



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:50 PM GMT

PDB ID : 4WRM
Title : Structure of the human CSF-1:CSF-1R complex
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Deposited on : 2014-10-24
Resolution : 6.85 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

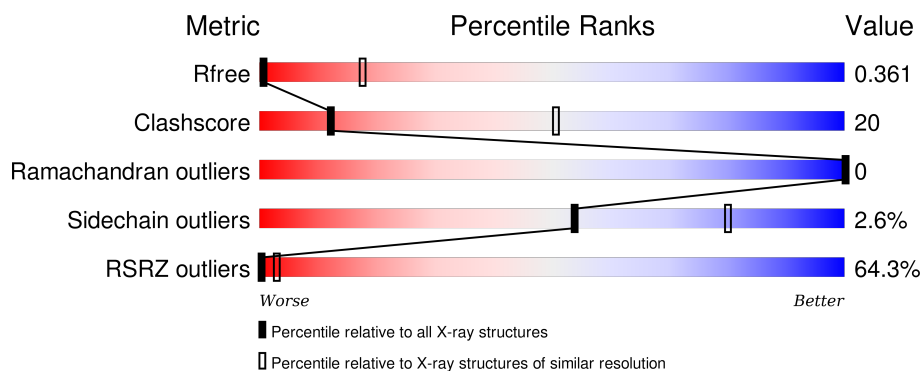
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.85 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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.

Mol	Chain	Length	Quality of chain
1	A	493	<div> <div>62%</div> <div>66% 23% 10%</div> </div>
2	B	170	<div> <div>41%</div> <div>74% 9% 17%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4524 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 colony-stimulating factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3422	2183	589	636	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	THR	-	expression tag	UNP P07333
A	506	LYS	-	expression tag	UNP P07333
A	507	HIS	-	expression tag	UNP P07333
A	508	HIS	-	expression tag	UNP P07333
A	509	HIS	-	expression tag	UNP P07333
A	510	HIS	-	expression tag	UNP P07333
A	511	HIS	-	expression tag	UNP P07333
A	512	HIS	-	expression tag	UNP P07333

- Molecule 2 is a protein called Macrophage colony-stimulating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	141	1102	691	185	215	11	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP P09603
B	-19	GLY	-	expression tag	UNP P09603
B	-18	SER	-	expression tag	UNP P09603
B	-17	SER	-	expression tag	UNP P09603
B	-16	HIS	-	expression tag	UNP P09603
B	-15	HIS	-	expression tag	UNP P09603
B	-14	HIS	-	expression tag	UNP P09603
B	-13	HIS	-	expression tag	UNP P09603

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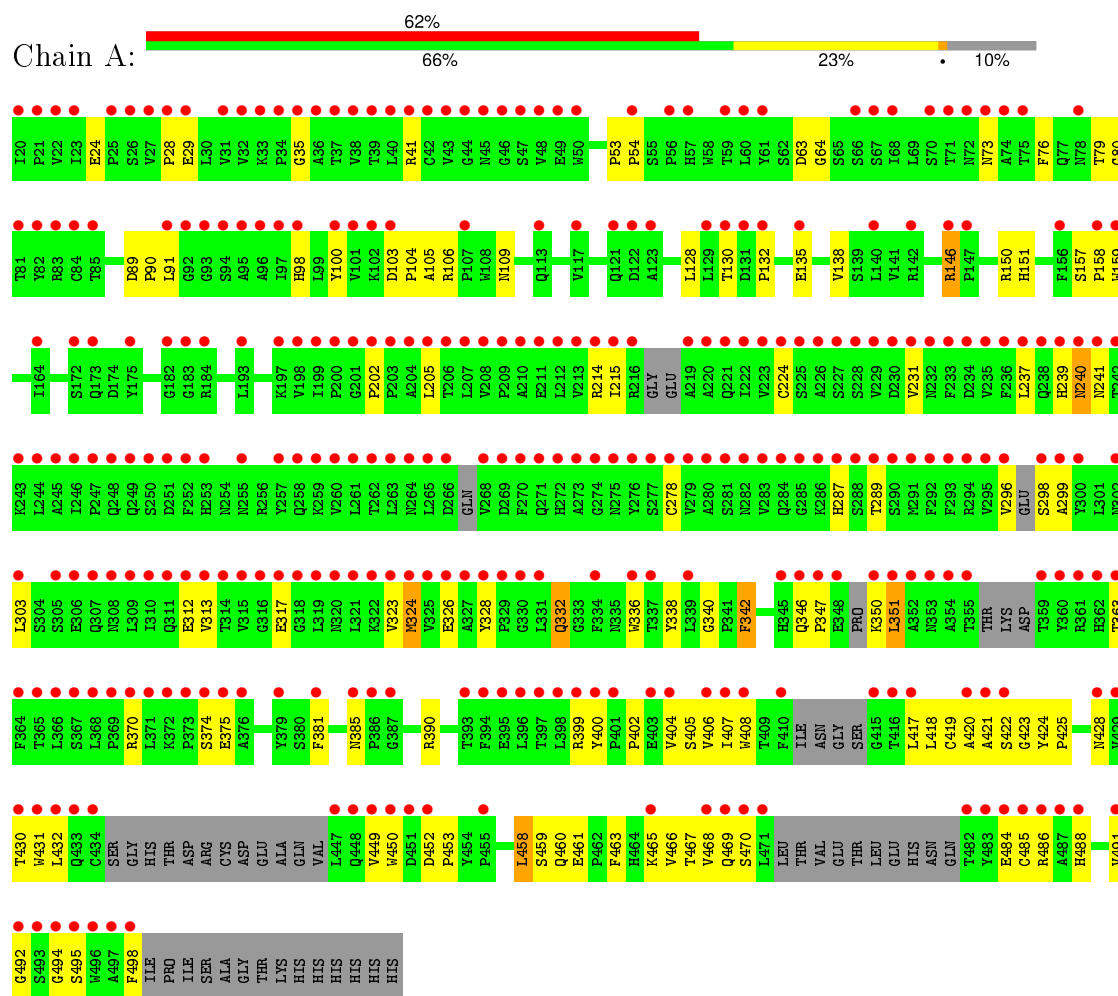
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P09603
B	-11	HIS	-	expression tag	UNP P09603
B	-10	SER	-	expression tag	UNP P09603
B	-9	SER	-	expression tag	UNP P09603
B	-8	GLY	-	expression tag	UNP P09603
B	-7	LEU	-	expression tag	UNP P09603
B	-6	VAL	-	expression tag	UNP P09603
B	-5	PRO	-	expression tag	UNP P09603
B	-4	ARG	-	expression tag	UNP P09603
B	-3	GLY	-	expression tag	UNP P09603
B	-2	SER	-	expression tag	UNP P09603
B	-1	HIS	-	expression tag	UNP P09603
B	0	MET	-	expression tag	UNP P09603

