wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 11:53 PM 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 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:
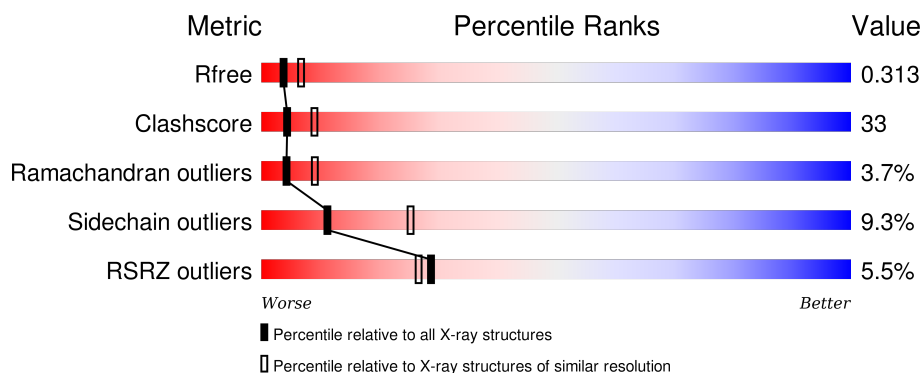
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 >=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 <=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	170	2% / 49% / 38% / 5% · 7%
1	B	170	% / 45% / 39% / 8% · 7%
1	C	170	2% / 42% / 42% / 7% · 7%
1	D	170	4% / 47% / 36% / 9% · 7%
1	E	170	7% / 47% / 35% / 11% · 7%

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Mol	Chain	Length	Quality of chain
1	F	170	8% / 38% / 45% / 10% / 7%
1	G	170	11% / 41% / 44% / 8% / 7%
1	H	170	44% / 43% / 6% / 7%
1	I	170	12% / 46% / 41% / 6% / 7%
1	J	170	4% / 49% / 38% / 5% / 7%

2 Entry composition (i)

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

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

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

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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

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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

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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

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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 16	O 16	0	0
2	B	27	Total 27	O 27	0	0
2	C	11	Total 11	O 11	0	0
2	D	16	Total 16	O 16	0	0
2	E	3	Total 3	O 3	0	0
2	F	5	Total 5	O 5	0	0
2	G	1	Total 1	O 1	0	0

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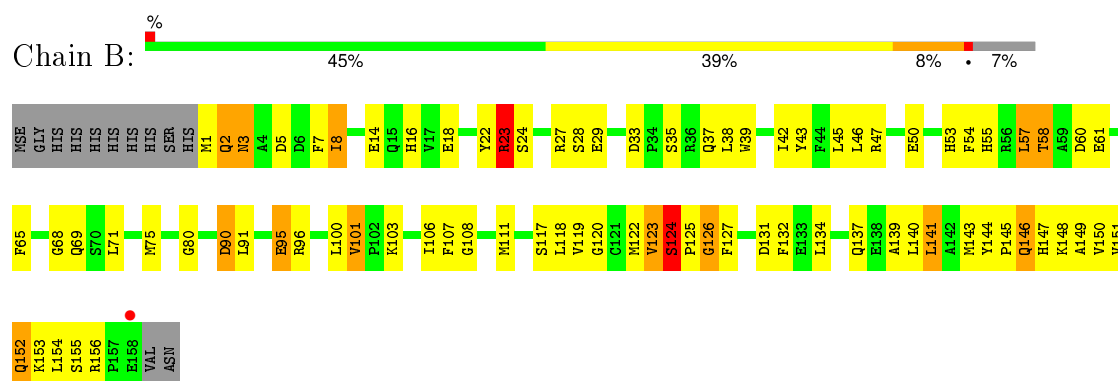| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	15	Total 15	O 15	0	0
2	I	6	Total 6	O 6	0	0
2	J	12	Total 12	O 12	0	0

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.
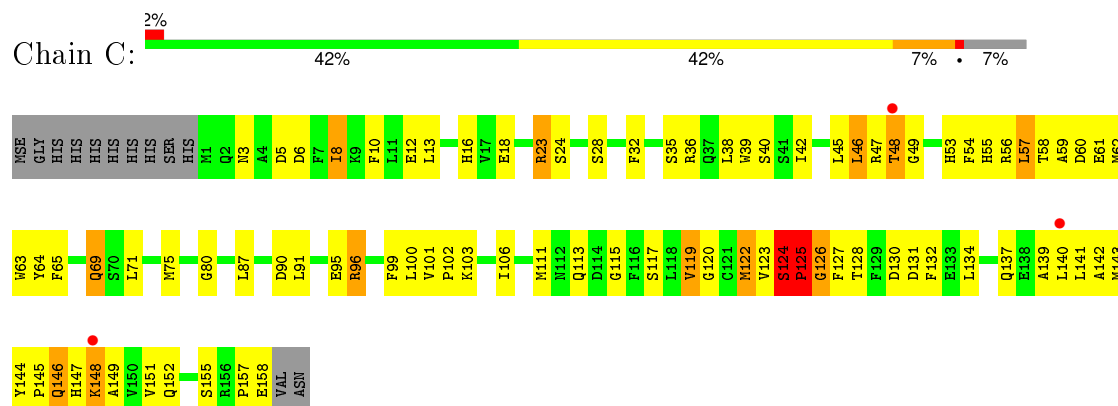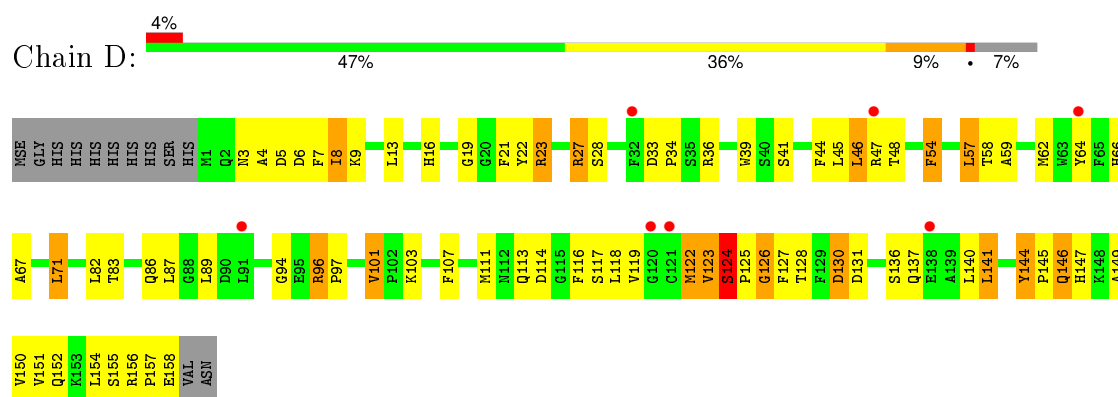
- Molecule 1: hypothetical protein SO0799

