wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 06:38 pm BST

PDB ID	:	3MCG
Title	:	THREE-DIMENSIONAL STRUCTURE OF A LIGHT CHAIN DIMER CRYSTALLIZED IN WATER. CONFORMATIONAL FLEXIBILITY OF A MOLECULE IN TWO CRYSTAL FORMS
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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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

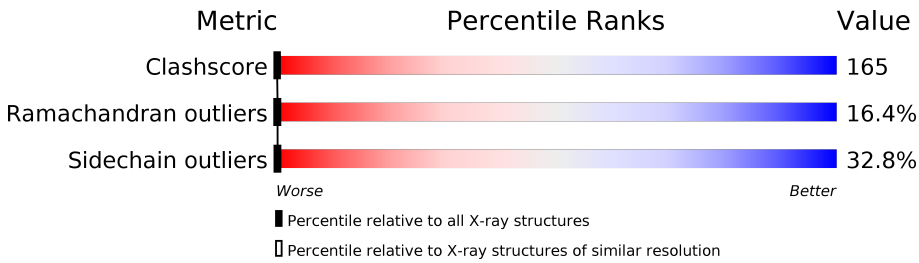
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	216	8% 38% 37% 17%
1	2	216	7% 40% 33% 19%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	1	216	1606	1000	266	335	5	0	0	0
1	2	216	1606	1000	266	335	5	0	0	0

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

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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
			Total	O		
2	1	123	123	123	0	0
			Total	O		
2	2	143	143	143	0	0

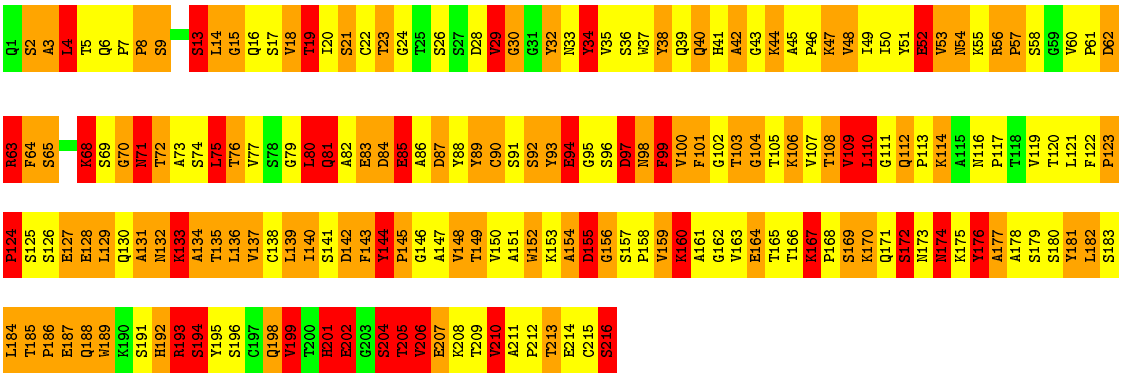
3 Residue-property plots (i)

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. 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. 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.

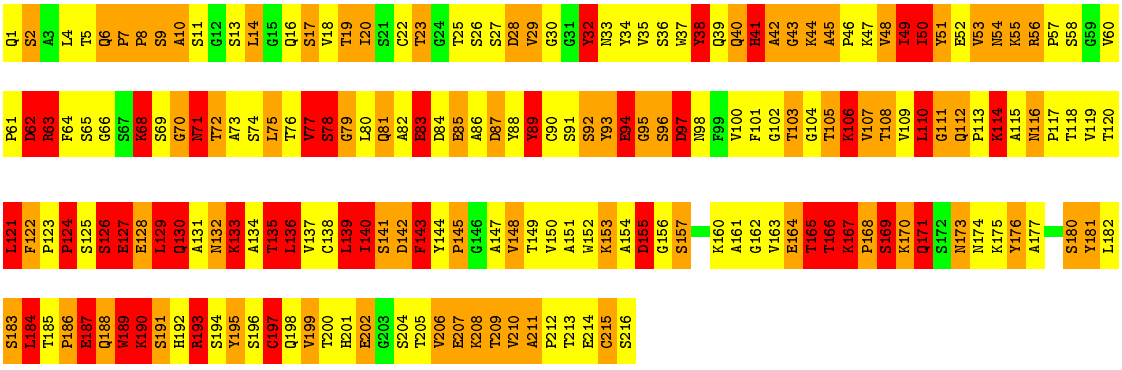
- Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)

Chain 1: 8% 38% 37% 17%



- Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)

Chain 2: 7% 40% 33% 19%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 (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	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

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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

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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 (i)

There are no RNA molecules in this entry.

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

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	7,8,9	3.65	4 (57%)	9,10,12	4.18	5 (55%)
1	PCA	2	1	1	7,8,9	3.21	3 (42%)	9,10,12	2.10	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	CD-N	8.46	1.57	1.34
1	2	1	PCA	CD-N	7.09	1.53	1.34
1	2	1	PCA	CA-N	3.37	1.50	1.46
1	1	1	PCA	OE-CD	2.85	1.29	1.23
1	1	1	PCA	CG-CD	2.46	1.57	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1	PCA	OE-CD-CG	-8.64	111.68	126.76
1	1	1	PCA	OE-CD-N	7.51	142.37	124.86
1	2	1	PCA	O-C-CA	-4.28	113.56	124.78
1	1	1	PCA	O-C-CA	-3.15	116.52	124.78
1	2	1	PCA	OE-CD-CG	-2.41	122.55	126.76

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.