



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 11:07 PM EST

PDB ID : 4JE0
Title : Structures of SdrD from Staphylococcus aureus reveal the molecular mechanism of how the cell surface receptors recognize their ligands
Authors : Wang, X.; Ge, J.; Yang, M.
Deposited on : 2013-02-25
Resolution : 1.70 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

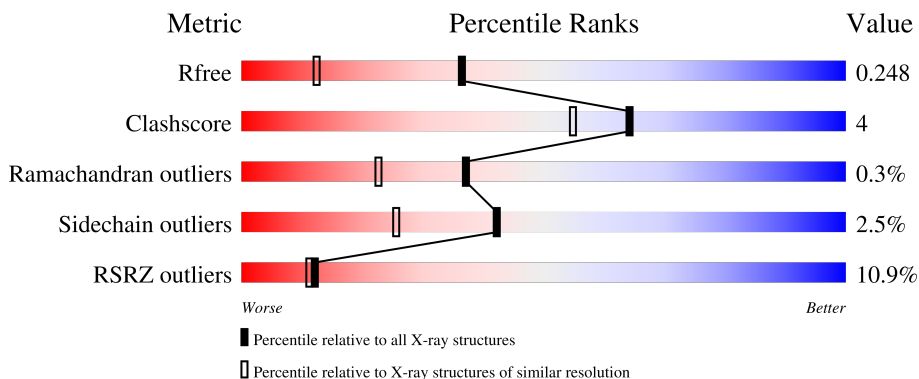
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	316	<div> <div>10%</div> <div>89%</div> <div>9%</div> <div>...</div> </div>
1	B	316	<div> <div>11%</div> <div>89%</div> <div>9%</div> <div>...</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5455 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 Ser-Asp rich fibrinogen/bone sialoprotein-binding protein SdrD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	Se	0	0	0
			2429	1515	396	514	4			
1	B	313	Total	C	N	O	Se	0	0	0
			2419	1506	395	514	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP E5QTK7
A	-3	PRO	-	expression tag	UNP E5QTK7
A	-2	LEU	-	expression tag	UNP E5QTK7
A	-1	GLY	-	expression tag	UNP E5QTK7
A	311	ALA	-	expression tag	UNP E5QTK7
B	-4	GLY	-	expression tag	UNP E5QTK7
B	-3	PRO	-	expression tag	UNP E5QTK7
B	-2	LEU	-	expression tag	UNP E5QTK7
B	-1	GLY	-	expression tag	UNP E5QTK7
B	311	ALA	-	expression tag	UNP E5QTK7

- 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		

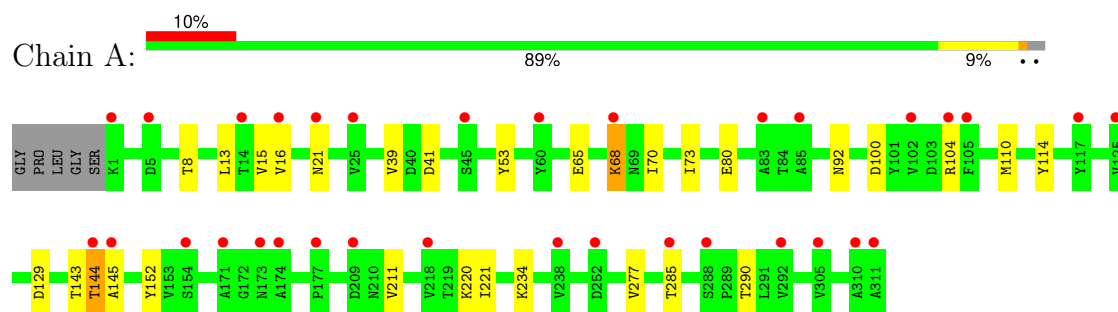
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total	O	0	0
			242	242		
3	B	364	Total	O	0	0
			364	364		

