



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 11:02 AM EDT

PDB ID : 2OV8
Title : Crystal Structure of StaL
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : unknown
Resolution : 2.58 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

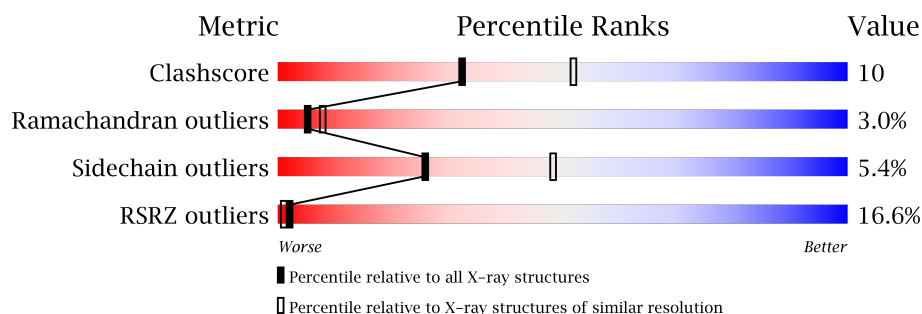
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	112137	3268 (2.60-2.56)
Ramachandran outliers	110173	3218 (2.60-2.56)
Sidechain outliers	110143	3218 (2.60-2.56)
RSRZ outliers	101464	2907 (2.60-2.56)

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. 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	288	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1781 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 StaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1768	1131	298	326	13			

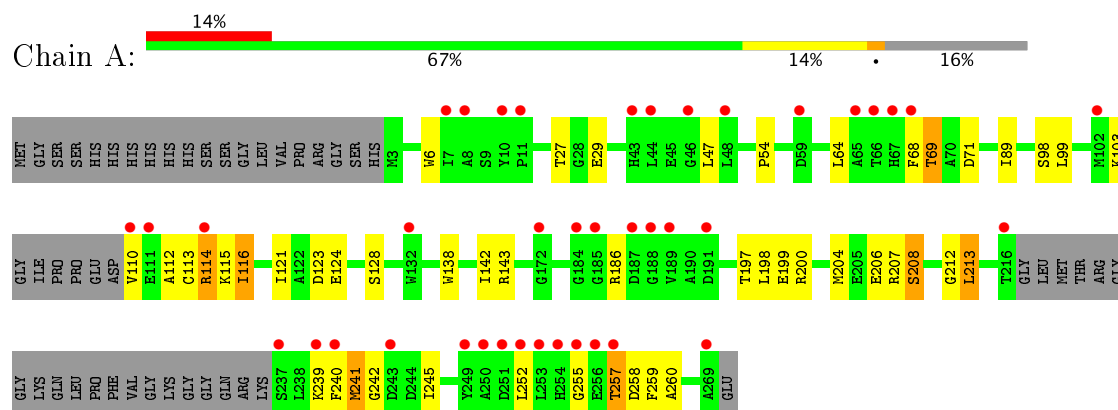
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	CLONING ARTIFACT	UNP Q8KLM3
A	-16	GLY	-	CLONING ARTIFACT	UNP Q8KLM3
A	-15	SER	-	CLONING ARTIFACT	UNP Q8KLM3
A	-14	SER	-	CLONING ARTIFACT	UNP Q8KLM3
A	-13	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-12	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-11	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-10	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-9	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-8	HIS	-	EXPRESSION TAG	UNP Q8KLM3
A	-7	SER	-	CLONING ARTIFACT	UNP Q8KLM3
A	-6	SER	-	CLONING ARTIFACT	UNP Q8KLM3
A	-5	GLY	-	CLONING ARTIFACT	UNP Q8KLM3
A	-4	LEU	-	CLONING ARTIFACT	UNP Q8KLM3
A	-3	VAL	-	CLONING ARTIFACT	UNP Q8KLM3
A	-2	PRO	-	CLONING ARTIFACT	UNP Q8KLM3
A	-1	ARG	-	CLONING ARTIFACT	UNP Q8KLM3
A	0	GLY	-	CLONING ARTIFACT	UNP Q8KLM3
A	1	SER	-	CLONING ARTIFACT	UNP Q8KLM3
A	2	HIS	-	CLONING ARTIFACT	UNP Q8KLM3
A	3	MET	-	CLONING ARTIFACT	UNP Q8KLM3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		

- Molecule 1: StaL



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.02Å 86.02Å 164.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.54 – 2.58 38.13 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.54-2.58) 94.0 (38.13-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.69 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.279 0.262 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.5	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	0.85	EDS
Total number of atoms	1781	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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](#)

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	0.67	1/1811 (0.1%)	0.71	0/2468

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	VAL	CB-CG1	5.73	1.64	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	PHE	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	1768	0	1631	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	0	0	0
All	All	1781	0	1631	34	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 10.

