



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2019 – 09:59 PM EST

PDB ID : 2MCG  
Title : THREE-DIMENSIONAL STRUCTURE OF A LIGHT CHAIN DIMER  
CRYSTALLIZED IN WATER. CONFORMATIONAL FLEXIBILITY OF A  
MOLECULE IN TWO CRYSTAL FORMS  
Authors : Ely, K.R.; Herron, J.N.; Edmundson, A.B.  
Deposited on : 1989-05-09  
Resolution : 2.00 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.

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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  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

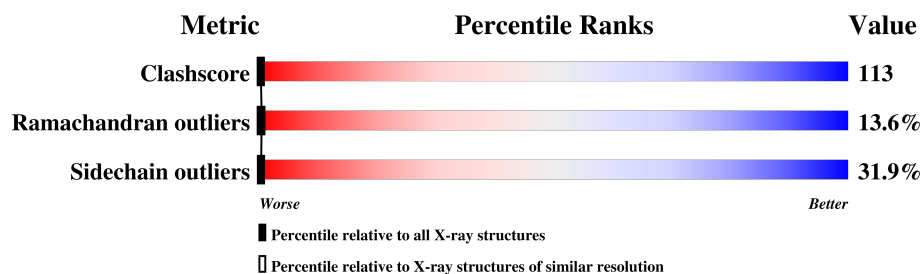
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

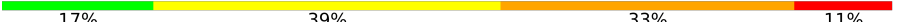

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	216	
1	2	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PCA	1	1	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3530 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 IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	216	Total	C	N	O	S	0	0	0
			1606	1000	266	335	5			
1	2	216	Total	C	N	O	S	0	0	0
			1606	1000	266	335	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	20	ILE	PHE	conflict	UNP P01709
1	23	THR	SER	conflict	UNP P01709
1	29	VAL	ILE	conflict	UNP P01709
1	31	GLY	ASN	conflict	UNP P01709
1	39	GLN	ARG	conflict	UNP P01709
1	42	ALA	PRO	conflict	UNP P01709
1	48	VAL	LEU	conflict	UNP P01709
1	49	ILE	MET	conflict	UNP P01709
1	54	ASN	THR	conflict	UNP P01709
1	62	ASP	ASN	conflict	UNP P01709
1	94	GLU	ALA	conflict	UNP P01709
1	97	ASP	ASN	conflict	UNP P01709
1	98	ASN	SER	conflict	UNP P01709
1	99	PHE	LEU	conflict	UNP P01709
1	100	VAL	ILE	conflict	UNP P01709
1	103	THR	GLY	conflict	UNP P01709
1	106	LYS	ARG	conflict	UNP P01709
1	107	VAL	LEU	conflict	UNP P01709
1	116	ASN	ALA	conflict	UNP P01709
1	118	THR	SER	conflict	UNP P01709
1	156	GLY	SER	conflict	UNP P01709
1	167	LYS	THR	conflict	UNP P01709
2	20	ILE	PHE	conflict	UNP P01709
2	23	THR	SER	conflict	UNP P01709

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Chain	Residue	Modelled	Actual	Comment	Reference
2	29	VAL	ILE	conflict	UNP P01709
2	31	GLY	ASN	conflict	UNP P01709
2	39	GLN	ARG	conflict	UNP P01709
2	42	ALA	PRO	conflict	UNP P01709
2	48	VAL	LEU	conflict	UNP P01709
2	49	ILE	MET	conflict	UNP P01709
2	54	ASN	THR	conflict	UNP P01709
2	62	ASP	ASN	conflict	UNP P01709
2	94	GLU	ALA	conflict	UNP P01709
2	97	ASP	ASN	conflict	UNP P01709
2	98	ASN	SER	conflict	UNP P01709
2	99	PHE	LEU	conflict	UNP P01709
2	100	VAL	ILE	conflict	UNP P01709
2	103	THR	GLY	conflict	UNP P01709
2	106	LYS	ARG	conflict	UNP P01709
2	107	VAL	LEU	conflict	UNP P01709
2	116	ASN	ALA	conflict	UNP P01709
2	118	THR	SER	conflict	UNP P01709
2	156	GLY	SER	conflict	UNP P01709
2	167	LYS	THR	conflict	UNP P01709

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	133	Total O 133 133	0	0
2	2	185	Total O 185 185	0	0



