



wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 07:45 pm BST

PDB ID : 1JHW
Title : Ca²⁺-binding Mimicry in the Crystal Structure of the Eu³⁺-Bound Mutant Human Macrophage Capping Protein Cap G
Authors : Vorobiev, S.M.; Southwick, F.S.; Almo, S.C.
Deposited on : 2001-06-28
Resolution : 2.80 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 ⓘ symbol.

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 : 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

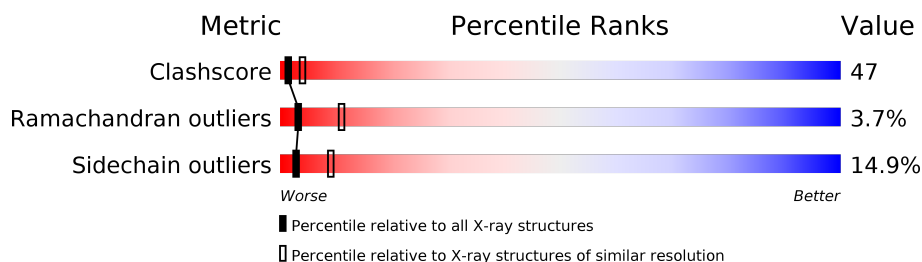
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	347	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2529 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 MACROPHAGE CAPPING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2436	1551	421	455	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	-	SEE REMARK 999	UNP P40121
A	84	LEU	-	SEE REMARK 999	UNP P40121
A	85	ASP	-	SEE REMARK 999	UNP P40121
A	86	ASP	-	SEE REMARK 999	UNP P40121
A	87	TYR	-	SEE REMARK 999	UNP P40121
A	88	LEU	-	SEE REMARK 999	UNP P40121
A	89	GLY	-	SEE REMARK 999	UNP P40121
A	90	GLY	-	SEE REMARK 999	UNP P40121
A	124	GLY	-	SEE REMARK 999	UNP P40121
A	125	PHE	-	SEE REMARK 999	UNP P40121
A	126	LYS	-	SEE REMARK 999	UNP P40121
A	127	HIS	-	SEE REMARK 999	UNP P40121
A	128	VAL	-	SEE REMARK 999	UNP P40121
A	129	VAL	-	SEE REMARK 999	UNP P40121
A	130	PRO	-	SEE REMARK 999	UNP P40121
A	131	ASN	-	SEE REMARK 999	UNP P40121
A	132	GLU	-	SEE REMARK 999	UNP P40121
A	133	VAL	-	SEE REMARK 999	UNP P40121
A	134	VAL	-	SEE REMARK 999	UNP P40121
A	135	VAL	-	SEE REMARK 999	UNP P40121
A	136	GLN	-	SEE REMARK 999	UNP P40121
A	137	ARG	-	SEE REMARK 999	UNP P40121

- Molecule 2 is EUROPIUM (III) ION (three-letter code: EU3) (formula: Eu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Eu 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total 91	O 91	0	0

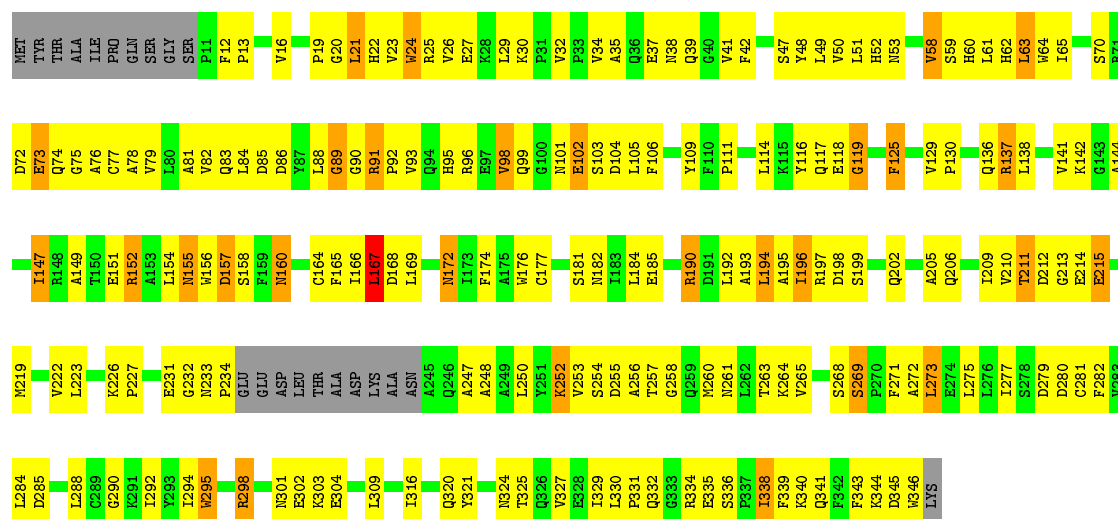
3 Residue-property plots [i](#)

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: MACROPHAGE CAPPING PROTEIN

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	205.60 Å 205.60 Å 56.42 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.73 – 2.80	Depositor
% Data completeness (in resolution range)	92.8 (24.73-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2529	wwPDB-VP
Average B, all atoms (Å ²)	76.0	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: EU3

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	0.90	1/2491 (0.0%)	0.97	3/3390 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TRP	CB-CG	5.04	1.59	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLY	N-CA-C	5.96	128.01	113.10
1	A	232	GLY	N-CA-C	5.86	127.74	113.10
1	A	167	LEU	CA-CB-CG	5.36	127.62	115.30

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	2436	0	2296	223	0
2	A	2	0	0	0	0
3	A	91	0	0	3	0
All	All	2529	0	2296	223	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 47.

The worst 5 of 223 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:253:VAL:HG12	1:A:260:MET:CE	1.85	1.04
1:A:152:ARG:HH11	1:A:152:ARG:HG2	1.22	1.00
1:A:155:ASN:HD22	1:A:157:ASP:H	1.11	0.96
1:A:253:VAL:HG12	1:A:260:MET:HE3	1.47	0.93
1:A:12:PHE:CE1	1:A:84:LEU:HB2	2.04	0.92

There are no symmetry-related clashes.

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	322/347 (93%)	256 (80%)	54 (17%)	12 (4%)	3 11

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	90	GLY
1	A	111	PRO
1	A	89	GLY
1	A	196	ILE

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	241/288 (84%)	205 (85%)	36 (15%)	3 9

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ASP
1	A	190	ARG
1	A	320	GLN
1	A	167	LEU
1	A	194	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	341	GLN
1	A	286	ASN
1	A	101	ASN
1	A	261	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.