

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 07:00 am BST

PDB ID 1BGC

> Title CRYSTAL STRUCTURE OF CANINE AND BOVINE GRANULOCYTE-

> > COLONY STIMULATING FACTOR (G-CSF)

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Deposited on 1993-04-27

1.70 Å(reported) Resolution

This is a Full wwPDB X-ray Structure Validation 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 (1)) were used in the production of this report:

4.02b-467MolProbity Xtriage (Phenix) 1.13

EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

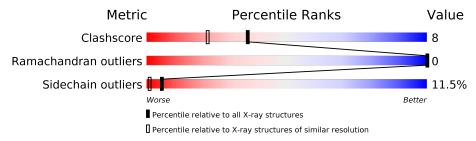
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.70 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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%

M	ol	Chain	Length	Quality of chain			
		A	174	62%	25%	•	9%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1734 atoms, of which 447 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 GRANULOCYTE COLONY-STIMULATING FACTOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	Α	158	Total	С	Н	N	О	S	0	0	0
_	11	100	1443	761	253	210	211	8			

• Molecule 2 is water.

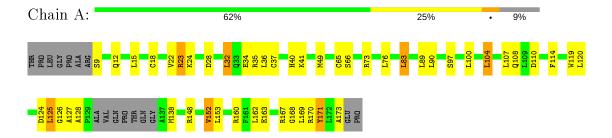
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	97	Total 291	H 194	O 97	0	0



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.

• Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	46.00Å 53.90Å 57.10Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 - 1.70	Depositor
Resolution (A)	46.00 - 1.59	EDS
% Data completeness	(Not available) (7.00-1.70)	Depositor
(in resolution range)	83.2 (46.00-1.59)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.71 (at 1.59Å)	Xtriage
Refinement program	X-PLOR	Depositor
D D.	0.213 , (Not available)	Depositor
R, R_{free}	0.426 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31,60.0	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	1734	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.18% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.87	0/1212	1.32	$14/1643 \ (0.9\%)$	

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	A	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	73	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	A	127	ALA	N-CA-C	8.88	134.97	111.00
1	A	119	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	A	35	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	119	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	A	171	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	A	73	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	125	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	163	GLU	CA-CB-CG	-5.59	101.09	113.40
1	A	126	GLY	C-N-CA	5.54	135.55	121.70
1	A	138	MET	CA-CB-CG	5.20	122.14	113.30
1	A	23	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	119	TRP	CG-CD1-NE1	-5.11	104.99	110.10
1	A	148	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	128	ALA	Peptide

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	1190	253	1190	19	5
2	A	97	194	0	5	3
All	All	1287	447	1190	19	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 8.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:22:VAL:HG23	2:A:231:HOH:O	1.92	0.69
1:A:49:MET:SD	1:A:153:LEU:HD22	2.35	0.66
1:A:66:SER:HA	2:A:203:HOH:O	1.96	0.66
1:A:36:LEU:HD13	1:A:152:VAL:HG12	1.86	0.57
1:A:171:TYR:HE2	2:A:203:HOH:O	1.91	0.52
1:A:40:HIS:HE1	1:A:97:SER:OG	1.98	0.47
1:A:24:LYS:NZ	1:A:28:ASP:OD1	2.48	0.46
1:A:32:LEU:HD23	1:A:100:LEU:HD12	1.97	0.46
1:A:23:ARG:HG2	2:A:231:HOH:O	2.14	0.46
1:A:24:LYS:NZ	1:A:110:ASP:OD2	2.41	0.46
1:A:90:LEU:HD22	1:A:104:LEU:HD21	2.00	0.43
1:A:9:SER:N	2:A:228:HOH:O	2.52	0.43
1:A:18:CYS:O	1:A:22:VAL:HG22	2.19	0.43
1:A:37:CYS:O	1:A:41:LYS:HA	2.19	0.42
1:A:104:LEU:O	1:A:108:GLN:HG3	2.20	0.41
1:A:83:LEU:HD21	1:A:114:PHE:CD2	2.55	0.41
1:A:12:GLN:HE22	1:A:173:ALA:HB1	1.84	0.41
1:A:32:LEU:CD2	1:A:100:LEU:HD12	2.50	0.41
1:A:65:CYS:HB3	1:A:168:GLY:HA3	2.01	0.41

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:124:ASP:OD1	1:A:167:ARG:HH12[2_335]	0.77	0.83
1:A:170:ARG:HH21	2:A:266:HOH:H2[3_457]	1.12	0.48
1:A:124:ASP:OD1	1:A:167:ARG:NH1[2_335]	1.72	0.48
1:A:170:ARG:NH2	2:A:266:HOH:O[3_457]	1.78	0.42
1:A:170:ARG:HH21	2:A:266:HOH:O[3_457]	1.49	0.11

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	3
1	A	154/174 (88%)	149 (97%)	5 (3%)	0	100 100	

There are no Ramachandran outliers to report.

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	122/142 (86%)	108 (88%)	14 (12%)	5 1

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	32	LEU

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Mol	Chain	Res	Type
1	A	34	GLU
1	A	76	LEU
1	A	83	LEU
1	A	89	LEU
1	A	104	LEU
1	A	107	LEU
1	A	120	LEU
1	A	125	LEU
1	A	152	VAL
1	A	160	ARG
1	A	162	LEU
1	A	169	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	12	GLN
1	A	21	GLN
1	A	40	HIS
1	A	77	ASN
1	A	87	GLN
1	A	121	GLN

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)

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

