



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:18 AM GMT

PDB ID : 3OPB
Title : Crystal structure of She4p
Authors : Shi, H.; Blobel, G.
Deposited on : 2010-08-31
Resolution : 2.90 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

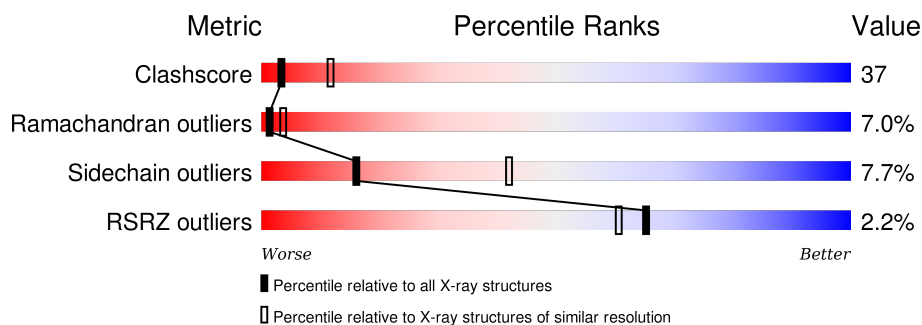
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	778	 3% 36% 52% 8% • •
1	B	778	 % 41% 45% 8% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12015 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 SWI5-dependent HO expression protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5954	3824	980	1124	26			
1	B	741	Total	C	N	O	S	0	0	0
			5920	3804	977	1113	26			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P51534
A	-3	SER	-	EXPRESSION TAG	UNP P51534
A	-2	PRO	-	EXPRESSION TAG	UNP P51534
A	-1	GLY	-	EXPRESSION TAG	UNP P51534
A	0	HIS	-	EXPRESSION TAG	UNP P51534
A	4	SER	CYS	ENGINEERED MUTATION	UNP P51534
A	?	-	MET	DELETION	UNP P51534
A	?	-	PRO	DELETION	UNP P51534
A	?	-	LYS	DELETION	UNP P51534
A	?	-	ILE	DELETION	UNP P51534
A	?	-	GLU	DELETION	UNP P51534
A	?	-	ASN	DELETION	UNP P51534
A	?	-	VAL	DELETION	UNP P51534
A	?	-	ASN	DELETION	UNP P51534
A	?	-	GLU	DELETION	UNP P51534
A	?	-	SER	DELETION	UNP P51534
A	?	-	ALA	DELETION	UNP P51534
A	?	-	VAL	DELETION	UNP P51534
A	?	-	LYS	DELETION	UNP P51534
A	?	-	LEU	DELETION	UNP P51534
A	?	-	GLU	DELETION	UNP P51534
A	?	-	GLU	DELETION	UNP P51534
A	406	UNK	SER	SEE REMARK 999	UNP P51534
A	407	UNK	ASN	SEE REMARK 999	UNP P51534
A	408	UNK	GLY	SEE REMARK 999	UNP P51534

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Chain	Residue	Modelled	Actual	Comment	Reference
A	409	UNK	SER	SEE REMARK 999	UNP P51534
A	410	UNK	SER	SEE REMARK 999	UNP P51534
A	411	UNK	GLN	SEE REMARK 999	UNP P51534
A	412	UNK	SER	SEE REMARK 999	UNP P51534
A	413	UNK	ILE	SEE REMARK 999	UNP P51534
A	414	UNK	ASN	SEE REMARK 999	UNP P51534
A	415	UNK	ASP	SEE REMARK 999	UNP P51534
A	416	UNK	LEU	SEE REMARK 999	UNP P51534
A	417	UNK	LYS	SEE REMARK 999	UNP P51534
A	418	UNK	ASN	SEE REMARK 999	UNP P51534
A	419	UNK	TYR	SEE REMARK 999	UNP P51534
A	420	UNK	ALA	SEE REMARK 999	UNP P51534
A	421	UNK	ASP	SEE REMARK 999	UNP P51534
A	422	UNK	LEU	SEE REMARK 999	UNP P51534
A	423	UNK	LYS	SEE REMARK 999	UNP P51534
A	424	UNK	GLY	SEE REMARK 999	UNP P51534
A	426	ALA	GLY	ENGINEERED MUTATION	UNP P51534
A	435	ALA	GLU	ENGINEERED MUTATION	UNP P51534
A	436	ALA	SER	ENGINEERED MUTATION	UNP P51534
A	475	ILE	VAL	ENGINEERED MUTATION	UNP P51534
A	489	LEU	CYS	ENGINEERED MUTATION	UNP P51534
A	490	ALA	ILE	ENGINEERED MUTATION	UNP P51534
A	491	GLN	SER	ENGINEERED MUTATION	UNP P51534
A	494	ALA	GLY	ENGINEERED MUTATION	UNP P51534
A	495	VAL	THR	ENGINEERED MUTATION	UNP P51534
A	496	LYS	THR	ENGINEERED MUTATION	UNP P51534
B	-4	GLY	-	EXPRESSION TAG	UNP P51534
B	-3	SER	-	EXPRESSION TAG	UNP P51534
B	-2	PRO	-	EXPRESSION TAG	UNP P51534
B	-1	GLY	-	EXPRESSION TAG	UNP P51534
B	0	HIS	-	EXPRESSION TAG	UNP P51534
B	4	SER	CYS	ENGINEERED MUTATION	UNP P51534
B	?	-	MET	DELETION	UNP P51534
B	?	-	PRO	DELETION	UNP P51534
B	?	-	LYS	DELETION	UNP P51534
B	?	-	ILE	DELETION	UNP P51534
B	?	-	GLU	DELETION	UNP P51534
B	?	-	ASN	DELETION	UNP P51534
B	?	-	VAL	DELETION	UNP P51534
B	?	-	ASN	DELETION	UNP P51534
B	?	-	GLU	DELETION	UNP P51534
B	?	-	SER	DELETION	UNP P51534

