



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 09:25 AM EST

PDB ID : 1EXZ
Title : STRUCTURE OF STEM CELL FACTOR
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Deposited on : 2000-05-05
Resolution : 2.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

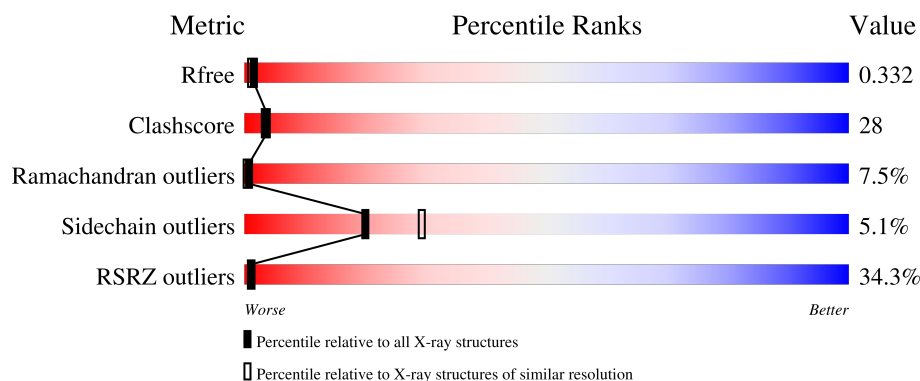
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>33%</div> <div>40%</div> <div>48%</div> <div>7%</div> <div>6%</div> </div>
1	B	141	<div> <div>34%</div> <div>55%</div> <div>40%</div> <div>5%</div> <div>•</div> </div>
1	C	141	<div> <div>30%</div> <div>57%</div> <div>29%</div> <div>6%</div> <div>•</div> <div>7%</div> </div>
1	D	141	<div> <div>31%</div> <div>46%</div> <div>35%</div> <div>6%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4236 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 STEM CELL FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1049	672	166	204	7			
1	B	140	Total	C	N	O	S	0	0	0
			1072	682	175	208	7			
1	C	131	Total	C	N	O	S	0	0	0
			998	638	157	197	6			
1	D	124	Total	C	N	O	S	0	0	0
			971	622	153	191	5			

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

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

- Molecule 3 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Sm	0	0
			2	2		
3	C	2	Total	Sm	0	0
			2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

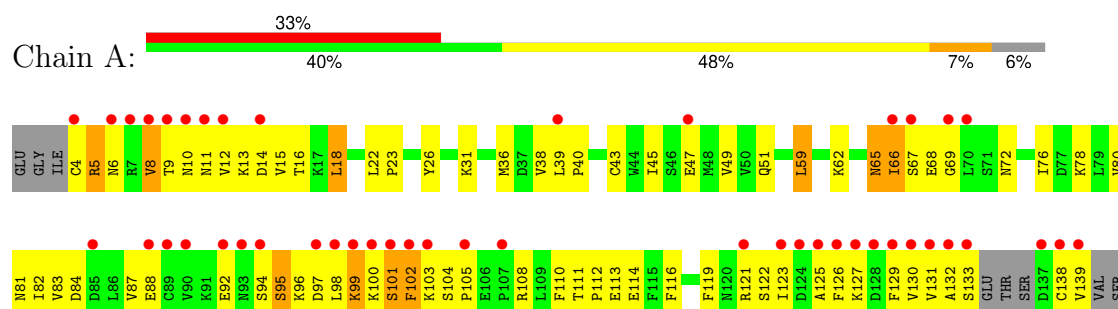
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	C	37	Total	O	0	0
			37	37		
5	D	28	Total	O	0	0
			28	28		

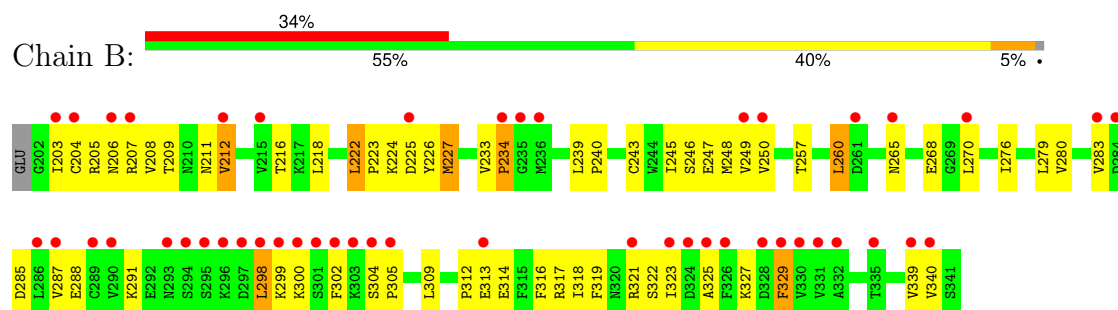
3 Residue-property plots

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. 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.

