



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:42 PM GMT

PDB ID : 1SCF
Title : HUMAN RECOMBINANT STEM CELL FACTOR
Authors : Jiang, X.; Gurel, O.; Langley, K.E.; Hendrickson, W.A.
Deposited on : 1998-06-04
Resolution : 2.20 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

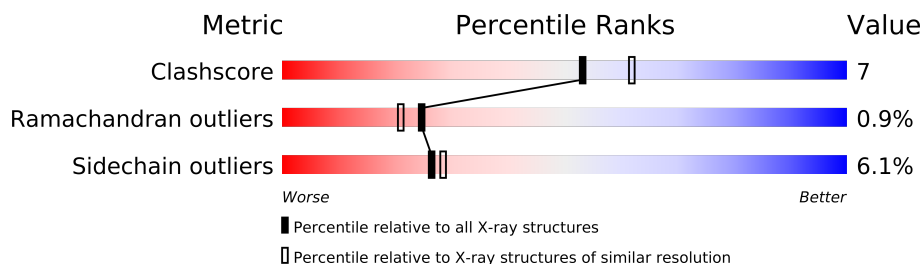
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3796 atoms, of which 0 are hydrogen and 0 are deuterium.

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 STEM CELL FACTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	Se	0	0	0
			925	594	142	183	3	3			
1	B	121	Total	C	N	O	S	Se	0	0	0
			947	612	148	181	3	3			
1	C	104	Total	C	N	O	S	Se	0	0	0
			824	532	128	159	2	3			
1	D	104	Total	C	N	O	S	Se	0	0	0
			817	528	127	157	2	3			

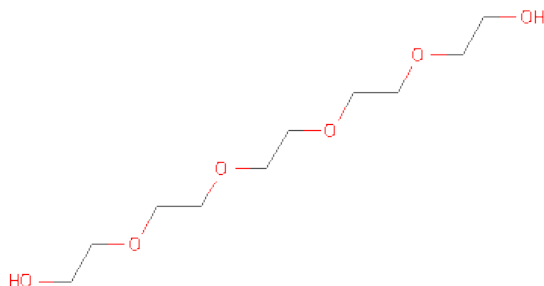
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	MET	MODIFIED	UNP P21583
A	36	MSE	MET	MODIFIED	UNP P21583
A	48	MSE	MET	MODIFIED	UNP P21583
B	27	MSE	MET	MODIFIED	UNP P21583
B	36	MSE	MET	MODIFIED	UNP P21583
B	48	MSE	MET	MODIFIED	UNP P21583
C	27	MSE	MET	MODIFIED	UNP P21583
C	36	MSE	MET	MODIFIED	UNP P21583
C	48	MSE	MET	MODIFIED	UNP P21583
D	27	MSE	MET	MODIFIED	UNP P21583
D	36	MSE	MET	MODIFIED	UNP P21583
D	48	MSE	MET	MODIFIED	UNP P21583

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Ca	0	0
			2	2		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	77	Total	O	0	0
			77	77		
4	C	57	Total	O	0	0
			57	57		
4	D	73	Total	O	0	0
			73	73		

SER ARG VAL SER VAL THR LYS PRO PHE MET LEU PRO VAL VAL ALA ALA SER SER LEU ARG ASN ASP SER SER SER SER ASN ARG LYS LYS ALA LYS ASN PRO PRO GLY GLY ASP SER SER LEU HIS TRP ALA MET ALA LEU PRO ALA LEU PHE SER LEU ILE ILE GLY PHE ALA PHE GLY ALA

LEU TYR TRP LYS LYS ARG GLN PRO SER LEU THR ARG ALA VAL GLU ASN ILE ILE ASN GLU ASP ASN GLU ILE SER ASN MET LEU GLN GLY LYS ARG GLU PHE GLN VAL

● Molecule 1: STEM CELL FACTOR

Chain D:

MET LYS LYS THR GLN THR TRP ILE LEU THR LYS CYS TYR ILE LEU GLN LEU LEU PHE ASN PRO LEU VAL VAL LYS THR GLU GLY ILE CYS ARG ASN ARG VAL VAL ASN N11 V12 T16 P23 Y26 L30 K31 Y32 V33 P34 C35 M36 H42 C43 V44 M48 E68 G69

L70 Y73 V83 L86 V87 V90 LYS GLU ASN SER SER LYS ASP LYS S104 P105 R108 L109 F110 T111 P112 R117 R121 S122 I123 F126 K127 ASP PHE VAL VAL ALA SER GLU THR ASP SER LEU TRP ALA ALA MET GLU THR LEU ASP CYS VAL VAL SER SER ILE THR LEU SER PRO GLU