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.30 Å 72.30 Å 185.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	1	1.42	7/1637 (0.4%)	2.51	82/2233 (3.7%)
1	2	1.40	1/1637 (0.1%)	2.44	94/2233 (4.2%)
All	All	1.41	8/3274 (0.2%)	2.48	176/4466 (3.9%)

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	1	0	2
1	2	0	1
All	All	0	3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	SER	C-O	6.03	1.34	1.23
1	1	4	LEU	CA-CB	-5.85	1.40	1.53
1	1	59	GLY	N-CA	5.62	1.54	1.46
1	1	196	SER	CB-OG	-5.54	1.35	1.42
1	1	157	SER	CB-OG	-5.25	1.35	1.42

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	63	ARG	CD-NE-CZ	23.28	156.19	123.60
1	1	4	LEU	CA-CB-CG	19.94	161.17	115.30
1	1	130	GLN	CB-CG-CD	17.04	155.90	111.60
1	1	55	LYS	CA-CB-CG	16.14	148.91	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	193	ARG	NE-CZ-NH2	-15.93	112.33	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	ARG	Sidechain
1	1	58	SER	Mainchain
1	2	163	VAL	Mainchain

## 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	1	1606	0	1538	368	4
1	2	1606	0	1536	356	1
2	1	133	0	0	35	2
2	2	185	0	0	41	1
All	All	3530	0	3074	712	5

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 113.

The worst 5 of 712 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)
1:1:177:ALA:HB3	2:1:347:HOH:O	1.32	1.26
1:1:19:THR:HG23	1:1:76:THR:CG2	1.66	1.26
2:1:314:HOH:O	1:2:141:SER:HB2	1.33	1.25
1:1:52:GLU:O	1:1:53:VAL:HG22	1.34	1.23
1:1:117:PRO:HB3	1:1:140:ILE:CD1	1.70	1.20

All (5) 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)
2:1:266:HOH:O	2:2:333:HOH:O[6_656]	1.54	0.66
1:1:81:GLN:NE2	2:1:242:HOH:O[4_646]	1.76	0.44
1:1:58:SER:O	1:1:215:CYS:CA[3_654]	2.11	0.09
1:1:32:TYR:OH	1:2:9:SER:CB[4_546]	2.14	0.06
1:1:59:GLY:O	1:1:216:SER:N[3_654]	2.19	0.01

## 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	1	214/216 (99%)	163 (76%)	28 (13%)	23 (11%)	0	0
1	2	214/216 (99%)	140 (65%)	39 (18%)	35 (16%)	0	0
All	All	428/432 (99%)	303 (71%)	67 (16%)	58 (14%)	0	0

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	2	SER
1	1	9	SER
1	1	14	LEU
1	1	26	SER
1	1	27	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	1	180/180 (100%)	116 (64%)	64 (36%)	0	0
1	2	180/180 (100%)	129 (72%)	51 (28%)	0	0
All	All	360/360 (100%)	245 (68%)	115 (32%)	0	0

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	181	TYR
1	2	2	SER
1	2	188	GLN
1	1	182	LEU
1	1	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	2	33	ASN
1	2	40	GLN
1	2	173	ASN
1	2	16	GLN
1	2	174	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PCA	1	1	1	8,8,9	3.27	2 (25%)	9,10,12	2.41	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PCA	2	1	1	8,8,9	2.95	4 (50%)	9,10,12	1.80	4 (44%)

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
1	PCA	1	1	1	-	0/0/11/13	0/1/1/1
1	PCA	2	1	1	-	0/0/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	PCA	CD-N	7.92	1.57	1.34
1	2	1	PCA	CD-N	6.67	1.53	1.34
1	2	1	PCA	CA-N	3.38	1.50	1.46
1	1	1	PCA	CA-N	3.32	1.50	1.46
1	2	1	PCA	CB-CG	2.55	1.58	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1	PCA	OE-CD-CG	-3.86	119.94	126.81
1	1	1	PCA	OE-CD-N	3.78	134.03	124.82
1	1	1	PCA	CA-N-CD	-3.49	101.62	113.58
1	2	1	PCA	CB-CA-N	2.75	111.18	103.30
1	2	1	PCA	CA-N-CD	-2.47	105.11	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1	PCA	8	0
1	2	1	PCA	1	0

## 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.