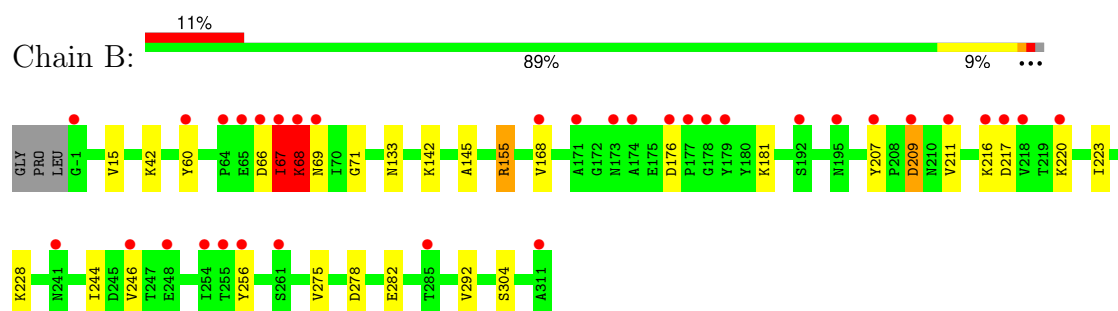
3 Residue-property plots

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 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: Ser-Asp rich fibrinogen/bone sialoprotein-binding protein SdrD



- Molecule 1: Ser-Asp rich fibrinogen/bone sialoprotein-binding protein SdrD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.31Å 58.36Å 112.36Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	31.44 – 1.70 31.44 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (31.44-1.70) 96.6 (31.44-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.208 , 0.246 0.210 , 0.248	Depositor DCC
R_{free} test set	4291 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5455	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: 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	0.32	0/2466	0.54	0/3353
1	B	0.37	0/2456	0.58	0/3344
All	All	0.35	0/4922	0.56	0/6697

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	68	LYS	Peptide

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	2429	0	2345	15	0
1	B	2419	0	2304	21	0
2	A	1	0	0	0	0
3	A	242	0	0	1	0
3	B	364	0	0	6	0
All	All	5455	0	4649	36	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 4.

All (36) 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:B:60:TYR:HB3	1:B:67:ILE:HG22	1.59	0.84
1:B:68:LYS:HE2	1:B:71:GLY:HA2	1.63	0.81
1:A:80:GLU:OE1	1:A:104:ARG:NH2	2.19	0.73
1:B:155:ARG:NH1	1:B:304:SER:O	2.24	0.71
1:B:216:LYS:HG2	1:B:256:TYR:CD1	2.29	0.67
1:B:68:LYS:NZ	3:B:677:HOH:O	2.26	0.65
1:B:209:ASP:OD1	1:B:209:ASP:N	2.19	0.63
1:A:221:ILE:HD13	1:A:277:VAL:HG22	1.81	0.60
1:B:15:VAL:HG21	1:B:145:ALA:HB2	1.84	0.59
1:B:211:VAL:HG13	1:B:282:GLU:HB2	1.86	0.58
1:A:41:ASP:O	3:A:502:HOH:O	2.17	0.56
1:A:73:ILE:HG21	1:A:110:MSE:HB3	1.86	0.56
1:A:100:ASP:OD1	1:A:104:ARG:NH1	2.38	0.55
1:B:220:LYS:NZ	3:B:743:HOH:O	2.26	0.54
1:A:100:ASP:O	1:A:104:ARG:HG3	2.07	0.54
1:A:152:TYR:CZ	1:A:234:LYS:HE3	2.44	0.53
1:A:129:ASP:HA	1:A:144:THR:HG23	1.92	0.52
1:B:176:ASP:OD2	3:B:537:HOH:O	2.18	0.52
1:A:65:GLU:O	1:A:68:LYS:HE3	2.10	0.52
1:B:67:ILE:HG13	1:B:67:ILE:O	2.12	0.50
1:A:13:LEU:HD23	1:A:143:THR:HG22	1.96	0.47
1:B:216:LYS:HG3	3:B:517:HOH:O	2.14	0.46
1:B:223:ILE:HG12	1:B:275:VAL:HG22	1.97	0.46
1:B:133:ASN:HB3	1:B:142:LYS:HG2	1.98	0.45
1:A:15:VAL:HG21	1:A:145:ALA:HB2	1.99	0.45
1:B:207:TYR:CD2	1:B:292:VAL:HG21	2.51	0.44
1:A:211:VAL:HG22	1:A:290:THR:O	2.17	0.44
1:B:244:ILE:O	1:B:246:VAL:HG23	2.18	0.44
1:A:70:ILE:HG23	1:A:114:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TYR:CZ	1:A:92:ASN:HA	2.53	0.43
1:B:66:ASP:C	1:B:68:LYS:H	2.22	0.43
1:B:181:LYS:NZ	1:B:278:ASP:OD2	2.52	0.42
1:B:42:LYS:NZ	3:B:761:HOH:O	2.53	0.41
1:A:39:VAL:CG2	1:A:110:MSE:HE2	2.50	0.41
1:B:155:ARG:NE	3:B:736:HOH:O	2.55	0.40
1:B:66:ASP:O	1:B:68:LYS:N	2.54	0.40