LYS ASP SER ARG VAL SER VAL THR LYS PRO PHE MET LEU THR PRO LEU ARG VAL VAL ALA SER SER LEU PHE ASN ARG ASP LYS SER SER SER SER SER ASN ASP LYS ALA LYS ASN PRO PRO ARG GLY ASP SER SER LEU HIS TRP ALA ALA MET ALA LEU PRO LEU ILE ILE GLY PHE ALA PHE

GLY ALA TYR TRP LYS LYS ARG GLN PRO SER THR ARG ALA VAL GLU ASN ILE GLN ILE ASN GLU ASP ASN GLU ILE SER MET LEU GLN GLY PHE GLN VAL

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.82Å 82.55Å 88.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.6 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3796	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 1PE

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	0.80	0/939	1.43	12/1274 (0.9%)
1	B	0.77	0/962	1.41	6/1298 (0.5%)
1	C	0.88	0/837	1.43	8/1132 (0.7%)
1	D	0.77	0/830	1.46	9/1124 (0.8%)
All	All	0.81	0/3568	1.43	35/4828 (0.7%)

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	TRP	CD1-CG-CD2	9.67	114.03	106.30
1	D	44	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	A	44	TRP	CD1-CG-CD2	8.63	113.21	106.30
1	B	44	TRP	CE2-CD2-CG	-8.33	100.63	107.30
1	A	44	TRP	CE2-CD2-CG	-8.31	100.66	107.30
1	D	108	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	D	44	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	C	44	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	C	44	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	32	TYR	CB-CG-CD1	-6.95	116.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	83	VAL	CG1-CB-CG2	-6.66	100.25	110.90
1	D	44	TRP	CG-CD2-CE3	6.49	139.74	133.90
1	D	44	TRP	CB-CG-CD1	-6.22	118.92	127.00
1	D	44	TRP	CG-CD1-NE1	-6.20	103.90	110.10
1	A	44	TRP	CG-CD2-CE3	6.08	139.37	133.90
1	B	61	ASP	CA-CB-CG	6.04	126.69	113.40
1	A	44	TRP	CB-CG-CD1	-6.03	119.17	127.00
1	B	44	TRP	CG-CD1-NE1	-6.00	104.10	110.10
1	A	26	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	D	121	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	38	VAL	N-CA-CB	-5.84	98.65	111.50
1	A	44	TRP	CG-CD1-NE1	-5.72	104.38	110.10
1	C	108	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	C	44	TRP	CB-CG-CD1	-5.57	119.77	127.00
1	B	44	TRP	CB-CG-CD1	-5.46	119.89	127.00
1	D	117	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	128	ASP	CA-CB-CG	5.36	125.19	113.40
1	A	32	TYR	CG-CD2-CE2	-5.35	117.02	121.30
1	A	83	VAL	CA-CB-CG2	5.29	118.83	110.90
1	B	48	MSE	CG-SE-CE	-5.28	87.28	98.90
1	C	44	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	A	49	VAL	CA-CB-CG1	-5.17	103.15	110.90
1	C	44	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	C	90	VAL	CA-CB-CG1	5.03	118.44	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	73	TYR	Sidechain
1	D	73	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	925	0	893	18	0
1	B	947	0	927	15	0
1	C	824	0	814	11	0
1	D	817	0	801	12	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	B	16	0	22	3	0
4	A	57	0	0	1	0
4	B	77	0	0	2	0
4	C	57	0	0	0	0
4	D	73	0	0	1	0
All	All	3796	0	3457	49	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:30:LEU:HD21	1:B:48:MSE:HE1	1.60	0.83
1:C:41:SER:HB2	1:C:125:ALA:HB1	1.76	0.66
1:B:31:LYS:HG2	1:B:105:PRO:O	2.02	0.60
1:A:31:LYS:HB3	1:A:105:PRO:HG2	1.84	0.58
1:B:99:LYS:HD3	1:B:102:PHE:CE2	2.39	0.58
1:D:83:VAL:O	1:D:87:VAL:HG23	2.05	0.56
1:A:83:VAL:HG22	1:A:119:PHE:HE2	1.71	0.55
1:A:26:TYR:O	1:A:112:PRO:HD3	2.07	0.54
1:A:70:LEU:HD13	1:B:68:GLU:OE1	2.07	0.54
1:C:26:TYR:O	1:C:112:PRO:HD3	2.07	0.54
1:B:126:PHE:HA	1:B:129:PHE:HD2	1.74	0.52
1:D:30:LEU:HD21	1:D:48:MSE:HE1	1.92	0.52
1:A:121:ARG:HD2	4:A:1393:HOH:O	2.11	0.50
1:C:63:PHE:CZ	1:D:23:PRO:HG3	2.48	0.49
3:B:249:1PE:H162	1:D:110:PHE:CE1	2.48	0.48
1:A:71:SER:HB3	1:A:74:SER:OG	2.13	0.48
1:C:36:MSE:SE	1:C:48:MSE:HE2	2.64	0.48
3:B:249:1PE:H232	3:B:249:1PE:H121	1.71	0.48
1:A:47:GLU:O	1:A:51:GLN:HG2	2.14	0.47
1:D:36:MSE:HE2	1:D:36:MSE:HB3	1.87	0.47
1:A:17:LYS:HD3	1:B:68:GLU:OE1	2.14	0.47
1:A:41:SER:HA	1:A:44:TRP:CE2	2.50	0.46
1:C:32:TYR:HA	1:C:48:MSE:HE1	1.97	0.46
1:B:68:GLU:HG2	1:B:69:GLY:N	2.30	0.46
1:B:100:LYS:HG2	4:B:1434:HOH:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:LEU:HD13	1:B:68:GLU:OE2	2.17	0.45
1:A:15:VAL:HG11	1:A:120:ASN:HD21	1.81	0.45
1:A:30:LEU:HB3	1:A:110:PHE:CE2	2.52	0.45
1:C:121:ARG:HG3	1:C:121:ARG:HH11	1.82	0.45
1:A:40:PRO:HG2	1:A:43:CYS:SG	2.57	0.44
1:A:79:LEU:O	1:A:83:VAL:HG23	2.18	0.44
1:B:31:LYS:HB3	1:B:105:PRO:HB2	1.99	0.44
1:A:40:PRO:HB2	1:A:42:HIS:HD2	1.82	0.43
1:D:26:TYR:O	1:D:112:PRO:HD3	2.18	0.43
1:C:83:VAL:O	1:C:87:VAL:HG23	2.18	0.42
1:D:42:HIS:HA	4:D:1291:HOH:O	2.19	0.42
1:B:17:LYS:HD2	4:B:1311:HOH:O	2.19	0.42
1:C:30:LEU:HB3	1:C:110:PHE:CE2	2.55	0.42
3:B:249:1PE:H241	1:D:108:ARG:HH12	1.85	0.42
1:B:47:GLU:HB2	1:B:102:PHE:CD1	2.55	0.42
1:C:72:ASN:O	1:C:76:ILE:HG13	2.20	0.41
1:A:63:PHE:CZ	1:B:23:PRO:HG3	2.55	0.41
1:A:70:LEU:HD13	1:B:68:GLU:CD	2.40	0.41
1:D:86:LEU:HD13	1:D:126:PHE:CD2	2.55	0.41
1:D:32:TYR:O	1:D:105:PRO:HB2	2.21	0.41
1:A:24:LYS:HG3	1:B:62:LYS:O	2.21	0.41
1:C:79:LEU:O	1:C:83:VAL:HG23	2.20	0.41
1:C:63:PHE:HZ	1:D:23:PRO:HG3	1.85	0.40
1:D:32:TYR:O	1:D:34:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

