Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 04:48 PM EST

PDB ID	:	2OV8
Title	:	Crystal Structure of StaL
Authors	:	Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2007-02-13
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
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:

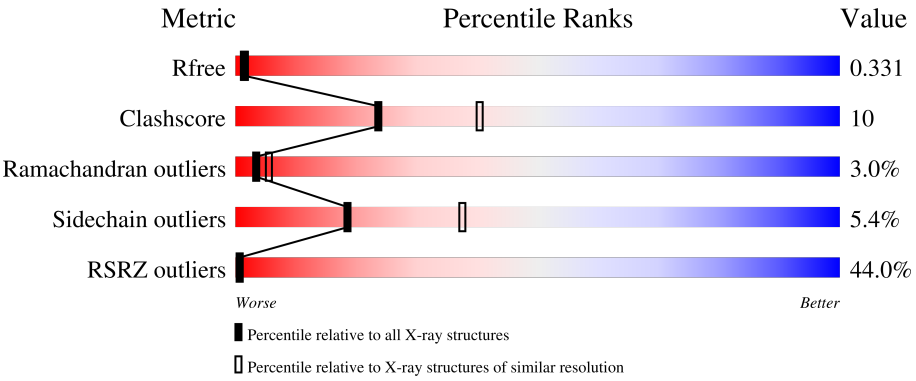
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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))
R_{free}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	288	37% 67% 14% • 16%

2 Entry composition (i)

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.

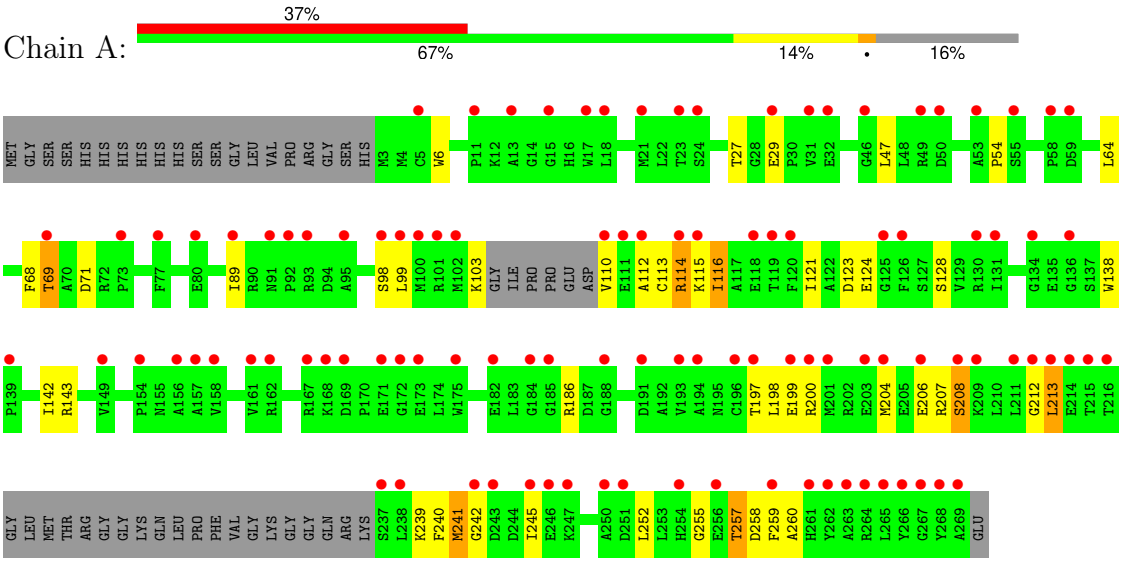
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		

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.

- Molecule 1: StaL

Chain A:



4 Data and refinement statistics (i)

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 74.49 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.54-2.58) 94.0 (74.49-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.38 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.279 (Not available) , 0.331	Depositor DCC
R_{free} test set	595 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 101.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

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

Continued on next page...

Continued from previous page...