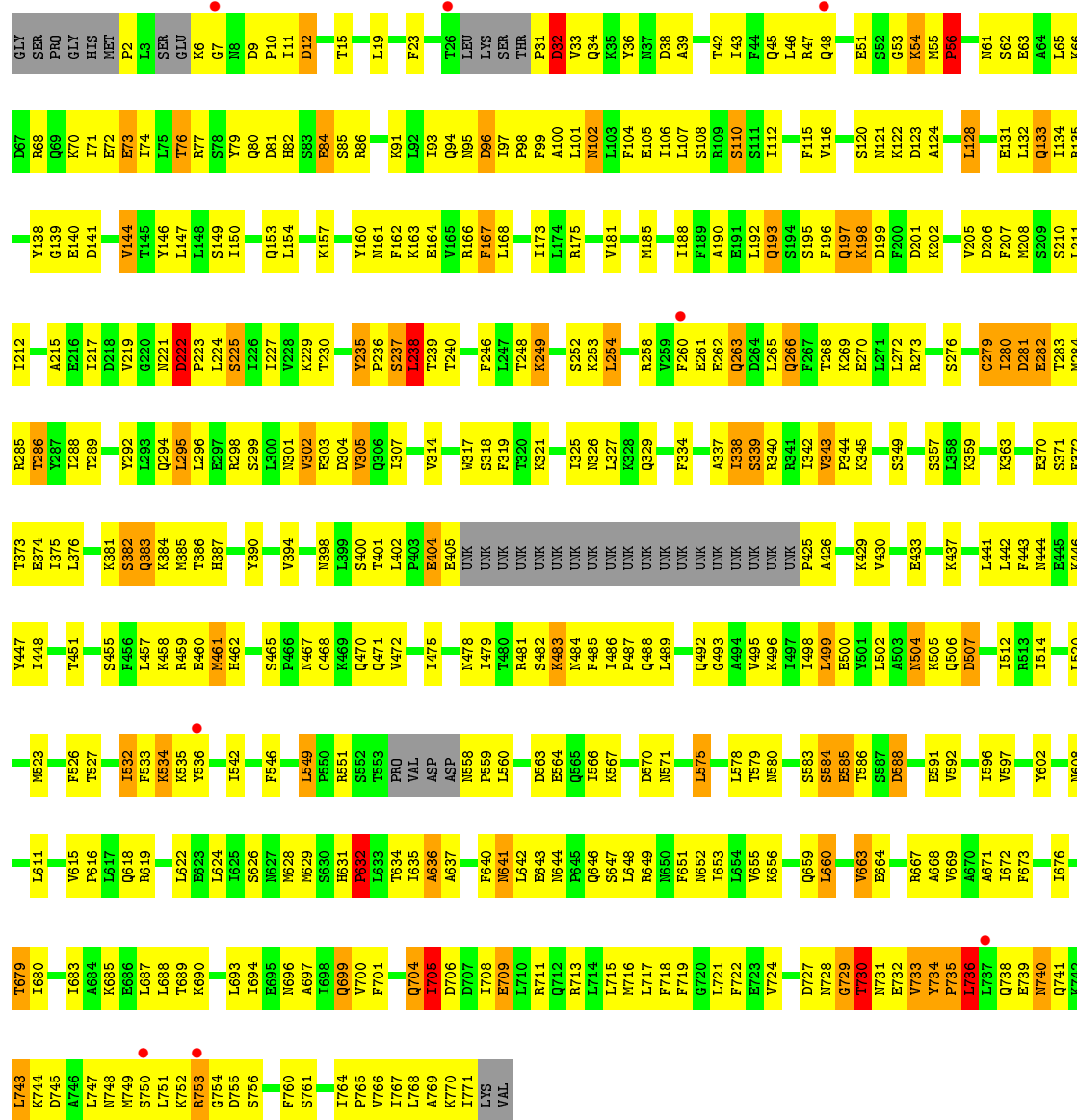
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	DELETION	UNP P51534
B	?	-	VAL	DELETION	UNP P51534
B	?	-	LYS	DELETION	UNP P51534
B	?	-	LEU	DELETION	UNP P51534
B	?	-	GLU	DELETION	UNP P51534
B	?	-	GLU	DELETION	UNP P51534
B	406	UNK	SER	SEE REMARK 999	UNP P51534
B	407	UNK	ASN	SEE REMARK 999	UNP P51534
B	408	UNK	GLY	SEE REMARK 999	UNP P51534
B	409	UNK	SER	SEE REMARK 999	UNP P51534
B	410	UNK	SER	SEE REMARK 999	UNP P51534
B	411	UNK	GLN	SEE REMARK 999	UNP P51534
B	412	UNK	SER	SEE REMARK 999	UNP P51534
B	413	UNK	ILE	SEE REMARK 999	UNP P51534
B	414	UNK	ASN	SEE REMARK 999	UNP P51534
B	415	UNK	ASP	SEE REMARK 999	UNP P51534
B	416	UNK	LEU	SEE REMARK 999	UNP P51534
B	417	UNK	LYS	SEE REMARK 999	UNP P51534
B	418	UNK	ASN	SEE REMARK 999	UNP P51534
B	419	UNK	TYR	SEE REMARK 999	UNP P51534
B	420	UNK	ALA	SEE REMARK 999	UNP P51534
B	421	UNK	ASP	SEE REMARK 999	UNP P51534
B	422	UNK	LEU	SEE REMARK 999	UNP P51534
B	423	UNK	LYS	SEE REMARK 999	UNP P51534
B	424	UNK	GLY	SEE REMARK 999	UNP P51534
B	426	ALA	GLY	ENGINEERED MUTATION	UNP P51534
B	435	ALA	GLU	ENGINEERED MUTATION	UNP P51534
B	436	ALA	SER	ENGINEERED MUTATION	UNP P51534
B	475	ILE	VAL	ENGINEERED MUTATION	UNP P51534
B	489	LEU	CYS	ENGINEERED MUTATION	UNP P51534
B	490	ALA	ILE	ENGINEERED MUTATION	UNP P51534
B	491	GLN	SER	ENGINEERED MUTATION	UNP P51534
B	494	ALA	GLY	ENGINEERED MUTATION	UNP P51534
B	495	VAL	THR	ENGINEERED MUTATION	UNP P51534
B	496	LYS	THR	ENGINEERED MUTATION	UNP P51534

