



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:51 PM UTC

PDB ID : 1DCL / pdb\_00001dcl  
Title : MCG, A LAMBDA V TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN), CRYSTALLIZED FROM AMMONIUM SULFATE  
Authors : Schiffer, M.; Xu, Z.B.  
Deposited on : 1995-10-16  
Resolution : 2.30 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

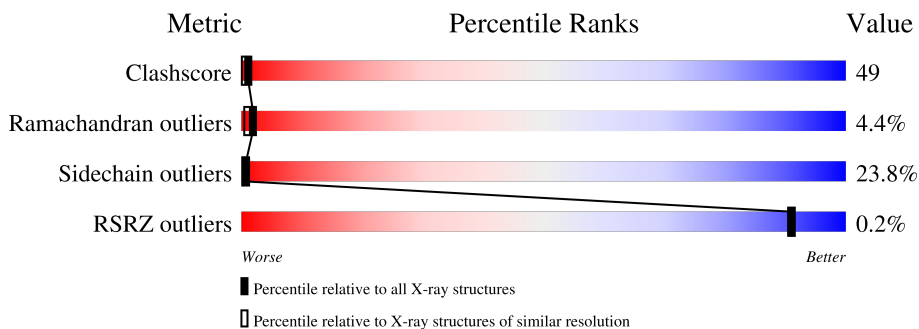
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

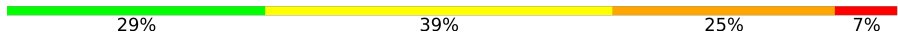
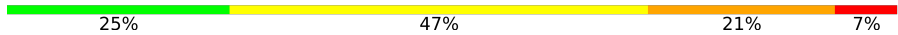
The reported resolution of this entry is 2.30 Å.

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	216	 29% 39% 25% 7%
1	B	216	 25% 47% 21% 7%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3621 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 MCG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1604	1000	267	332	5	0	0	0
1	B	216	1604	1000	267	332	5	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ILE	PHE	conflict	UNP P01709
A	23	THR	SER	conflict	UNP P01709
A	28	ASN	ASP	conflict	UNP P01709
A	29	VAL	ILE	conflict	UNP P01709
A	31	GLY	ASN	conflict	UNP P01709
A	39	GLN	ARG	conflict	UNP P01709
A	42	ALA	PRO	conflict	UNP P01709
A	48	VAL	LEU	conflict	UNP P01709
A	49	ILE	MET	conflict	UNP P01709
A	54	ASN	THR	conflict	UNP P01709
A	62	ASP	ASN	conflict	UNP P01709
A	94	GLU	ALA	conflict	UNP P01709
A	97	ASP	ASN	conflict	UNP P01709
A	98	ASN	SER	conflict	UNP P01709
A	99	PHE	LEU	conflict	UNP P01709
A	100	VAL	ILE	conflict	UNP P01709
A	103	THR	GLY	conflict	UNP P01709
A	106	LYS	ARG	conflict	UNP P01709
A	107	VAL	LEU	conflict	UNP P01709
A	116	ASN	ALA	conflict	UNP P01709
A	118	THR	SER	conflict	UNP P01709
A	156	GLY	SER	conflict	UNP P01709
A	167	LYS	THR	conflict	UNP P01709
B	20	ILE	PHE	conflict	UNP P01709
B	23	THR	SER	conflict	UNP P01709

