wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 10:43 AM EST

PDB ID	:	1CD9
Title	:	2:2 COMPLEX OF G-CSF WITH ITS RECEPTOR
Authors	:	Aritomi, M.; Kunishima, N.; Okamoto, T.; Kuroki, R.; Ota, Y.; Morikawa, K.
Deposited on	:	1999-03-08
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

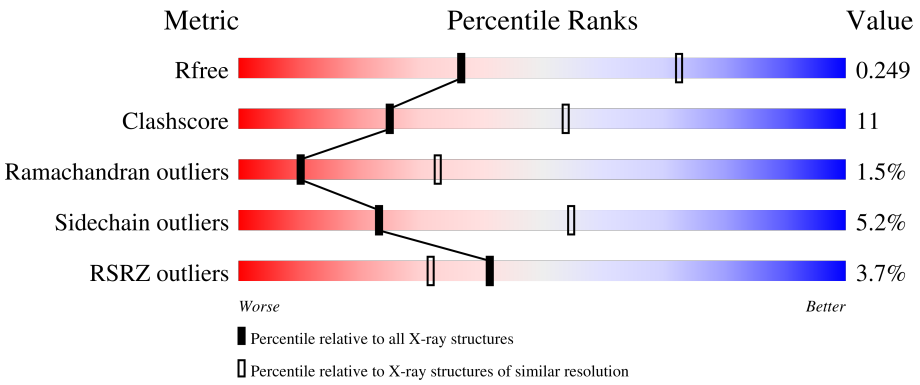
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of 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% 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.

Mol	Chain	Length	Quality of chain
1	A	175	6% 77% 21%
1	C	175	2% 71% 23%
2	B	215	70% 24%
2	D	215	7% 67% 23% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6080 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 PROTEIN (GRANULOCYTE COLONY-STIMULATING FACTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1283	820	218	237	8	0	0	0
1	C	169	1254	800	212	234	8	0	0	0

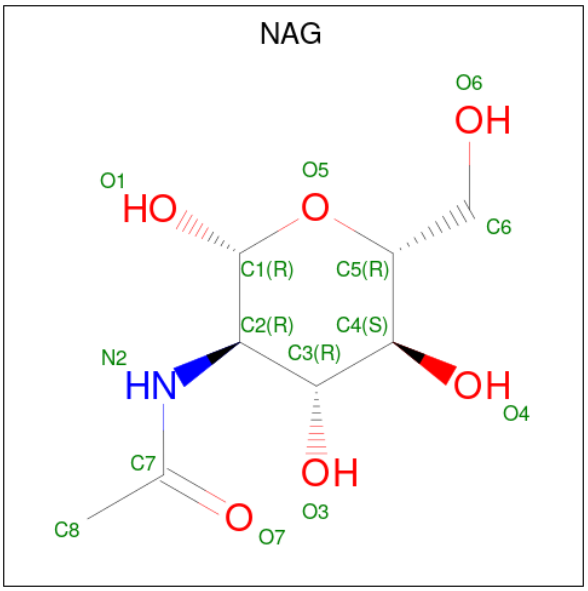
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	ALA	cloning artifact	UNP P09919
C	1	MET	ALA	cloning artifact	UNP P09919

- Molecule 2 is a protein called PROTEIN (G-CSF RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	206	1638	1050	274	296	18	0	0	0
2	D	204	1617	1036	270	293	18	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0

- Molecule 4 is water.

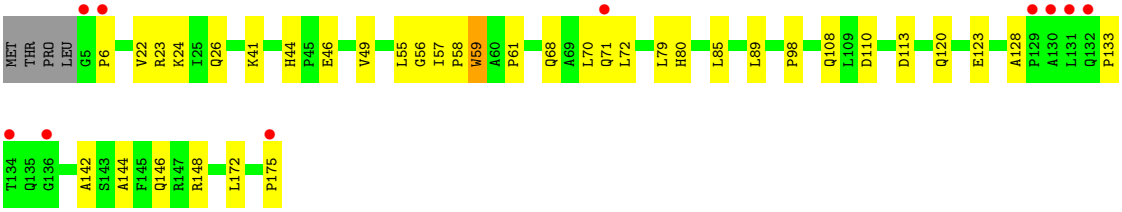
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
			Total	O		
4	B	108	108	108	0	0
			Total	O		
4	C	37	37	37	0	0
			Total	O		
4	D	69	69	69	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