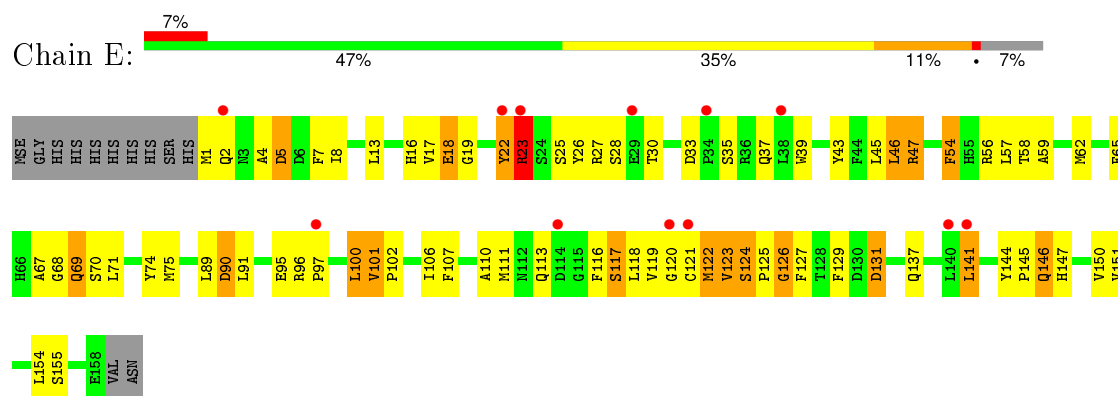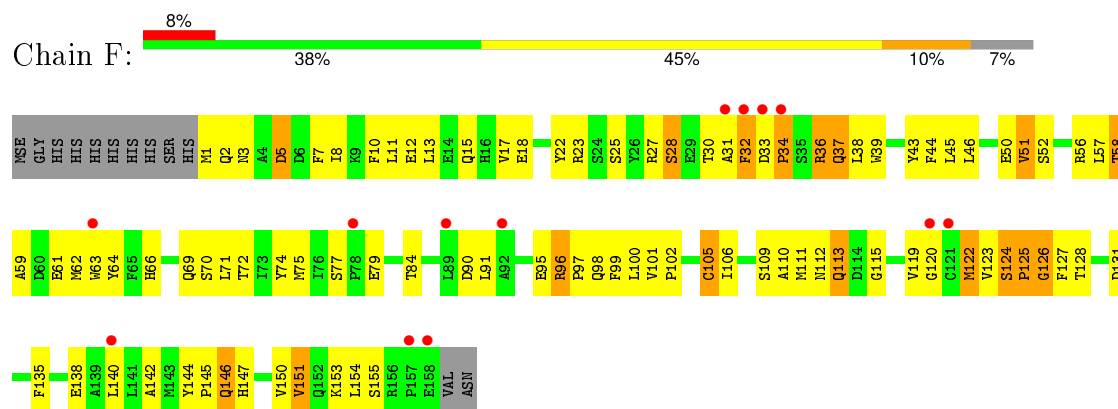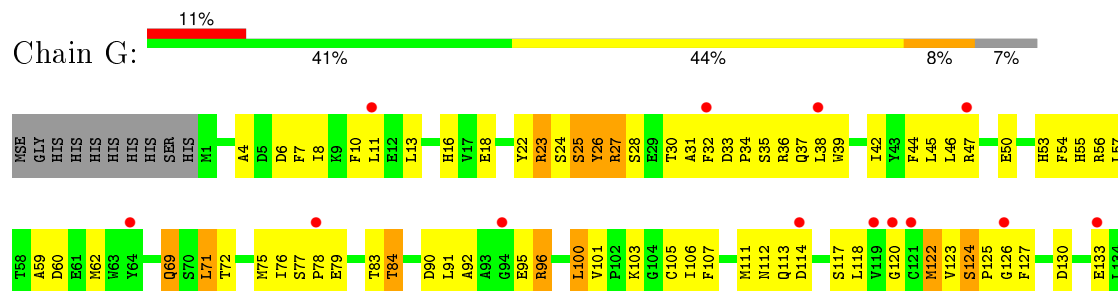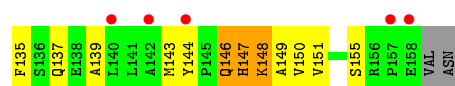- Molecule 1: hypothetical protein SO0799

- Molecule 1: hypothetical protein SO0799

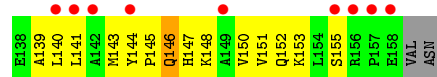- