



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 07:46 AM GMT

PDB ID : 1YUD  
Title : X-ray Crystal Structure of Protein SO0799 from Shewanella oneidensis. Northeast Structural Genomics Consortium Target SoR12.  
Authors : Kuzin, A.P.; Vorobiev, S.; Chen, Y.; Forouhar, F.; Acton, T.; Ma, L.-C.; Xiao, R.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2005-02-14  
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

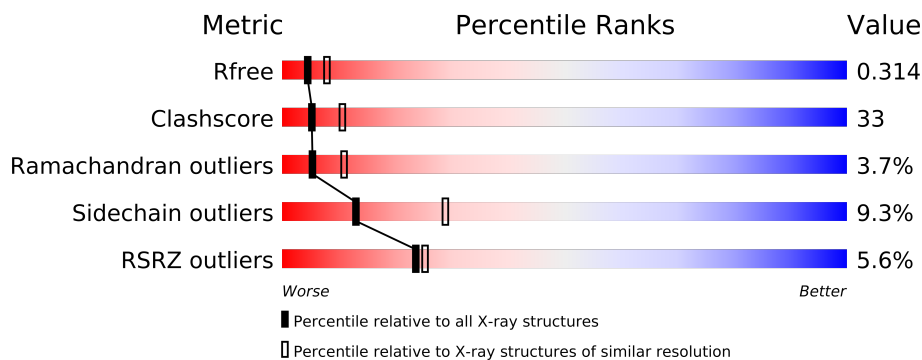
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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  $\geq 3$ , 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	170	
1	B	170	
1	C	170	
1	D	170	
1	E	170	
1	F	170	
1	G	170	
1	H	170	
1	I	170	
1	J	170	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12762 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 hypothetical protein SO0799.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	B	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	C	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	D	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	E	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	F	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	G	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	H	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	I	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			
1	J	158	Total	C	N	O	S	Se	0	0	0
			1265	813	207	237	2	6			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
A	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
A	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
A	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
A	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
A	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
B	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
B	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
B	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
B	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
B	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
B	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
B	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
C	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
C	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
C	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
C	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
C	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
C	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
C	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
C	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
C	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
D	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
D	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
D	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
D	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
D	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
D	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
D	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
D	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
D	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
D	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
D	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
D	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
D	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
D	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
E	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
E	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
E	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
E	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
E	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
E	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
E	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
E	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
E	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
F	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
F	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
F	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
F	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
F	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
F	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
F	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
F	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
G	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
G	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
G	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
G	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
G	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
G	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
G	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
G	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
G	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
H	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
H	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
H	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
H	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
H	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
H	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
H	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
H	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
H	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
I	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
I	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
I	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
I	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
I	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
I	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
I	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
I	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
I	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
I	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
I	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
I	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
I	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
I	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
I	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
J	-9	MSE	-	EXPRESSION TAG	UNP Q8EIN8
J	-8	GLY	-	EXPRESSION TAG	UNP Q8EIN8
J	-7	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	-6	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	-5	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	-4	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	-3	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	-2	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	-1	SER	-	EXPRESSION TAG	UNP Q8EIN8
J	0	HIS	-	EXPRESSION TAG	UNP Q8EIN8
J	1	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
J	62	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
J	75	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
J	111	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
J	122	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8
J	143	MSE	MET	MODIFIED RESIDUE	UNP Q8EIN8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	27	Total O 27 27	0	0
2	C	11	Total O 11 11	0	0
2	D	16	Total O 16 16	0	0
2	E	3	Total O 3 3	0	0
2	F	5	Total O 5 5	0	0
2	G	1	Total O 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

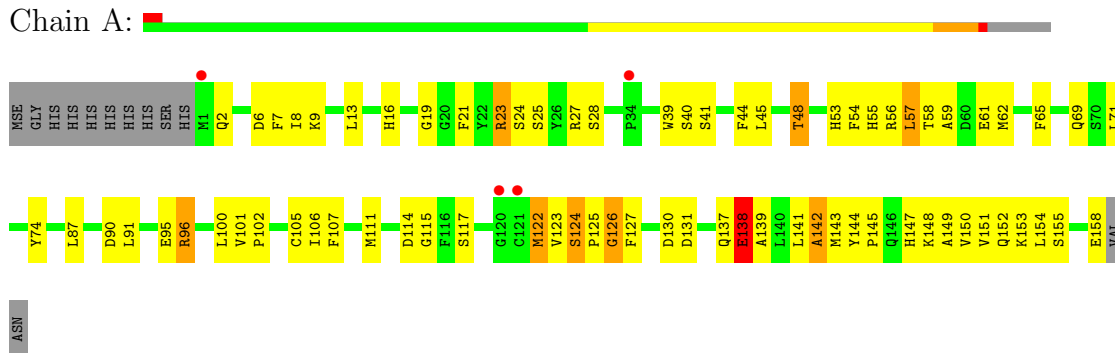
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	15	Total 15	O 15	0	0
2	I	6	Total 6	O 6	0	0
2	J	12	Total 12	O 12	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

