



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 06:35 am GMT

PDB ID : 3MCG
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : recalc28949

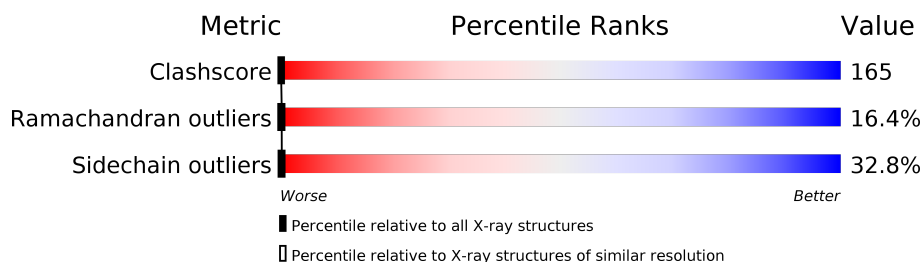
1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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 ≥ 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	1	216	
1	2	216	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3478 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	PIR S14675
1	23	THR	SER	CONFLICT	PIR S14675
1	29	VAL	ILE	CONFLICT	PIR S14675
1	31	GLY	ASN	CONFLICT	PIR S14675
1	39	GLN	ARG	CONFLICT	PIR S14675
1	42	ALA	PRO	CONFLICT	PIR S14675
1	48	VAL	LEU	CONFLICT	PIR S14675
1	49	ILE	MET	CONFLICT	PIR S14675
1	54	ASN	THR	CONFLICT	PIR S14675
1	62	ASP	ASN	CONFLICT	PIR S14675
1	94	GLU	ALA	CONFLICT	PIR S14675
1	97	ASP	ASN	CONFLICT	PIR S14675
1	98	ASN	SER	CONFLICT	PIR S14675
1	99	PHE	LEU	CONFLICT	PIR S14675
1	100	VAL	ILE	CONFLICT	PIR S14675
1	103	THR	GLY	CONFLICT	PIR S14675
1	106	LYS	ARG	CONFLICT	PIR S14675
1	107	VAL	LEU	CONFLICT	PIR S14675
1	116	ASN	ALA	CONFLICT	PIR S14675
1	118	THR	SER	CONFLICT	PIR S14675
1	156	GLY	SER	CONFLICT	PIR S14675
1	167	LYS	THR	CONFLICT	PIR S14675
2	20	ILE	PHE	CONFLICT	PIR S14675
2	23	THR	SER	CONFLICT	PIR S14675

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2	29	VAL	ILE	CONFLICT	PIR S14675
2	31	GLY	ASN	CONFLICT	PIR S14675
2	39	GLN	ARG	CONFLICT	PIR S14675
2	42	ALA	PRO	CONFLICT	PIR S14675
2	48	VAL	LEU	CONFLICT	PIR S14675
2	49	ILE	MET	CONFLICT	PIR S14675
2	54	ASN	THR	CONFLICT	PIR S14675
2	62	ASP	ASN	CONFLICT	PIR S14675
2	94	GLU	ALA	CONFLICT	PIR S14675
2	97	ASP	ASN	CONFLICT	PIR S14675
2	98	ASN	SER	CONFLICT	PIR S14675
2	99	PHE	LEU	CONFLICT	PIR S14675
2	100	VAL	ILE	CONFLICT	PIR S14675
2	103	THR	GLY	CONFLICT	PIR S14675
2	106	LYS	ARG	CONFLICT	PIR S14675
2	107	VAL	LEU	CONFLICT	PIR S14675
2	116	ASN	ALA	CONFLICT	PIR S14675
2	118	THR	SER	CONFLICT	PIR S14675
2	156	GLY	SER	CONFLICT	PIR S14675
2	167	LYS	THR	CONFLICT	PIR S14675