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:113:CYS:HA	1:A:116:ILE:CG2	2.34	0.58
1:A:114:ARG:HA	1:A:245:ILE:HD11	1.84	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

Continued on next page...

Continued from previous page...

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%)	3 5

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%)	18 37

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

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	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 oligosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.3341, which does not match the depositor's R factor of 0.249. Please interpret the results in this section carefully.

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, 95^{th} 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%)	2.01	106 (43%) 1 1	63, 78, 93, 96	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ASP	5.3
1	A	199	GLU	5.2
1	A	263	ALA	5.1
1	A	185	GLY	4.9
1	A	188	GLY	4.9
1	A	246	GLU	4.9
1	A	269	ALA	4.9
1	A	262	TYR	4.4
1	A	115	LYS	4.4
1	A	130	ARG	4.3
1	A	114	ARG	4.2
1	A	216	THR	4.0
1	A	46	GLY	3.9
1	A	191	ASP	3.9
1	A	265	LEU	3.9
1	A	156	ALA	3.8
1	A	24	SER	3.8
1	A	238	LEU	3.7
1	A	110	VAL	3.7
1	A	136	GLY	3.7
1	A	194	ALA	3.6
1	A	266	TYR	3.6
1	A	237	SER	3.5
1	A	215	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	184	GLY	3.4
1	A	134	GLY	3.4
1	A	55	SER	3.4
1	A	243	ASP	3.4
1	A	50	ASP	3.3
1	A	32	GLU	3.3
1	A	111	GLU	3.3
1	A	203	GLU	3.3
1	A	168	LYS	3.3
1	A	167	ARG	3.2
1	A	92	PRO	3.2
1	A	245	ILE	3.2
1	A	53	ALA	3.2
1	A	208	SER	3.1
1	A	196	CYS	3.1
1	A	268	TYR	3.1
1	A	175	TRP	3.1
1	A	158	VAL	3.1
1	A	102	MET	3.0
1	A	172	GLY	2.9
1	A	154	PRO	2.9
1	A	214	GLU	2.9
1	A	80	GLU	2.8
1	A	139	PRO	2.8
1	A	31	VAL	2.8
1	A	101	ARG	2.8
1	A	157	ALA	2.8
1	A	112	ALA	2.7
1	A	256	GLU	2.7
1	A	95	ALA	2.7
1	A	182	GLU	2.7
1	A	120	PHE	2.7
1	A	211	LEU	2.7
1	A	169	ASP	2.7
1	A	261	HIS	2.7
1	A	242	GLY	2.7
1	A	93	ARG	2.6
1	A	197	THR	2.6
1	A	91	ASN	2.6
1	A	98	SER	2.6
1	A	131	ILE	2.6
1	A	173	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	201	MET	2.6
1	A	204	MET	2.6
1	A	89	ILE	2.6
1	A	29	GLU	2.5
1	A	125	GLY	2.5
1	A	250	ALA	2.5
1	A	209	LYS	2.5
1	A	126	PHE	2.5
1	A	69	THR	2.5
1	A	13	ALA	2.4
1	A	99	LEU	2.4
1	A	5	CYS	2.4
1	A	212	GLY	2.4
1	A	259	PHE	2.4
1	A	23	THR	2.3
1	A	254	HIS	2.3
1	A	49	ARG	2.3
1	A	200	ARG	2.3
1	A	77	PHE	2.2
1	A	11	PRO	2.2
1	A	58	PRO	2.2
1	A	247	LYS	2.2
1	A	118	GLU	2.2
1	A	161	VAL	2.2
1	A	213	LEU	2.2
1	A	21	MET	2.2
1	A	17	TRP	2.2
1	A	15	GLY	2.1
1	A	206	GLU	2.1
1	A	73	PRO	2.1
1	A	193	VAL	2.1
1	A	267	GLY	2.1
1	A	18	LEU	2.1
1	A	162	ARG	2.1
1	A	171	GLU	2.1
1	A	251	ASP	2.1
1	A	149	VAL	2.0
1	A	264	ARG	2.0
1	A	119	THR	2.0
1	A	100	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.