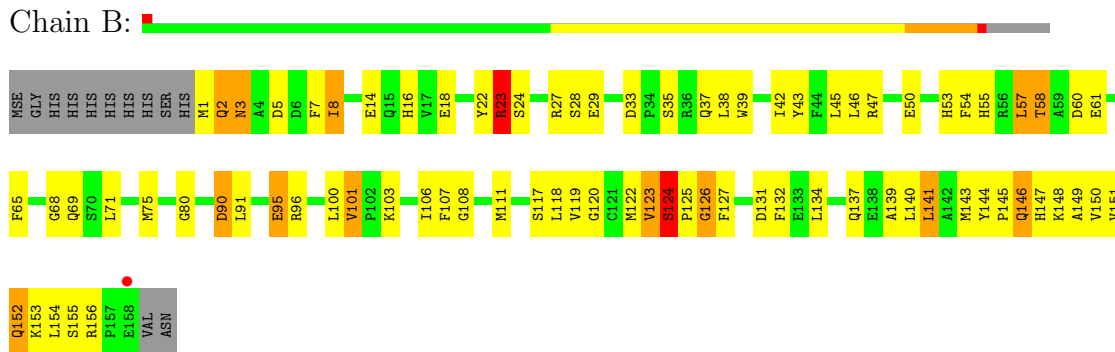
#### • Molecule 1: hypothetical protein SO0799

Chain A:



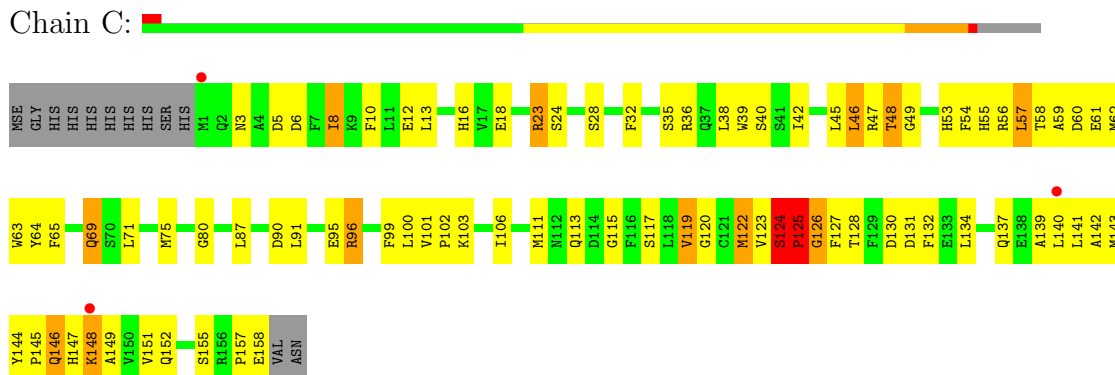
#### • Molecule 1: hypothetical protein SO0799

Chain B:



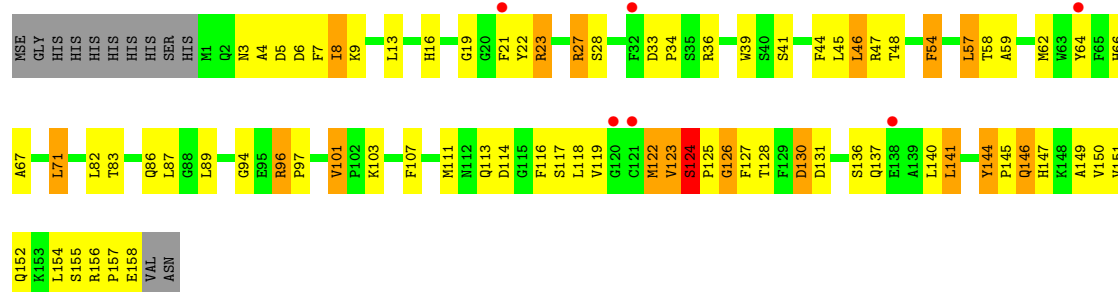
#### • Molecule 1: hypothetical protein SO0799