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	123	Total O 123 123	0	0
2	2	143	Total O 143 143	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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.80Å 81.90Å 71.00Å 90.00° 90.00° 90.00°	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}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3478	wwPDB-VP
Average B, all atoms (Å ²)	7.0	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	1.39	9/1637 (0.5%)	2.68	126/2233 (5.6%)
1	2	1.38	5/1637 (0.3%)	2.54	109/2233 (4.9%)
All	All	1.39	14/3274 (0.4%)	2.61	235/4466 (5.3%)

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	1	0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2	SER	CB-OG	7.02	1.51	1.42
1	2	79	GLY	N-CA	6.40	1.55	1.46
1	1	136	LEU	N-CA	6.02	1.58	1.46
1	2	138	CYS	CB-SG	-5.98	1.72	1.81
1	1	127	GLU	CD-OE1	-5.66	1.19	1.25

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	136	LEU	CA-CB-CG	26.67	176.65	115.30
1	1	40	GLN	CA-CB-CG	13.46	143.01	113.40
1	1	14	LEU	CA-CB-CG	13.29	145.86	115.30
1	2	40	GLN	CA-CB-CG	13.07	142.15	113.40
1	1	136	LEU	CB-CA-C	12.82	134.55	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	148	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	1	1606	0	1537	460	8
1	2	1606	0	1536	613	8
2	1	123	0	0	49	5
2	2	143	0	0	73	6
All	All	3478	0	3073	1035	18

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 165.

The worst 5 of 1035 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)
1:2:56:ARG:HB2	1:2:60:VAL:CG2	1.62	1.29
1:1:92:SER:OG	1:1:100:VAL:HB	1.31	1.29
1:2:137:VAL:HG11	2:2:252:HOH:O	1.32	1.25
1:2:56:ARG:CB	1:2:60:VAL:HG21	1.66	1.25
1:2:154:ALA:HA	2:2:308:HOH:O	1.39	1.21

The worst 5 of 18 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)
1:1:34:TYR:OH	1:1:157:SER:OG[3_455]	1.40	0.80
1:1:51:TYR:OH	2:1:281:HOH:O[3_455]	1.45	0.75
2:1:221:HOH:O	2:1:334:HOH:O[3_455]	1.59	0.61
1:2:1:PCA:CG	2:1:234:HOH:O[2_555]	1.63	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:93:TYR:OH	1:1:156:GLY:CA[3_455]	1.66	0.54

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%)	138 (64%)	42 (20%)	34 (16%)	0	0
1	2	214/216 (99%)	135 (63%)	43 (20%)	36 (17%)	0	0
All	All	428/432 (99%)	273 (64%)	85 (20%)	70 (16%)	0	0

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	15	GLY
1	1	52	GLU
1	1	53	VAL
1	1	70	GLY
1	1	71	ASN

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%)	125 (69%)	55 (31%)	0	0
1	2	180/180 (100%)	117 (65%)	63 (35%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	360/360 (100%)	242 (67%)	118 (33%)	0 0

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	215	CYS
1	2	48	VAL
1	2	188	GLN
1	1	216	SER
1	2	22	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	81	GLN
1	1	201	HIS
1	2	41	HIS
1	2	130	GLN
1	2	192	HIS

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	3.19	4 (50%)	9,10,12	4.00	4 (44%)
1	PCA	2	1	1	8,8,9	2.81	3 (37%)	9,10,12	2.25	3 (33%)

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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	PCA	CB-CG	2.02	1.57	1.53
1	1	1	PCA	CG-CD	2.25	1.57	1.50
1	2	1	PCA	CB-CG	2.42	1.58	1.53
1	1	1	PCA	OE-CD	2.78	1.29	1.23
1	2	1	PCA	CA-N	3.33	1.50	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1	PCA	OE-CD-CG	-8.24	111.68	126.86
1	2	1	PCA	O-C-CA	-4.97	113.56	125.15
1	1	1	PCA	O-C-CA	-3.70	116.52	125.15
1	2	1	PCA	OE-CD-CG	-2.34	122.55	126.86
1	2	1	PCA	CA-N-CD	-2.04	106.59	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

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.