



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7YZX / pdb_00007yzx
Title : ScpA from Streptococcus pyogenes, D783A mutant.
Authors : Kagawa, T.F.; Cooney, J.C.; Jain, M.
Deposited on : 2022-02-21
Resolution : 1.90 Å(reported)

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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

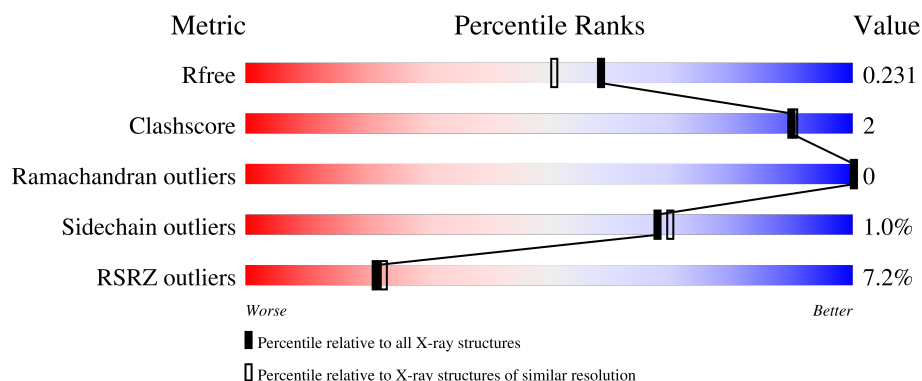
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	1002	6% 88% 5% 7%
1	B	1002	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7433 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 C5a peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	930	Total	C	N	O	S	0	11	0
			7030	4422	1187	1403	18			
1	B	5	Total	C	N	O		0	0	0
			27	17	5	5				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	783	ALA	ASP	engineered mutation	UNP B6ETQ5
B	783	ALA	ASP	engineered mutation	UNP B6ETQ5

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

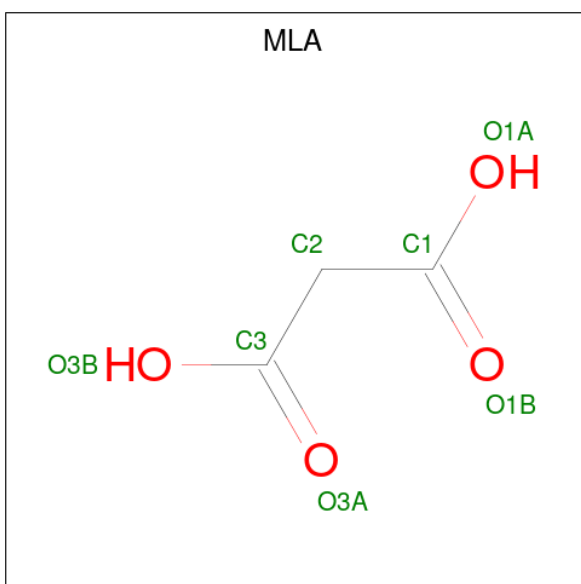
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	A	1	Total	C	O	0	1
			14	6	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	326	Total	O	0	0
			326	326		
6	B	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.42Å 169.42Å 141.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 1.90 45.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.00-1.90) 99.6 (45.00-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.198 , 0.229 0.201 , 0.231	Depositor DCC
R_{free} test set	4685 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7433	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MLA, SO4, NA

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	0.15	0/7197	0.36	0/9782
1	B	0.12	0/27	0.21	0/37
All	All	0.15	0/7224	0.36	0/9819

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	7030	0	6637	25	0
1	B	27	0	20	0	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	25	0	0	1	0
5	A	21	0	6	0	0
6	A	326	0	0	2	0
6	B	2	0	0	0	0
All	All	7433	0	6663	25	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 2.