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	309/316 (98%)	305 (99%)	3 (1%)	1 (0%)	37	23
1	B	311/316 (98%)	303 (97%)	7 (2%)	1 (0%)	37	23
All	All	620/632 (98%)	608 (98%)	10 (2%)	2 (0%)	37	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	ILE
1	A	21	ASN

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	278/277 (100%)	272 (98%)	6 (2%)	47	30
1	B	273/277 (99%)	265 (97%)	8 (3%)	37	20
All	All	551/554 (100%)	537 (98%)	14 (2%)	42	25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	16	VAL
1	A	68	LYS
1	A	144	THR
1	A	220	LYS
1	A	285	THR
1	B	67	ILE
1	B	68	LYS
1	B	69	ASN
1	B	155	ARG
1	B	168	VAL
1	B	209	ASP
1	B	217	ASP
1	B	228	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

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	307/316 (97%)	1.07	33 (10%)	12 12	36, 47, 66, 91	0
1	B	309/316 (97%)	0.87	34 (11%)	12 11	27, 39, 59, 81	0
All	All	616/632 (97%)	0.97	67 (10%)	12 11	27, 44, 64, 91	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	ILE	6.0
1	B	68	LYS	4.9
1	A	311	ALA	4.3
1	B	254	ILE	4.0
1	B	69	ASN	3.7
1	B	311	ALA	3.7
1	A	171	ALA	3.6
1	B	174	ALA	3.5
1	B	246	VAL	3.4
1	A	252	ASP	3.4
1	B	285	THR	3.4
1	B	177	PRO	3.3
1	A	125	VAL	3.3
1	B	216	LYS	3.3
1	B	209	ASP	3.3
1	B	171	ALA	3.3
1	B	261	SER	3.3
1	B	168	VAL	3.2
1	A	174	ALA	3.2
1	A	1	LYS	3.2
1	A	68	LYS	3.0
1	A	209	ASP	2.9
1	B	220	LYS	2.8
1	A	292	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	238	VAL	2.7
1	B	-1	GLY	2.7
1	B	64	PRO	2.6
1	B	65	GLU	2.6
1	A	21	ASN	2.6
1	B	66	ASP	2.6
1	B	217	ASP	2.6
1	B	173	ASN	2.5
1	B	195	ASN	2.5
1	A	288	SER	2.5
1	A	102	VAL	2.5
1	A	104	ARG	2.4
1	A	16	VAL	2.4
1	B	211	VAL	2.4
1	B	241	ASN	2.4
1	B	207	TYR	2.4
1	A	105	PHE	2.4
1	A	5	ASP	2.4
1	B	218	VAL	2.4
1	B	60	TYR	2.4
1	B	179	TYR	2.4
1	B	255	THR	2.3
1	A	25	VAL	2.3
1	A	117	TYR	2.3
1	A	45	SER	2.3
1	A	145	ALA	2.3
1	A	285	THR	2.3
1	A	177	PRO	2.3
1	A	173	ASN	2.3
1	A	310	ALA	2.3
1	A	14	THR	2.2
1	A	218	VAL	2.2
1	B	248	GLU	2.2
1	A	85	ALA	2.2
1	A	60	TYR	2.2
1	B	178	GLY	2.1
1	A	305	VAL	2.1
1	B	256	TYR	2.1
1	A	83	ALA	2.0
1	A	144	THR	2.0
1	B	176	ASP	2.0
1	A	154	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	192	SER	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 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
2	CA	A	401	1/1	0.96	0.13	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.