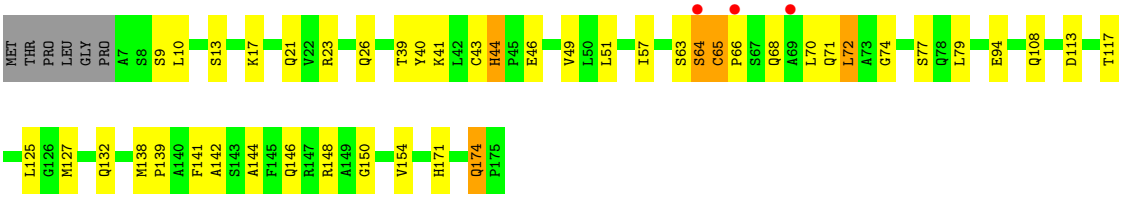
• Molecule 1: PROTEIN (GRANULOCYTE COLONY-STIMULATING FACTOR)

Chain A:



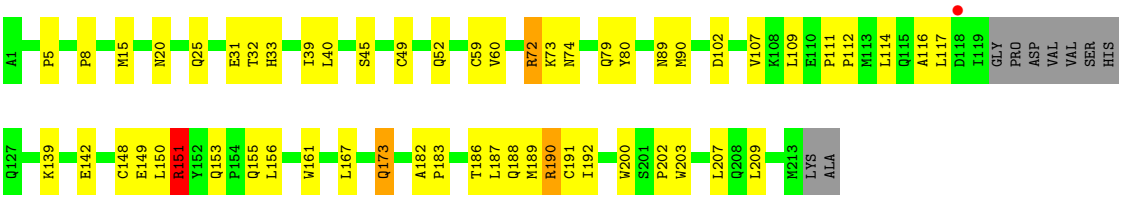
• Molecule 1: PROTEIN (GRANULOCYTE COLONY-STIMULATING FACTOR)

Chain C:



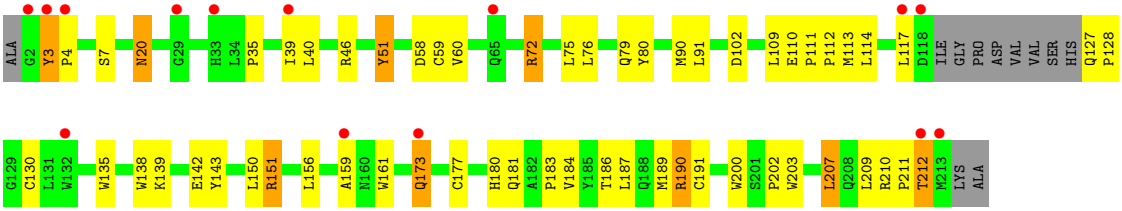
• Molecule 2: PROTEIN (G-CSF RECEPTOR)

Chain B:



• Molecule 2: PROTEIN (G-CSF RECEPTOR)

Chain D:


ALA
G2
Y3
P4
S7
N20
G29
H33
L34
P35
I39
L40
R46
Y51
D58
C59
V60
Q65
R72
L75
L76
Q79
Y80
M90
L91
D102
L109
E110
P111
P112
M113
L114
L117
D118
ILE
GLY
PRO
ASP
VAL
VAL
SER
HIS
Q127
P128
G129
C130
L131
W132
W135
W138
K139
E142
Y143
L150
R151
L156
A159
N160
W161
Q173
C177
H180
Q181
A182
P183
V184
Y185
T186
L187
Q188
M189
R190
C191
W200
S201
P202
W203
L207
Q208
L209
R210
P211
T212
M213
LYS
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	125.47Å 125.47Å 372.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 44.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (15.00-2.80) 78.3 (44.14-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.319 0.198 , 0.249	Depositor DCC
R_{free} test set	425 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 73.6	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	0.93	EDS
Total number of atoms	6080	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