Chain C:



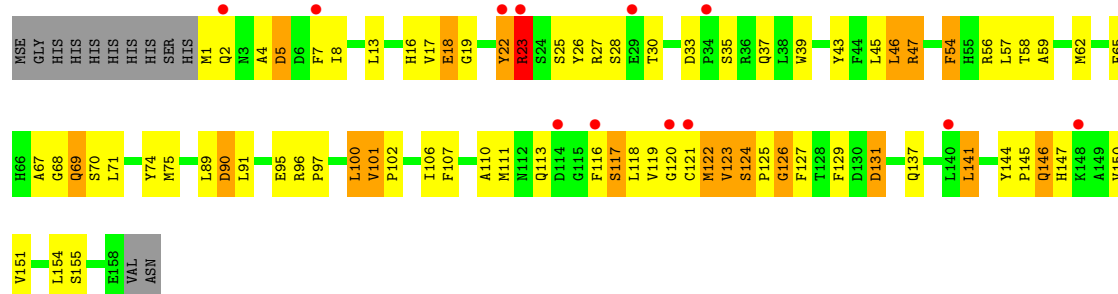
#### • Molecule 1: hypothetical protein SO0799

Chain D:



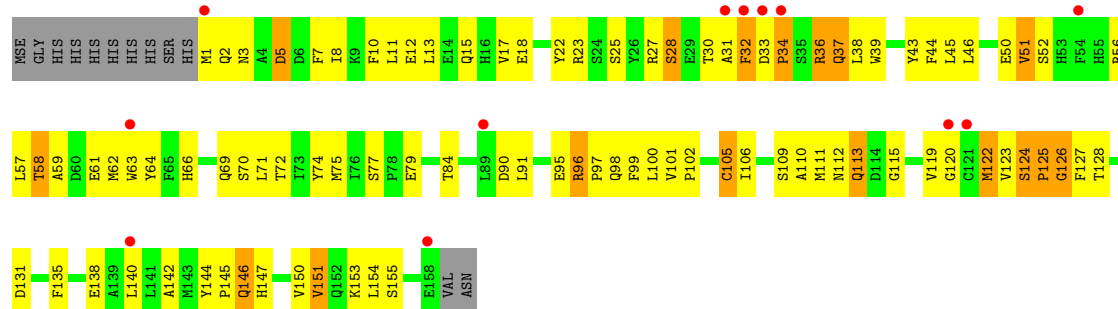
• Molecule 1: hypothetical protein SO0799

Chain E:



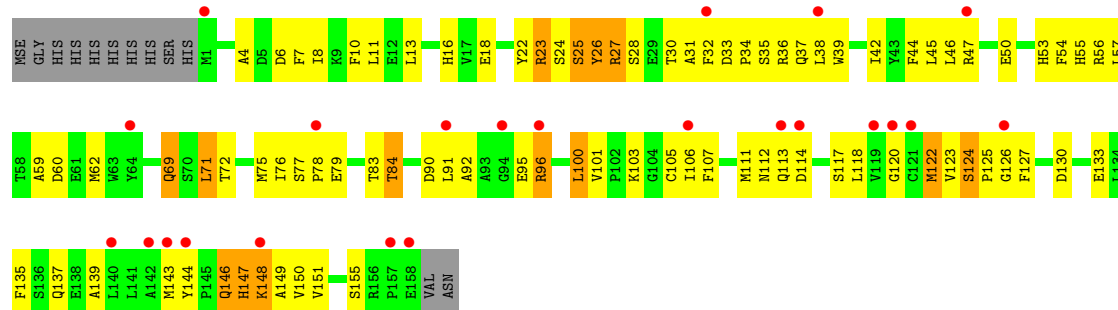
• Molecule 1: hypothetical protein SO0799

Chain F:

