



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 12:56 PM GMT

PDB ID : 3G06
Title : The Salmonella Virulence Effector SspH2 Functions As A Novel E3 Ligase
Authors : Quezada, C.M.; Stebbins, C.E.
Deposited on : 2009-01-27
Resolution : 1.90 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>

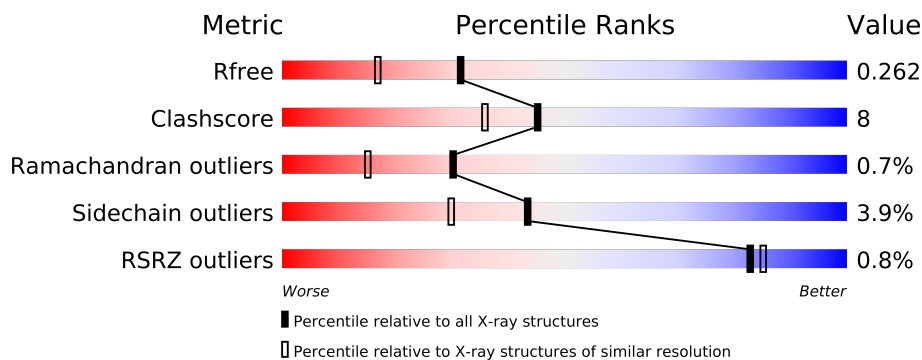
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 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.

Mol	Chain	Length	Quality of chain
1	A	622	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5069 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 SspH2 (Leucine-rich repeat protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4663	2951	803	891	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	GLY	-	expression tag	UNP Q9RPH0
A	163	PRO	-	expression tag	UNP Q9RPH0
A	164	VAL	-	expression tag	UNP Q9RPH0
A	165	ASP	-	expression tag	UNP Q9RPH0

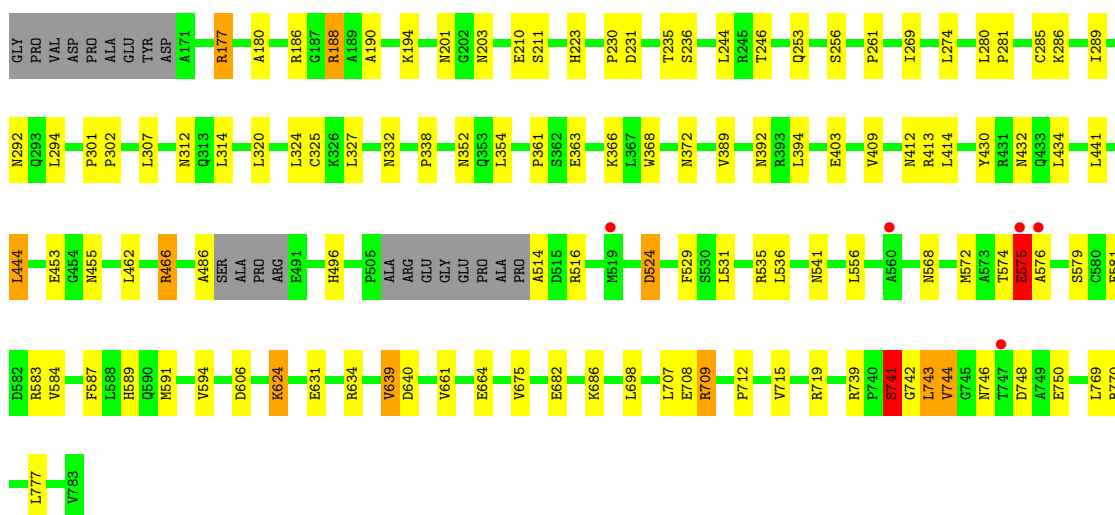
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	406	Total	O	0	0
			406	406		

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- Molecule 1: SspH2 (Leucine-rich repeat protein)

Age Group	Percentage
18-29	90%
30-49	85%
50-64	75%
65+	65%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.89Å 76.89Å 281.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 35.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-1.90) 98.1 (35.49-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.4.0063	Depositor
R, R_{free}	0.219 , 0.264 0.218 , 0.262	Depositor DCC
R_{free} test set	3369 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 66510 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5069	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.99	3/4753 (0.1%)	0.98	13/6468 (0.2%)