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: NAG

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	0.60	0/1312	0.73	0/1784
1	C	0.66	0/1279	0.76	0/1738
2	B	0.65	0/1690	0.84	2/2306 (0.1%)
2	D	0.58	0/1669	0.81	2/2279 (0.1%)
All	All	0.62	0/5950	0.79	4/8107 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	151	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	B	151	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	B	102	ASP	N-CA-C	-5.50	96.17	111.00
2	D	102	ASP	N-CA-C	-5.13	97.15	111.00

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	1283	0	1283	20	0
1	C	1254	0	1254	25	0
2	B	1638	0	1593	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1617	0	1557	39	0
3	B	14	0	13	2	0
3	D	14	0	13	0	0
4	A	46	0	0	0	0
4	B	108	0	0	2	0
4	C	37	0	0	0	0
4	D	69	0	0	0	0
All	All	6080	0	5713	124	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 11.

The worst 5 of 124 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:C:23:ARG:HA	1:C:26:GLN:HE21	1.43	0.84
2:D:3:TYR:HB2	2:D:91:LEU:HD12	1.58	0.84
2:D:114:LEU:HD13	2:D:189:MET:HE3	1.61	0.81
2:B:5:PRO:CG	2:B:89:ASN:HB2	2.12	0.79
2:B:114:LEU:HD13	2:B:189:MET:HE3	1.67	0.75

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	169/175 (97%)	155 (92%)	13 (8%)	1 (1%)	25 56
1	C	167/175 (95%)	150 (90%)	11 (7%)	6 (4%)	3 11
2	B	202/215 (94%)	191 (95%)	11 (5%)	0	100 100
2	D	200/215 (93%)	185 (92%)	11 (6%)	4 (2%)	7 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	738/780 (95%)	681 (92%)	46 (6%)	11 (2%)	10	33

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	51	TYR
1	C	41	LYS
1	C	63	SER
2	D	159	ALA
1	A	41	LYS

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	136/142 (96%)	130 (96%)	6 (4%)	28	61
1	C	132/142 (93%)	126 (96%)	6 (4%)	27	60
2	B	186/195 (95%)	178 (96%)	8 (4%)	29	62
2	D	183/195 (94%)	170 (93%)	13 (7%)	14	39
All	All	637/674 (94%)	604 (95%)	33 (5%)	23	55

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	177	CYS
2	D	180	HIS
2	D	212	THR
2	B	173	GLN
2	B	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
2	D	79	GLN
2	D	155	GLN
2	D	153	GLN
2	B	20	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
3	NAG	B	323	2	14,14,15	1.25	1 (7%)	17,19,21	1.22	1 (5%)
3	NAG	D	923	2	14,14,15	0.91	1 (7%)	17,19,21	0.72	0

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
3	NAG	B	323	2	-	2/6/23/26	0/1/1/1
3	NAG	D	923	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	323	NAG	C1-C2	3.79	1.58	1.52
3	D	923	NAG	C1-C2	2.52	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	323	NAG	O7-C7-C8	-2.50	117.42	122.06

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	323	NAG	C1-C2-N2-C7
3	B	323	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	323	NAG	2	0

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	171/175 (97%)	-0.25	10 (5%)	23	15	3, 20, 115, 192	0
1	C	169/175 (96%)	-0.26	3 (1%)	68	61	5, 24, 114, 146	0
2	B	206/215 (95%)	-0.52	1 (0%)	91	88	3, 16, 57, 95	0
2	D	204/215 (94%)	0.07	14 (6%)	16	10	4, 34, 97, 199	0
All	All	750/780 (96%)	-0.24	28 (3%)	41	31	3, 23, 99, 199	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	7.0
1	A	175	PRO	5.9
2	D	33	HIS	4.7
1	C	69	ALA	4.4
1	A	130	ALA	4.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	923	14/15	0.51	0.27	70,103,108,112	0
3	NAG	B	323	14/15	0.80	0.14	63,87,127,128	0

6.5 Other polymers (i)

There are no such residues in this entry.