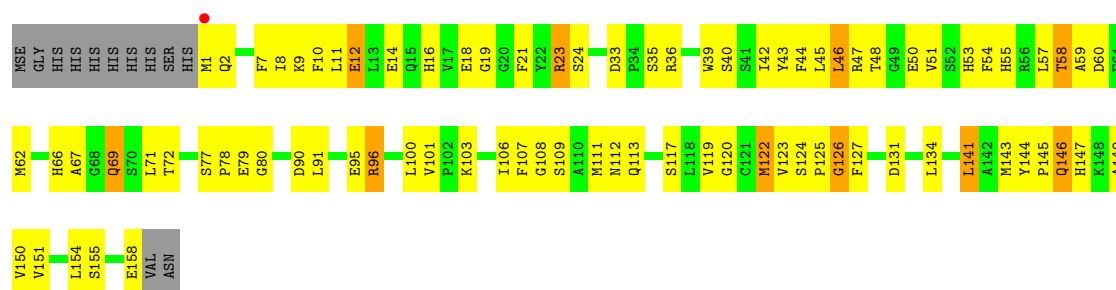


• Molecule 1: hypothetical protein SO0799

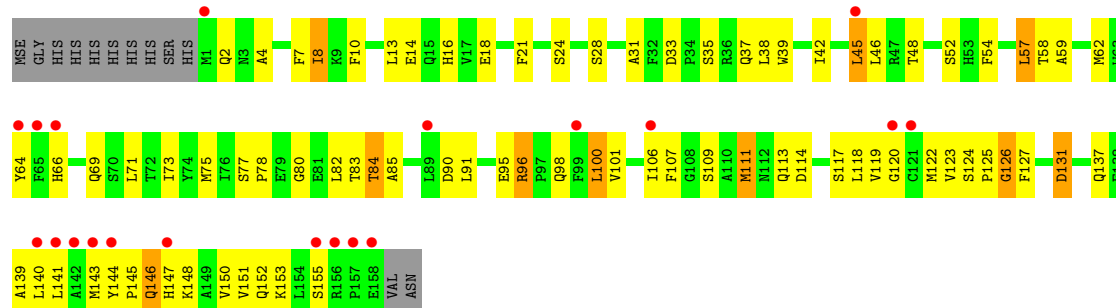
Chain G:



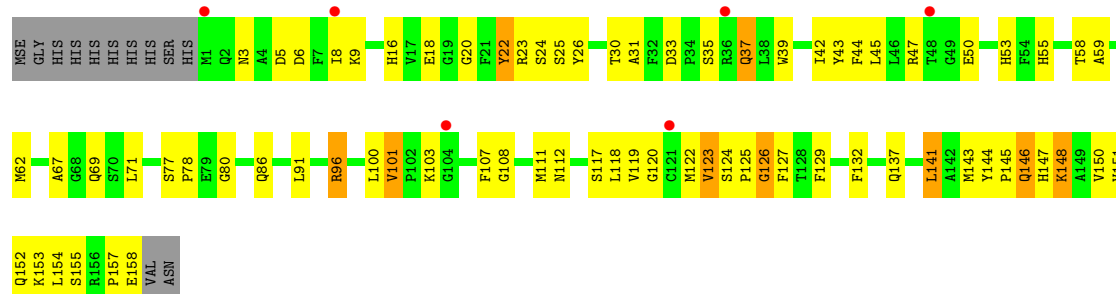
- Molecule 1: hypothetical protein SO0799

Chain H: 

- Molecule 1: hypothetical protein SO0799

Chain I: 

- Molecule 1: hypothetical protein SO0799

Chain J: 

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.44Å 94.10Å 117.10Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	29.93 – 2.70 29.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.9 (29.93-2.70) 97.6 (29.93-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.292 0.256 , 0.314	Depositor DCC
$R_{free}$ test set	2583 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 105354 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.42	0/1295	0.66	0/1742
1	B	0.53	0/1295	0.76	2/1742 (0.1%)
1	C	0.43	0/1295	0.73	0/1742
1	D	0.42	0/1295	0.68	1/1742 (0.1%)
1	E	0.41	0/1295	0.63	0/1742
1	F	0.40	0/1295	0.63	0/1742
1	G	0.37	0/1295	0.63	0/1742
1	H	0.48	0/1295	0.74	1/1742 (0.1%)
1	I	0.37	0/1295	0.63	0/1742
1	J	0.45	0/1295	0.72	0/1742
All	All	0.43	0/12950	0.68	4/17420 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	SER	C-N-CD	6.28	141.59	128.40
1	B	43	TYR	N-CA-C	-5.53	96.07	111.00
1	H	43	TYR	N-CA-C	-5.14	97.12	111.00
1	D	124	SER	C-N-CD	5.07	139.05	128.40

There are no chirality outliers.

There are no planarity outliers.