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	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	CYS	CB-SG	-9.06	1.66	1.82
1	A	581	GLU	CB-CG	-6.46	1.39	1.52
1	A	529	PHE	CE2-CZ	5.13	1.47	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	ARG	NE-CZ-NH2	-13.33	113.63	120.30
1	A	709	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	A	639	VAL	CB-CA-C	-7.46	97.23	111.40
1	A	186	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	186	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	739	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	640	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	444	LEU	CB-CG-CD1	5.45	120.27	111.00
1	A	188	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	536	LEU	CA-CB-CG	5.29	127.48	115.30
1	A	739	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	575	GLU	N-CA-C	-5.08	97.30	111.00
1	A	709	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	THR	Peptide
1	A	575	GLU	Peptide
1	A	741	SER	Peptide

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	4663	0	4711	79	0
2	A	406	0	0	13	0
All	All	5069	0	4711	79	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 8.

All (79) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:246:THR:HG22	2:A:967:HOH:O	1.45	1.16
1:A:576:ALA:HB2	1:A:587:PHE:HB2	1.46	0.95
1:A:742:GLY:HA3	1:A:743:LEU:HG	1.49	0.95
1:A:742:GLY:CA	1:A:743:LEU:HG	2.04	0.86
1:A:576:ALA:HB1	1:A:584:VAL:HA	1.60	0.84
1:A:414:LEU:H	1:A:432:ASN:HD22	1.31	0.78
1:A:352:ASN:HB2	1:A:372:ASN:HD21	1.50	0.74
1:A:631:GLU:OE2	1:A:634:ARG:NH1	2.20	0.74
1:A:434:LEU:H	1:A:455:ASN:HD22	1.35	0.74
1:A:413:ARG:HD2	2:A:975:HOH:O	1.87	0.74
1:A:496:HIS:HD2	2:A:898:HOH:O	1.72	0.72
1:A:177:ARG:CD	2:A:970:HOH:O	2.37	0.71
1:A:576:ALA:HB2	1:A:587:PHE:CB	2.20	0.70
1:A:392:ASN:HB2	1:A:412:ASN:HD21	1.58	0.69
1:A:432:ASN:HB2	1:A:455:ASN:HD21	1.59	0.68
1:A:177:ARG:HD3	2:A:970:HOH:O	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:741:SER:HB2	1:A:742:GLY:HA3	1.78	0.66
1:A:742:GLY:HA3	1:A:743:LEU:CG	2.24	0.66
1:A:514:ALA:N	2:A:971:HOH:O	2.30	0.64
1:A:741:SER:CB	1:A:742:GLY:HA3	2.28	0.63
1:A:675:VAL:HG23	2:A:1000:HOH:O	1.97	0.63
1:A:403:GLU:HB2	2:A:122:HOH:O	1.99	0.63
1:A:535:ARG:NH2	1:A:579:SER:O	2.34	0.61
1:A:312:ASN:HB2	1:A:332:ASN:HD21	1.64	0.60
1:A:177:ARG:HD2	2:A:970:HOH:O	1.98	0.59
1:A:587:PHE:O	1:A:591:MET:HG3	2.03	0.58
1:A:180:ALA:HB2	1:A:188:ARG:HD2	1.85	0.58
1:A:332:ASN:HB2	1:A:352:ASN:HD21	1.68	0.58
1:A:742:GLY:HA2	1:A:743:LEU:HG	1.85	0.57
1:A:572:MET:O	1:A:575:GLU:O	2.22	0.56
1:A:432:ASN:CB	1:A:455:ASN:HD21	2.18	0.55
1:A:576:ALA:CB	1:A:584:VAL:HA	2.35	0.55
1:A:606:ASP:OD2	1:A:709:ARG:HD2	2.07	0.55
1:A:412:ASN:HB2	1:A:432:ASN:HD21	1.71	0.54
1:A:363:GLU:HG3	2:A:1018:HOH:O	2.09	0.52
1:A:244:LEU:HB3	1:A:261:PRO:HG2	1.91	0.51
1:A:589:HIS:CE1	1:A:661:VAL:HG13	2.46	0.51
1:A:392:ASN:CB	1:A:412:ASN:HD21	2.22	0.51
1:A:541:ASN:HD21	1:A:664:GLU:H	1.60	0.50