All (25) 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:332:SER:HB2	1:A:494:GLN:HG3	1.66	0.77
1:A:902:THR:HG22	1:A:926:ILE:HG12	1.74	0.69
1:A:940:PHE:HZ	1:A:945:ARG:HH11	1.46	0.64
1:A:691:ARG:NH1	4:A:1103:SO4:O4	2.38	0.53
1:A:850:LEU:HB2	1:A:904:THR:HB	1.91	0.53
1:A:338:THR:HG21	1:A:354:PRO:HB3	1.91	0.52
1:A:585:MET:HG2	1:A:614:ASN:HA	1.93	0.51
1:A:534:PRO:HA	1:A:541:ARG:HH21	1.75	0.50
1:A:181:TYR:HE1	1:A:227[B]:MET:HG2	1.77	0.49
1:A:113:THR:HG21	1:A:578:LYS:HG3	1.97	0.47
1:A:959:ILE:HG21	1:A:962:GLU:HG3	1.97	0.46
1:A:471:LEU:HD22	1:A:569:GLN:HG2	1.98	0.45
1:A:522[B]:MET:SD	1:A:549:LEU:HD22	2.57	0.45
1:A:857:VAL:O	1:A:893:LYS:HG3	2.17	0.45
1:A:810:HIS:HE1	6:A:1363:HOH:O	1.98	0.45
1:A:932:PRO:HD3	1:A:1018:ASN:HB3	2.00	0.44
1:A:908:ARG:HD2	1:A:918:GLU:OE2	2.19	0.43
1:A:1008:PHE:HB2	1:A:1024:VAL:HG11	2.02	0.42
1:A:771:ILE:O	1:A:775:LYS:HD3	2.20	0.42
1:A:414:LEU:HD23	1:A:436:ALA:HB3	2.02	0.41
1:A:623:TYR:HA	1:A:651:GLN:O	2.20	0.41
1:A:263:ASN:O	1:A:317:GLY:HA3	2.21	0.41
1:A:721:LYS:NZ	6:A:1218:HOH:O	2.53	0.41
1:A:965:ALA:O	1:A:1008:PHE:HA	2.21	0.41
1:A:563:ALA:HB2	1:A:644:ALA:HB2	2.03	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	933/1002 (93%)	900 (96%)	33 (4%)	0	100	100
1	B	3/1002 (0%)	3 (100%)	0	0	100	100
All	All	936/2004 (47%)	903 (96%)	33 (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	715/837 (85%)	708 (99%)	7 (1%)	68	70
1	B	1/837 (0%)	1 (100%)	0	100	100
All	All	716/1674 (43%)	709 (99%)	7 (1%)	68	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LEU
1	A	184	ASP
1	A	406	LYS
1	A	471	LEU
1	A	549	LEU
1	A	776	GLU
1	A	781	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	494	GLN
1	A	592	ASN
1	A	658	ASN
1	A	810	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	SO4	A	1103	-	4,4,4	0.25	0	6,6,6	0.08	0
5	MLA	A	1109[A]	-	6,6,6	1.42	0	7,7,7	1.37	0
5	MLA	A	1109[B]	-	6,6,6	1.41	0	7,7,7	1.35	0
5	MLA	A	1108	-	6,6,6	1.37	0	7,7,7	1.37	1 (14%)
4	SO4	A	1104	-	4,4,4	0.24	0	6,6,6	0.13	0
4	SO4	A	1106	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	A	1105	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	A	1107	-	4,4,4	0.25	0	6,6,6	0.09	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
5	MLA	A	1109[A]	-	-	0/4/4/4	-
5	MLA	A	1109[B]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLA	A	1108	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1108	MLA	O1A-C1-C2	2.04	120.82	114.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1108	MLA	O1B-C1-C2-C3
5	A	1108	MLA	C1-C2-C3-O3A
5	A	1108	MLA	O1A-C1-C2-C3
5	A	1108	MLA	C1-C2-C3-O3B
5	A	1109[B]	MLA	C1-C2-C3-O3A
5	A	1109[B]	MLA	C1-C2-C3-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	SO4	1	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

6.1 Protein, DNA and RNA chains

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	930/1002 (92%)	0.39	64 (6%) 23 24	18, 44, 83, 108	11 (1%)
1	B	5/1002 (0%)	2.92	3 (60%) 0 0	59, 62, 74, 79	0
All	All	935/2004 (46%)	0.40	67 (7%) 21 23	18, 44, 83, 108	11 (1%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	974	PRO	5.2
1	A	995	THR	5.1
1	A	233[A]	ASN	5.0
1	A	972	ASP	5.0
1	A	781	ILE	4.7
1	B	87	ALA	4.6
1	A	1000	THR	4.4
1	B	83	LEU	4.3
1	A	1001	VAL	4.3
1	A	737	ASN	4.2
1	A	94	THR	4.2
1	A	95	PRO	4.0
1	A	934	VAL	3.9
1	A	970	ASP	3.7
1	A	96	ALA	3.7
1	A	232[A]	VAL	3.5
1	A	785	GLU	3.3
1	A	969	MET	3.2
1	A	1003	LEU	3.2
1	A	895	GLY	3.2
1	A	975	THR	3.0
1	A	348	HIS	3.0
1	A	371	TYR	3.0
1	A	777	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	940	PHE	2.9
1	A	1008	PHE	2.9
1	A	97	THR	2.8
1	A	935	ALA	2.8
1	B	84	ALA	2.8
1	A	967	THR	2.8
1	A	959	ILE	2.6
1	A	739	ASP	2.6
1	A	1024	VAL	2.6
1	A	956	SER	2.6
1	A	999	GLY	2.5
1	A	813	ALA	2.5
1	A	384	VAL	2.5
1	A	942	THR	2.5
1	A	778	VAL	2.5
1	A	738	SER	2.4
1	A	1028	LEU	2.4
1	A	187	THR	2.4
1	A	771	ILE	2.4
1	A	1030	GLY	2.4
1	A	989	LEU	2.3
1	A	786	SER	2.3
1	A	1025	THR	2.3
1	A	382	LYS	2.3
1	A	184	ASP	2.3
1	A	774	VAL	2.3
1	A	188	ALA	2.2
1	A	993	ALA	2.2
1	A	350	ALA	2.2
1	A	780	ASN	2.2
1	A	897	VAL	2.2
1	A	898	VAL	2.2
1	A	899	VAL	2.2
1	A	949	LEU	2.2
1	A	1027	LEU	2.2
1	A	903	TYR	2.1
1	A	968	TYR	2.1
1	A	803	ASP	2.1
1	A	894	ASP	2.1
1	A	854	GLY	2.1
1	A	343	VAL	2.1
1	A	742	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	971	GLU	2.0

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 oligosaccharides 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	SO4	A	1107	5/5	0.60	0.12	65,73,103,106	0
5	MLA	A	1109[A]	7/7	0.64	0.19	51,59,61,61	7
5	MLA	A	1109[B]	7/7	0.64	0.19	56,57,60,60	7
5	MLA	A	1108	7/7	0.67	0.15	55,62,67,67	0
4	SO4	A	1105	5/5	0.74	0.10	59,72,86,88	0
4	SO4	A	1106	5/5	0.79	0.12	53,65,79,80	0
4	SO4	A	1104	5/5	0.83	0.09	76,76,80,89	0
4	SO4	A	1103	5/5	0.86	0.09	50,56,67,73	0
2	CA	A	1101	1/1	0.98	0.04	55,55,55,55	0
3	NA	A	1102	1/1	0.99	0.05	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.