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	75	Total O 75 75	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.02Å 149.94Å 158.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 2.90 42.95 – 2.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.00-2.90) 83.0 (42.95-2.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.296 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 45269 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12015	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.71 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.0958e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/6012	0.65	0/8121
1	B	0.42	0/6006	0.67	2/8109 (0.0%)
All	All	0.41	0/12018	0.66	2/16230 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	PRO	N-CA-CB	5.67	110.10	103.30
1	B	222	ASP	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

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	5954	0	6152	471	0
1	B	5920	0	6132	436	0
2	A	66	0	0	22	0
2	B	75	0	0	21	0
All	All	12015	0	12284	890	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 37.

The worst 5 of 890 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:61:ASN:CG	1:A:62:SER:H	1.65	0.99
1:B:655:VAL:HG12	1:B:693:LEU:HD13	1.44	0.98
1:B:667:ARG:HD2	1:B:709:GLU:HB3	1.45	0.98
1:B:99:PHE:HA	1:B:102:ASN:HD21	1.28	0.97
1:A:363:LYS:HE3	1:A:398:ASN:O	1.65	0.96

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	733/778 (94%)	562 (77%)	119 (16%)	52 (7%)	1	3
1	B	729/778 (94%)	570 (78%)	109 (15%)	50 (7%)	1	4
All	All	1462/1556 (94%)	1132 (77%)	228 (16%)	102 (7%)	1	4

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	13	SER
1	A	30	THR
1	A	32	ASP
1	A	51	GLU

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	680/694 (98%)	627 (92%)	53 (8%)	16	41
1	B	676/694 (97%)	625 (92%)	51 (8%)	17	44
All	All	1356/1388 (98%)	1252 (92%)	104 (8%)	16	42

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	719	PHE
1	B	76	THR
1	B	705	ILE
1	A	724	VAL
1	A	749	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	740	ASN
1	B	102	ASN
1	B	704	GLN
1	B	41	ASN
1	B	82	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 [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	741/778 (95%)	0.17	25 (3%) 49 41	71, 97, 132, 155	0
1	B	741/778 (95%)	0.05	8 (1%) 82 80	31, 91, 125, 149	0
All	All	1482/1556 (95%)	0.11	33 (2%) 65 60	31, 94, 128, 155	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	760	PHE	8.3
1	A	47	ARG	5.7
1	A	338	ILE	4.6
1	B	536	TYR	4.5
1	B	26	THR	4.2

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.