



wwPDB X-ray Structure Validation Summary Report

Feb 4, 2024 – 10:09 PM EST

PDB ID : 1SRR
Title : CRYSTAL STRUCTURE OF A PHOSPHATASE RESISTANT MUTANT OF SPORULATION RESPONSE REGULATOR SPO0F FROM BACILLUS SUBTILIS
Authors : Madhusudan; Whiteley, J.M.; Hoch, J.A.; Zapf, J.; Xuong, N.H.; Varughese, K.I.
Deposited on : 1996-04-10
Resolution : 1.90 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

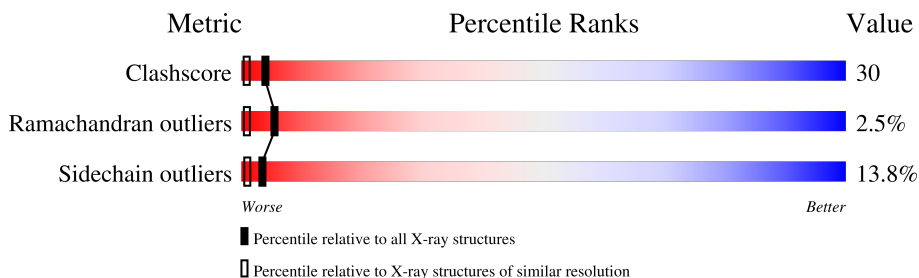
1 Overall quality at a glance

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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	124	50% 38% 8% .
1	B	124	27% 51% 17% . .
1	C	124	48% 35% 9% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3039 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 SPORULATION RESPONSE REGULATORY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	119	937	600	155	177	5	0	0	0
1	B	120	907	587	144	171	5	0	0	0
1	C	121	933	596	152	180	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	SER	TYR	conflict	UNP P06628
B	13	SER	TYR	conflict	UNP P06628
C	13	SER	TYR	conflict	UNP P06628

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total 97	O 97	0	0
3	B	83	Total 83	O 83	0	0
3	C	80	Total 80	O 80	0	0

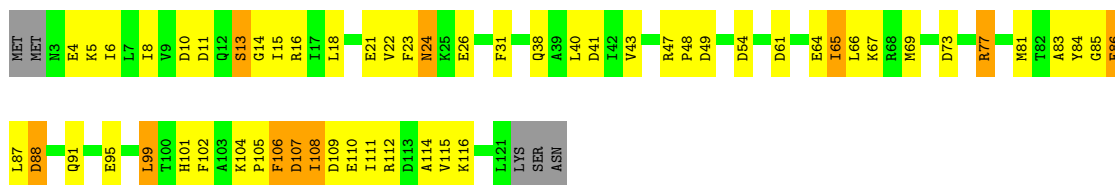
3 Residue-property plots [i](#)

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.

Note EDS was not executed.

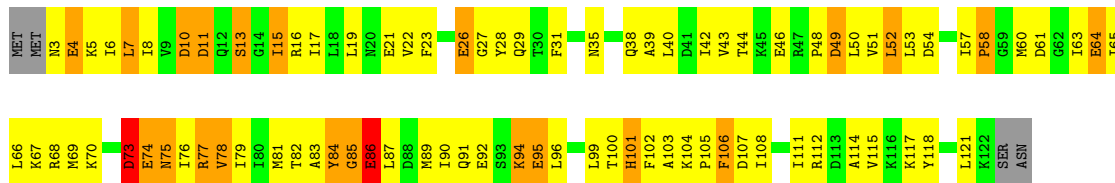
- Molecule 1: SPORULATION RESPONSE REGULATORY PROTEIN

Chain A: 



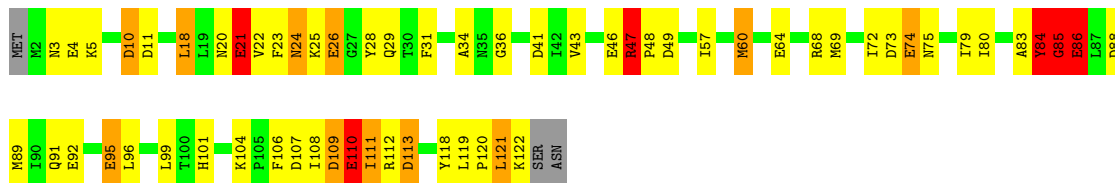
- Molecule 1: SPORULATION RESPONSE REGULATORY PROTEIN

Chain B: 



- Molecule 1: SPORULATION RESPONSE REGULATORY PROTEIN

Chain C: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.99Å 101.99Å 82.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.5 (10.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.219 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3039	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

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	1.09	5/948 (0.5%)	1.49	18/1276 (1.4%)
1	B	1.08	7/918 (0.8%)	1.45	10/1243 (0.8%)
1	C	1.18	10/944 (1.1%)	1.50	19/1278 (1.5%)
All	All	1.12	22/2810 (0.8%)	1.48	47/3797 (1.2%)

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	1	0

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	GLY	N-CA	8.19	1.58	1.46
1	B	64	GLU	CD-OE1	7.52	1.33	1.25
1	C	110	GLU	CD-OE1	7.20	1.33	1.25
1	C	84	TYR	C-N	7.08	1.45	1.33
1	C	46	GLU	CD-OE1	6.64	1.32	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	TYR	C-N-CA	10.14	143.60	122.30
1	B	16	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	49	ASP	CB-CG-OD1	-8.17	110.94	118.30
1	A	61	ASP	CB-CG-OD1	-8.14	110.97	118.30
1	A	61	ASP	CB-CG-OD2	8.06	125.55	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	86	GLU	CA

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	937	0	961	35	0
1	B	907	0	897	88	0
1	C	933	0	920	51	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	97	0	0	5	0
3	B	83	0	0	2	0
3	C	80	0	0	2	0
All	All	3039	0	2778	169	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 30.

The worst 5 of 169 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:121:LEU:HD13	1:C:122:LYS:N	1.93	0.82
1:B:26:GLU:OE1	1:B:112:ARG:HG2	1.80	0.82
1:B:35:ASN:OD1	1:B:38:GLN:HG3	1.82	0.79
1:C:104:LYS:HG2	1:C:106:PHE:CE2	2.19	0.78
1:B:95:GLU:HA	1:C:99:LEU:CD2	2.16	0.76

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	117/124 (94%)	114 (97%)	2 (2%)	1 (1%)	17	7
1	B	118/124 (95%)	104 (88%)	9 (8%)	5 (4%)	3	0
1	C	119/124 (96%)	107 (90%)	9 (8%)	3 (2%)	5	1
All	All	354/372 (95%)	325 (92%)	20 (6%)	9 (2%)	5	1

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLY
1	B	58	PRO
1	B	84	TYR
1	C	84	TYR
1	C	85	GLY

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	101/110 (92%)	91 (90%)	10 (10%)	8	3
1	B	91/110 (83%)	76 (84%)	15 (16%)	2	0
1	C	97/110 (88%)	82 (84%)	15 (16%)	2	1
All	All	289/330 (88%)	249 (86%)	40 (14%)	3	1

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	25	LYS
1	C	108	ILE
1	C	47	ARG
1	C	84	TYR
1	C	110	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	75	ASN
1	C	24	ASN
1	C	38	GLN
1	C	29	GLN
1	B	20	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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 [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.