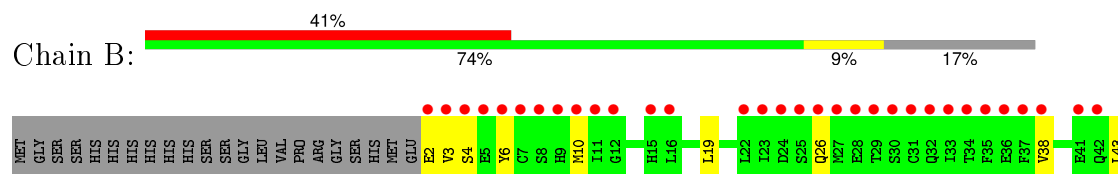
3 Residue-property plots

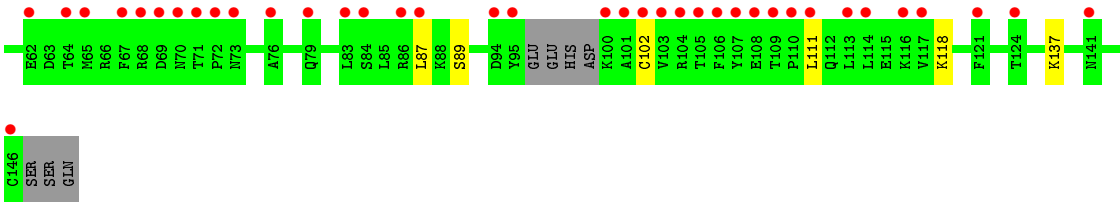
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: Macrophage colony-stimulating factor 1 receptor



• Molecule 2: Macrophage colony-stimulating factor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	281.47Å 281.47Å 91.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.75 – 6.85 48.75 – 6.80	Depositor EDS
% Data completeness (in resolution range)	82.7 (48.75-6.85) 99.9 (48.75-6.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1685)	Depositor
R, R_{free}	0.326 , 0.359 0.342 , 0.361	Depositor DCC
R_{free} test set	384 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	446.7	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 560.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 3953 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4524	wwPDB-VP
Average B, all atoms (Å ²)	313.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.43	0/3509	0.61	0/4788
2	B	0.25	0/1118	0.39	0/1513
All	All	0.40	0/4627	0.56	0/6301

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	A	3422	0	3286	163	3
2	B	1102	0	1034	13	0
All	All	4524	0	4320	175	3

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 20.

The worst 5 of 175 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:215:ILE:CG2	1:A:298:SER:CA	1.74	1.65
1:A:28:PRO:O	1:A:159:TRP:CZ2	1.64	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD13	1:A:299:ALA:N	1.18	1.44
1:A:215:ILE:CG2	1:A:298:SER:HA	1.32	1.42
1:A:215:ILE:CD1	1:A:299:ALA:HA	1.51	1.40

All (3) 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:A:370:ARG:NH2	1:A:375:GLU:OE2[9_554]	1.67	0.53
1:A:370:ARG:NH1	1:A:375:GLU:OE1[9_554]	2.11	0.09
1:A:91:LEU:CD2	1:A:452:ASP:OD1[12_565]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	423/493 (86%)	406 (96%)	17 (4%)	0	100	100
2	B	137/170 (81%)	132 (96%)	5 (4%)	0	100	100
All	All	560/663 (84%)	538 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	372/429 (87%)	359 (96%)	13 (4%)	43	74
2	B	122/160 (76%)	122 (100%)	0	100	100
All	All	494/589 (84%)	481 (97%)	13 (3%)	54	80

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	PHE
1	A	346	GLN
1	A	460	GLN
1	A	332	GLN
1	A	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	239	HIS
1	A	320	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	399:ARG	C	400:TYR	N	4.38
1	A	104:PRO	C	105:ALA	N	4.10

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	445/493 (90%)	4.48	307 (68%) 0 3	216, 314, 410, 458	0
2	B	141/170 (82%)	2.54	70 (49%) 0 4	213, 290, 416, 477	0
All	All	586/663 (88%)	4.01	377 (64%) 0 3	213, 307, 411, 477	0

The worst 5 of 377 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ALA	19.0
1	A	295	VAL	18.1
1	A	268	VAL	18.0
1	A	203	PRO	17.3
1	A	204	ALA	16.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.