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Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASN	ASP	conflict	UNP P01709
B	29	VAL	ILE	conflict	UNP P01709
B	31	GLY	ASN	conflict	UNP P01709
B	39	GLN	ARG	conflict	UNP P01709
B	42	ALA	PRO	conflict	UNP P01709
B	48	VAL	LEU	conflict	UNP P01709
B	49	ILE	MET	conflict	UNP P01709
B	54	ASN	THR	conflict	UNP P01709
B	62	ASP	ASN	conflict	UNP P01709
B	94	GLU	ALA	conflict	UNP P01709
B	97	ASP	ASN	conflict	UNP P01709
B	98	ASN	SER	conflict	UNP P01709
B	99	PHE	LEU	conflict	UNP P01709
B	100	VAL	ILE	conflict	UNP P01709
B	103	THR	GLY	conflict	UNP P01709
B	106	LYS	ARG	conflict	UNP P01709
B	107	VAL	LEU	conflict	UNP P01709
B	116	ASN	ALA	conflict	UNP P01709
B	118	THR	SER	conflict	UNP P01709
B	156	GLY	SER	conflict	UNP P01709
B	167	LYS	THR	conflict	UNP P01709

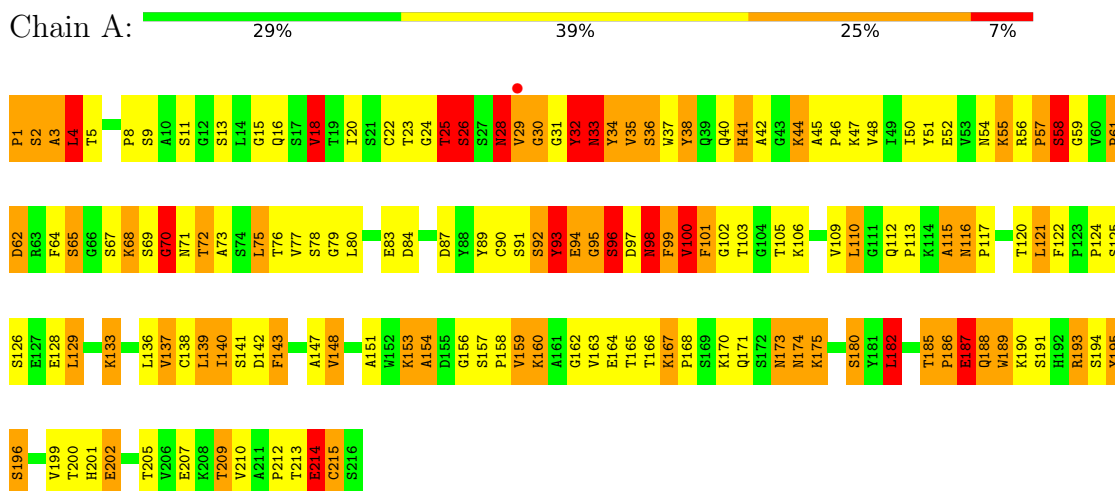
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	195	Total O 195 195	0	0
2	B	218	Total O 218 218	0	0