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	115/273 (42%)	107 (93%)	7 (6%)	1 (1%)	25	21
1	B	117/273 (43%)	110 (94%)	6 (5%)	1 (1%)	25	21
1	C	100/273 (37%)	97 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	100/273 (37%)	95 (95%)	3 (3%)	2 (2%)	11	6
All	All	432/1092 (40%)	409 (95%)	19 (4%)	4 (1%)	25	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	ASN
1	A	137	ASP
1	D	105	PRO
1	D	12	VAL

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	108/251 (43%)	102 (94%)	6 (6%)	30	33
1	B	109/251 (43%)	102 (94%)	7 (6%)	25	26
1	C	97/251 (39%)	91 (94%)	6 (6%)	26	27
1	D	95/251 (38%)	89 (94%)	6 (6%)	25	27
All	All	409/1004 (41%)	384 (94%)	25 (6%)	26	28

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	59	LEU
1	A	68	GLU
1	A	121	ARG
1	A	129	PHE
1	A	139	VAL
1	B	36	MSE
1	B	61	ASP
1	B	89	CYS
1	B	104	SER
1	B	117	ARG

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Mol	Chain	Res	Type
1	B	121	ARG
1	B	129	PHE
1	C	38	VAL
1	C	43	CYS
1	C	46	SER
1	C	78	LYS
1	C	90	VAL
1	C	124	ASP
1	D	16	THR
1	D	36	MSE
1	D	68	GLU
1	D	70	LEU
1	D	123	ILE
1	D	126	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	120	ASN
1	B	65	ASN
1	C	120	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	1PE	B	249	-	15,15,15	0.61	0	14,14,14	0.69	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	1PE	B	249	-	-	0/13/13/13	0/0/0/0

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.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.