1:A:314:LEU:H	1:A:332:ASN:HD22	1.60	0.49
1:A:210:GLU:HG3	1:A:230:PRO:HB2	1.94	0.49
1:A:707:LEU:HD13	1:A:769:LEU:HD22	1.95	0.48
1:A:715:VAL:O	1:A:719:ARG:HG2	2.14	0.47
1:A:414:LEU:H	1:A:432:ASN:ND2	2.04	0.47
1:A:294:LEU:H	1:A:312:ASN:HD22	1.63	0.47
1:A:285:CYS:O	1:A:286:LYS:HD3	2.15	0.47
1:A:466:ARG:HB2	1:A:466:ARG:HE	1.33	0.46
1:A:568:ASN:O	1:A:572:MET:HG3	2.15	0.46
1:A:320:LEU:HG	1:A:338:PRO:HG2	1.97	0.46
1:A:575:GLU:HG2	1:A:575:GLU:H	1.67	0.46
1:A:190:ALA:O	1:A:194:LYS:HG3	2.17	0.45
1:A:579:SER:HB3	1:A:583:ARG:HB3	1.98	0.45
1:A:430:TYR:HA	1:A:453:GLU:O	2.16	0.45
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.56	0.45
1:A:269:ILE:CG2	1:A:289:ILE:HG22	2.48	0.44
1:A:708:GLU:OE1	1:A:719:ARG:NH2	2.47	0.44
1:A:307:LEU:HD23	1:A:327:LEU:HD13	2.00	0.43
1:A:698:LEU:HD21	1:A:770:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:HIS:CD2	1:A:223:HIS:H	2.34	0.43
1:A:354:LEU:H	1:A:372:ASN:HD22	1.64	0.43
1:A:572:MET:SD	1:A:594:VAL:HG21	2.58	0.43
1:A:434:LEU:H	1:A:455:ASN:ND2	2.09	0.43
1:A:741:SER:CB	1:A:742:GLY:CA	2.97	0.43
1:A:203:ASN:O	1:A:223:HIS:HE1	2.02	0.42
1:A:361:PRO:HB2	2:A:966:HOH:O	2.19	0.42
1:A:394:LEU:H	1:A:412:ASN:HD22	1.66	0.42
1:A:441:LEU:O	1:A:441:LEU:HD12	2.20	0.42
1:A:744:VAL:O	1:A:750:GLU:OE1	2.38	0.42
1:A:486:ALA:C	2:A:968:HOH:O	2.58	0.42
1:A:389:VAL:CG2	1:A:409:VAL:HG12	2.50	0.41
1:A:201:ASN:OD1	1:A:203:ASN:HB2	2.20	0.41
1:A:280:LEU:HA	1:A:281:PRO:HD3	1.88	0.41
1:A:682:GLU:OE2	1:A:686:LYS:HE3	2.21	0.41
1:A:624:LYS:HD3	2:A:877:HOH:O	2.20	0.41
1:A:301:PRO:HA	1:A:302:PRO:HD3	1.98	0.41
1:A:292:ASN:H	1:A:312:ASN:HD21	1.68	0.41
1:A:256:SER:HA	1:A:274:LEU:HD11	2.02	0.41
1:A:366:LYS:HE3	1:A:368:TRP:CD2	2.56	0.40
1:A:556:LEU:HA	1:A:556:LEU:HD23	1.91	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	595/622 (96%)	565 (95%)	26 (4%)	4 (1%)	30	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	ASP
1	A	743	LEU

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Mol	Chain	Res	Type
1	A	741	SER
1	A	746	ASN

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	516/531 (97%)	496 (96%)	20 (4%)	43	30

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	211	SER
1	A	231	ASP
1	A	235	THR
1	A	236	SER
1	A	253	GLN
1	A	324	LEU
1	A	444	LEU
1	A	462	LEU
1	A	466	ARG
1	A	516	ARG
1	A	524	ASP
1	A	531	LEU
1	A	575	GLU
1	A	624	LYS
1	A	639	VAL
1	A	712	PRO
1	A	744	VAL
1	A	748	ASP
1	A	777	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	312	ASN
1	A	332	ASN
1	A	352	ASN
1	A	372	ASN
1	A	412	ASN
1	A	432	ASN
1	A	455	ASN
1	A	541	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 ⓘ

There are no ligands in this entry.

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	601/622 (96%)	-0.01	5 (0%) 83 85	21, 33, 51, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	ALA	3.7
1	A	519	MET	2.5
1	A	575	GLU	2.4
1	A	747	THR	2.1
1	A	560	ALA	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.