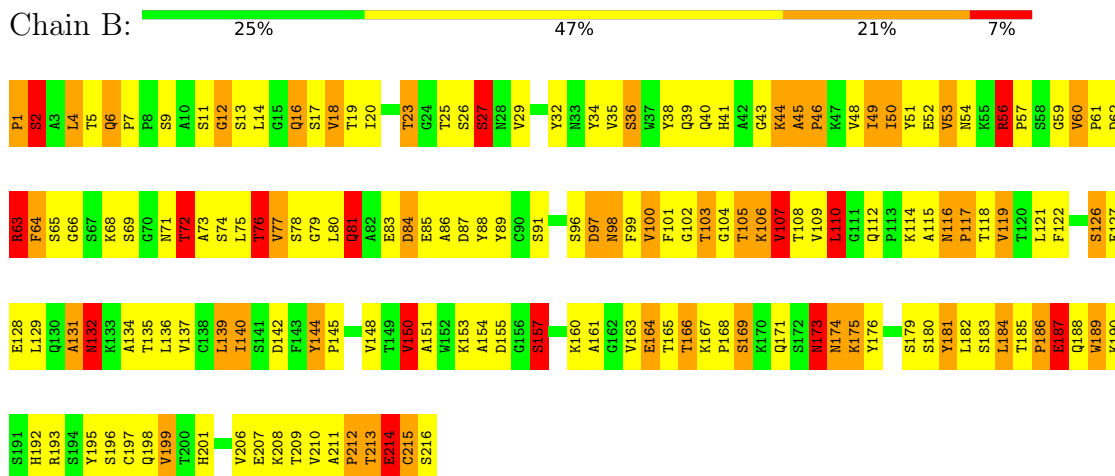
### 3 Residue-property plots

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: MCG



- Molecule 1: MCG



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.30Å 72.30Å 185.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30 62.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30) 49.7 (62.61-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.140 , (Not available) 0.149 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , 14.8	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Theoretical 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](#)

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	1.34	2/1643 (0.1%)	2.56	125/2241 (5.6%)
1	B	1.36	7/1643 (0.4%)	2.53	120/2241 (5.4%)
All	All	1.35	9/3286 (0.3%)	2.54	245/4482 (5.5%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	GLY	N-CA	7.78	1.52	1.44
1	A	57	PRO	C-O	6.24	1.32	1.24
1	A	5	THR	CA-CB	6.14	1.61	1.53
1	B	103	THR	C-O	5.89	1.31	1.24
1	B	5	THR	CA-CB	5.68	1.60	1.53

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PRO	CA-C-N	14.16	148.58	121.54
1	B	1	PRO	C-N-CA	14.16	148.58	121.54
1	B	174	ASN	CA-CB-CG	-13.03	99.57	112.60
1	A	159	VAL	CB-CA-C	12.10	125.24	111.08
1	A	92	SER	CA-C-N	11.18	142.89	121.54

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	1604	0	1542	176	0
1	B	1604	0	1542	145	1
2	A	195	0	0	24	4
2	B	218	0	0	15	2
All	All	3621	0	3084	308	4

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 49.

The worst 5 of 308 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:31:GLY:O	1:A:32:TYR:HB2	1.42	1.14
1:A:93:TYR:CE1	1:A:96:SER:HB3	1.84	1.12
1:B:23:THR:HG23	1:B:72:THR:HG22	1.36	1.07
1:A:213:THR:O	1:A:214:GLU:HB2	1.55	1.06
1:B:160:LYS:H	1:B:160:LYS:HD3	1.11	1.05

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:769:HOH:O	2:B:820:HOH:O[6_656]	0.99	1.21
2:A:597:HOH:O	2:A:903:HOH:O[6_656]	1.69	0.51
2:A:647:HOH:O	2:B:901:HOH:O[6_656]	1.76	0.44
1:B:216:SER:O	2:A:526:HOH:O[2_545]	1.94	0.26

## 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	214/216 (99%)	183 (86%)	16 (8%)	15 (7%)	<b>1</b> <b>0</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	214/216 (99%)	189 (88%)	21 (10%)	4 (2%)	6	5
All	All	428/432 (99%)	372 (87%)	37 (9%)	19 (4%)	2	1

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	29	VAL
1	A	32	TYR
1	A	33	ASN
1	A	96	SER

### 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	181/181 (100%)	136 (75%)	45 (25%)	0	0
1	B	181/181 (100%)	140 (77%)	41 (23%)	1	1
All	All	362/362 (100%)	276 (76%)	86 (24%)	1	0

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	LEU
1	B	150	VAL
1	B	78	SER
1	B	110	LEU
1	B	164	GLU

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

Mol	Chain	Res	Type
1	A	192	HIS
1	B	81	GLN

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Mol	Chain	Res	Type
1	B	198	GLN
1	B	132	ASN
1	B	173	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](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	216/216 (100%)	-0.82	1 (0%) 87   87	8, 19, 47, 53	0
1	B	216/216 (100%)	-0.82	0 100   100	8, 21, 38, 55	0
All	All	432/432 (100%)	-0.82	1 (0%) 91   91	8, 20, 45, 55	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	VAL	2.4

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.