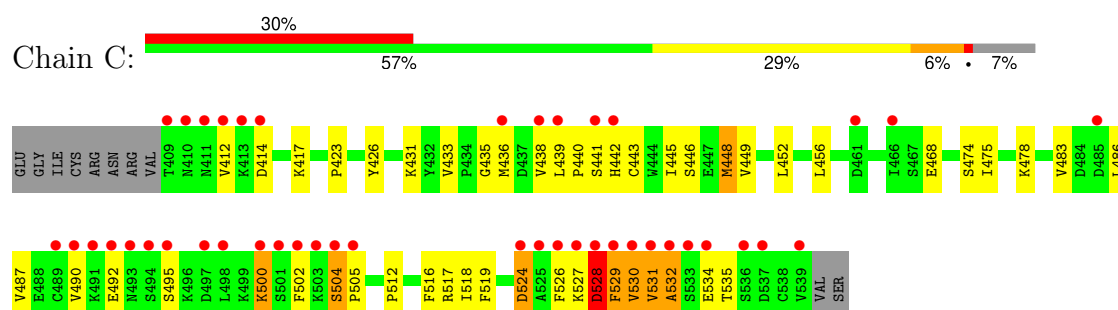
• Molecule 1: STEM CELL FACTOR



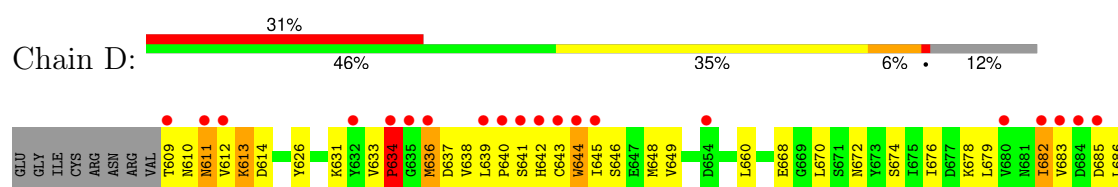
• Molecule 1: STEM CELL FACTOR



• Molecule 1: STEM CELL FACTOR



• Molecule 1: STEM CELL FACTOR





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.15Å 87.53Å 79.43Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	10.0 (40.00-2.30) 98.0 (40.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.294 0.295 , 0.332	Depositor DCC
R_{free} test set	1067 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4236	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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, 0.333 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: SM, TRS, CA

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	0.37	0/1067	0.58	0/1444
1	B	0.35	0/1090	0.58	0/1483
1	C	0.39	0/1016	0.62	0/1385
1	D	0.35	0/988	0.56	0/1342
All	All	0.37	0/4161	0.59	0/5654

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 [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	1049	0	1042	82	1
1	B	1072	0	1033	54	0
1	C	998	0	948	52	0
1	D	971	0	949	50	1
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	B	2	0	0	0	1
3	C	2	0	0	0	1
4	D	8	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	35	0	0	2	0
5	B	32	0	0	1	0
5	C	37	0	0	3	0
5	D	28	0	0	1	0
All	All	4236	0	3983	230	2

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 28.

The worst 5 of 230 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:531:VAL:HG12	1:C:532:ALA:H	1.12	1.15
1:C:423:PRO:HG2	1:C:426:TYR:HB2	1.48	0.94
1:A:65:ASN:HD22	1:A:66:ILE:H	1.16	0.93
1:C:452:LEU:O	1:C:456:LEU:HD23	1.72	0.90
1:C:527:LYS:HG3	1:C:528:ASP:H	1.38	0.89

All (2) 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:D:713:GLU:OE1	3:B:803:SM:SM[2_645]	2.12	0.08
1:A:88:GLU:OE2	3:C:801:SM:SM[2_656]	2.17	0.03

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	129/141 (92%)	103 (80%)	13 (10%)	13 (10%)	0	0
1	B	138/141 (98%)	113 (82%)	20 (14%)	5 (4%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	129/141 (92%)	105 (81%)	15 (12%)	9 (7%)	1	0
1	D	121/141 (86%)	98 (81%)	11 (9%)	12 (10%)	0	0
All	All	517/564 (92%)	419 (81%)	59 (11%)	39 (8%)	1	0

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	66	ILE
1	A	67	SER
1	A	132	ALA
1	B	291	LYS

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	125/135 (93%)	120 (96%)	5 (4%)	27	40
1	B	121/135 (90%)	112 (93%)	9 (7%)	11	15
1	C	112/135 (83%)	107 (96%)	5 (4%)	23	34
1	D	113/135 (84%)	108 (96%)	5 (4%)	24	35
All	All	471/540 (87%)	447 (95%)	24 (5%)	20	29

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	417	LYS
1	C	528	ASP
1	C	524	ASP
1	C	529	PHE
1	B	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	520	ASN
1	D	642	HIS
1	D	720	ASN
1	B	211	ASN
1	B	242	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 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	$\# Z > 2$
4	TRS	D	807	-	7,7,7	1.84	1 (14%)	9,9,9	1.49	1 (11%)

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
4	TRS	D	807	-	-	1/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	807	TRS	C2-C	-4.32	1.41	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	807	TRS	O2-C2-C	2.86	118.85	110.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	807	TRS	C3-C-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	731:VAL	C	732:ALA	N	8.59

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Warning: The R factor obtained from EDS is 0.3001, which does not match the depositor's R factor of 0.223. Please interpret the results in this section carefully.

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	133/141 (94%)	1.62	46 (34%) 1 1	18, 41, 88, 109	0
1	B	140/141 (99%)	1.74	48 (34%) 1 1	21, 48, 100, 104	0
1	C	131/141 (92%)	1.62	43 (32%) 1 1	18, 37, 92, 119	0
1	D	124/141 (87%)	1.77	44 (35%) 1 1	19, 47, 105, 114	0
All	All	528/564 (93%)	1.69	181 (34%) 1 1	18, 45, 99, 119	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	412	VAL	7.0
1	C	501	SER	6.7
1	D	641	SER	6.3
1	A	10	ASN	6.1
1	A	89	CYS	5.8

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
4	TRS	D	807	8/8	0.63	0.16	65,65,66,67	0
2	CA	A	806	1/1	0.77	0.24	29,29,29,29	0
3	SM	B	802	1/1	0.96	0.36	46,46,46,46	0
3	SM	C	804	1/1	0.98	0.37	29,29,29,29	0
2	CA	C	805	1/1	0.98	0.27	13,13,13,13	0
3	SM	B	803	1/1	0.99	0.37	31,31,31,31	0
3	SM	C	801	1/1	1.00	0.28	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.