All (34) 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:69:THR:CG2	1:A:71:ASP:OD1	2.21	0.89
1:A:69:THR:HG21	1:A:71:ASP:OD1	1.72	0.88
1:A:99:LEU:O	1:A:103:LYS:HB2	1.91	0.70
1:A:212:GLY:O	1:A:213:LEU:O	2.13	0.67
1:A:112:ALA:O	1:A:116:ILE:HG22	1.96	0.65
1:A:239:LYS:O	1:A:241:MET:N	2.28	0.65
1:A:204:MET:HA	1:A:207:ARG:HH11	1.62	0.64
1:A:69:THR:CG2	1:A:71:ASP:CG	2.67	0.63
1:A:239:LYS:C	1:A:241:MET:H	2.02	0.62
1:A:204:MET:HA	1:A:207:ARG:NH1	2.15	0.62
1:A:114:ARG:HA	1:A:245:ILE:HD11	1.84	0.58
1:A:113:CYS:HA	1:A:116:ILE:CG2	2.34	0.58
1:A:27:THR:HG22	1:A:29:GLU:H	1.72	0.55
1:A:197:THR:HG22	1:A:199:GLU:H	1.74	0.51
1:A:255:GLY:O	1:A:257:THR:HG22	2.11	0.50
1:A:89:ILE:HG12	1:A:142:ILE:CD1	2.41	0.50
1:A:197:THR:HB	1:A:200:ARG:H	1.78	0.48
1:A:69:THR:HG23	1:A:71:ASP:CG	2.33	0.47
1:A:47:LEU:HD13	1:A:54:PRO:HD3	1.96	0.47
1:A:197:THR:C	1:A:199:GLU:N	2.69	0.47
1:A:252:LEU:O	1:A:260:ALA:HB2	2.15	0.47
1:A:197:THR:O	1:A:199:GLU:N	2.49	0.46
1:A:257:THR:O	1:A:259:PHE:N	2.48	0.46
1:A:89:ILE:HG12	1:A:142:ILE:HD12	1.98	0.45
1:A:186:ARG:HG2	1:A:186:ARG:O	2.17	0.45
1:A:6:TRP:HA	1:A:64:LEU:O	2.17	0.44
1:A:27:THR:HG22	1:A:29:GLU:N	2.32	0.44
1:A:197:THR:C	1:A:199:GLU:H	2.21	0.44
1:A:239:LYS:C	1:A:241:MET:N	2.70	0.43
1:A:123:ASP:O	1:A:124:GLU:HB2	2.19	0.43
1:A:138:TRP:O	1:A:142:ILE:HG12	2.20	0.42
1:A:113:CYS:C	1:A:115:LYS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MET:O	1:A:208:SER:OG	2.38	0.41
1:A:99:LEU:O	1:A:103:LYS:CB	2.64	0.41

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	235/288 (82%)	211 (90%)	17 (7%)	7 (3%)	5 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	LEU
1	A	240	PHE
1	A	242	GLY
1	A	258	ASP
1	A	198	LEU
1	A	114	ARG
1	A	241	MET

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	166/236 (70%)	157 (95%)	9 (5%)	26	48

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	98	SER
1	A	116	ILE
1	A	121	ILE
1	A	128	SER
1	A	143	ARG
1	A	206	GLU
1	A	208	SER
1	A	257	THR

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

Mol	Chain	Res	Type
1	A	261	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 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	241/288 (83%)	1.04	40 (16%) 2 1	63, 78, 93, 96	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	SER	6.3
1	A	252	LEU	6.1
1	A	269	ALA	5.5
1	A	110	VAL	5.0
1	A	256	GLU	4.7
1	A	185	GLY	3.4
1	A	255	GLY	3.4
1	A	66	THR	3.3
1	A	184	GLY	3.0
1	A	243	ASP	2.9
1	A	8	ALA	2.9
1	A	59	ASP	2.8
1	A	251	ASP	2.7
1	A	65	ALA	2.7
1	A	240	PHE	2.6
1	A	111	GLU	2.6
1	A	114	ARG	2.6
1	A	44	LEU	2.5
1	A	188	GLY	2.5
1	A	7	ILE	2.4
1	A	187	ASP	2.4
1	A	132	TRP	2.4
1	A	239	LYS	2.3
1	A	68	PHE	2.3
1	A	257	THR	2.3
1	A	43	HIS	2.3
1	A	191	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	10	TYR	2.2
1	A	11	PRO	2.2
1	A	250	ALA	2.1
1	A	48	LEU	2.1
1	A	254	HIS	2.1
1	A	102	MET	2.1
1	A	189	VAL	2.1
1	A	216	THR	2.1
1	A	67	HIS	2.1
1	A	46	GLY	2.1
1	A	172	GLY	2.0
1	A	253	LEU	2.0
1	A	249	TYR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.