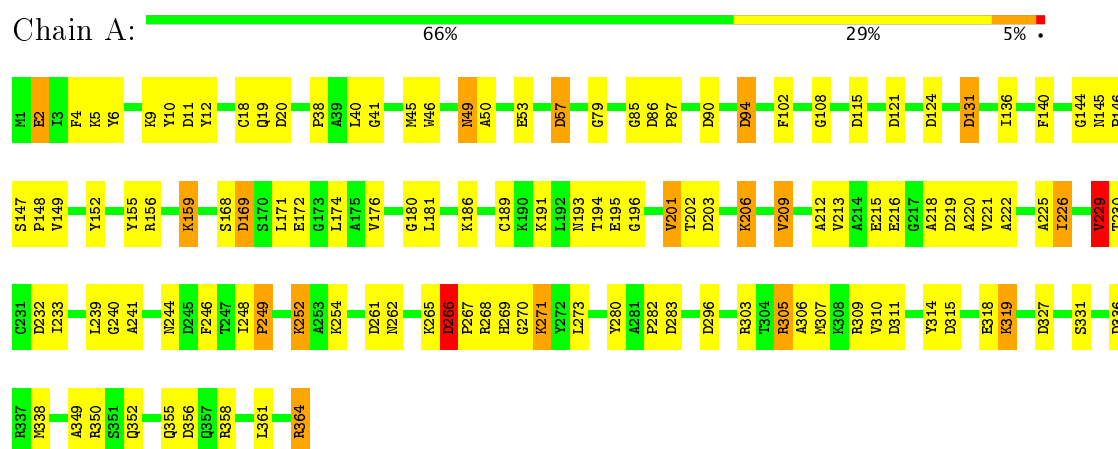
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	46	Total	O	0	0
			46	46		

### 3 Residue-property plots

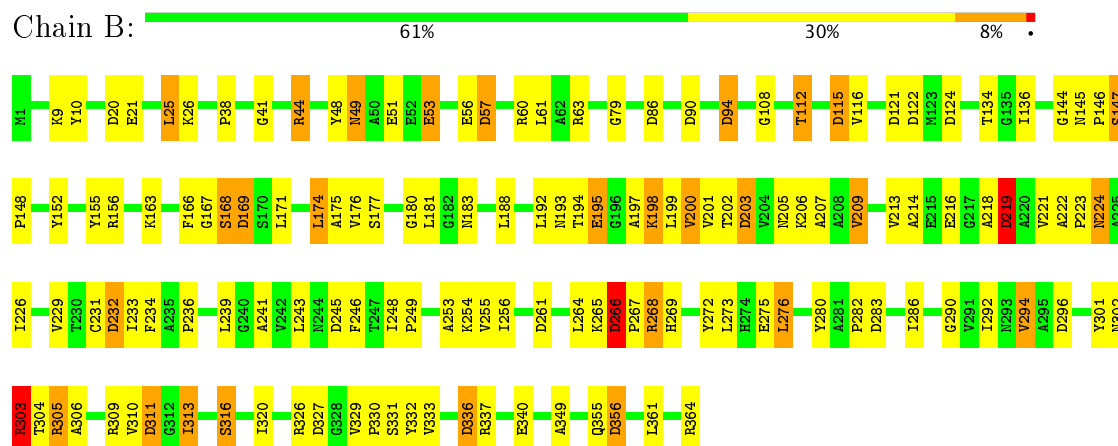
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: LEUCINE DEHYDROGENASE



#### • Molecule 1: LEUCINE DEHYDROGENASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.40 Å   138.40 Å   121.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	97.0 (10.00-2.20)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 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	0.71	0/2788	1.28	44/3769 (1.2%)
1	B	0.71	1/2788 (0.0%)	1.31	48/3769 (1.3%)
All	All	0.71	1/5576 (0.0%)	1.30	92/7538 (1.2%)

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	A	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	ARG	CZ-NH2	5.06	1.39	1.33

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	B	44	ARG	NE-CZ-NH1	-10.69	114.96	120.30
1	A	311	ASP	CB-CG-OD2	-10.12	109.19	118.30
1	B	44	ARG	NE-CZ-NH2	9.42	125.01	120.30
1	B	94	ASP	CB-CG-OD2	8.54	125.98	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	229	VAL	CA

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	A	2744	0	2725	84	0
1	B	2744	0	2725	106	0
2	A	70	0	0	0	0
2	B	46	0	0	1	0
All	All	5604	0	5450	188	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 17.

The worst 5 of 188 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:B:166:PHE:HE2	1:B:232:ASP:HB3	1.07	1.13
1:B:166:PHE:CE2	1:B:232:ASP:HB3	1.95	1.01
1:B:9:LYS:HD3	1:B:10:TYR:CE2	2.01	0.96
1:A:268:ARG:HA	1:A:271:LYS:HE2	1.48	0.94
1:B:171:LEU:HD13	1:B:192:LEU:HD21	1.48	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	362/364 (100%)	340 (94%)	19 (5%)	3 (1%)	22	21
1	B	362/364 (100%)	324 (90%)	30 (8%)	8 (2%)	8	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	724/728 (100%)	664 (92%)	49 (7%)	11 (2%)	12	9

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	GLY
1	B	174	LEU
1	B	214	ALA
1	B	253	ALA
1	A	49	ASN

### 5.3.2 Protein sidechains ⓘ

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	277/277 (100%)	252 (91%)	25 (9%)	11	11
1	B	277/277 (100%)	249 (90%)	28 (10%)	9	8
All	All	554/554 (100%)	501 (90%)	53 (10%)	10	9

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	MET
1	B	112	THR
1	B	303	ARG
1	A	355	GLN
1	B	49	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	49	ASN
1	B	179	GLN

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Mol	Chain	Res	Type
1	A	357	GLN
1	B	145	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 carbohydrates 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.