### 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	1265	0	1204	78	0
1	B	1265	0	1204	84	0
1	C	1265	0	1204	94	0
1	D	1265	0	1204	80	0
1	E	1265	0	1204	88	0
1	F	1265	0	1204	90	0
1	G	1265	0	1204	92	0
1	H	1265	0	1204	95	0
1	I	1265	0	1204	88	0
1	J	1265	0	1204	75	0
2	A	16	0	0	2	0
2	B	27	0	0	4	0
2	C	11	0	0	1	0
2	D	16	0	0	2	0
2	E	3	0	0	0	0
2	F	5	0	0	1	0
2	G	1	0	0	0	0
2	H	15	0	0	1	0
2	I	6	0	0	1	0
2	J	12	0	0	2	0
All	All	12762	0	12040	811	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 33.

The worst 5 of 811 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:TRP:HB2	1:A:122:MSE:HE3	1.29	1.14
1:A:124:SER:HB3	1:A:125:PRO:HD3	1.31	1.10
1:A:122:MSE:HE1	1:A:124:SER:HA	1.25	1.09
1:G:59:ALA:HB1	1:G:124:SER:HB3	1.35	1.08
1:B:146:GLN:H	1:B:146:GLN:NE2	1.55	1.03

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	156/170 (92%)	134 (86%)	17 (11%)	5 (3%)	6	14
1	B	156/170 (92%)	139 (89%)	11 (7%)	6 (4%)	5	10
1	C	156/170 (92%)	136 (87%)	14 (9%)	6 (4%)	5	10
1	D	156/170 (92%)	132 (85%)	18 (12%)	6 (4%)	5	10
1	E	156/170 (92%)	134 (86%)	15 (10%)	7 (4%)	4	7
1	F	156/170 (92%)	123 (79%)	24 (15%)	9 (6%)	3	4
1	G	156/170 (92%)	117 (75%)	30 (19%)	9 (6%)	3	4
1	H	156/170 (92%)	137 (88%)	18 (12%)	1 (1%)	33	66
1	I	156/170 (92%)	129 (83%)	22 (14%)	5 (3%)	6	14
1	J	156/170 (92%)	140 (90%)	12 (8%)	4 (3%)	8	20
All	All	1560/1700 (92%)	1321 (85%)	181 (12%)	58 (4%)	5	11

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	THR
1	C	125	PRO
1	C	126	GLY
1	D	124	SER
1	E	124	SER

### 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	135/139 (97%)	125 (93%)	10 (7%)	20	43
1	B	135/139 (97%)	121 (90%)	14 (10%)	10	23
1	C	135/139 (97%)	120 (89%)	15 (11%)	9	20
1	D	135/139 (97%)	119 (88%)	16 (12%)	8	18
1	E	135/139 (97%)	120 (89%)	15 (11%)	9	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	135/139 (97%)	123 (91%)	12 (9%)	14	31
1	G	135/139 (97%)	124 (92%)	11 (8%)	17	36
1	H	135/139 (97%)	123 (91%)	12 (9%)	14	31
1	I	135/139 (97%)	127 (94%)	8 (6%)	28	56
1	J	135/139 (97%)	122 (90%)	13 (10%)	12	27
All	All	1350/1390 (97%)	1224 (91%)	126 (9%)	13	29

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	GLU
1	F	5	ASP
1	J	37	GLN
1	E	23	ARG
1	E	100	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	15	GLN
1	F	15	GLN
1	J	55	HIS
1	E	37	GLN
1	E	137	GLN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	158/170 (92%)	0.29	4 (2%) 54 61	24, 62, 88, 130	0
1	B	158/170 (92%)	-0.19	1 (0%) 86 90	16, 39, 73, 124	0
1	C	158/170 (92%)	-0.01	3 (1%) 64 70	27, 55, 91, 130	0
1	D	158/170 (92%)	0.28	6 (3%) 38 43	36, 60, 87, 127	0
1	E	158/170 (92%)	0.56	12 (7%) 14 14	39, 72, 99, 130	0
1	F	158/170 (92%)	0.63	12 (7%) 14 14	43, 77, 112, 144	0
1	G	158/170 (92%)	0.92	23 (14%) 3 4	65, 89, 117, 149	0
1	H	158/170 (92%)	0.06	1 (0%) 86 90	23, 48, 82, 130	0
1	I	158/170 (92%)	0.89	20 (12%) 4 4	53, 86, 119, 144	0
1	J	158/170 (92%)	0.34	6 (3%) 38 43	33, 59, 87, 139	0
All	All	1580/1700 (92%)	0.38	88 (5%) 24 25	16, 66, 108, 149	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	PRO	6.3
1	F	33	ASP	5.7
1	G	157	PRO	4.8
1	G	144	TYR	4.3
1	G	126	GLY	4.3

### 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.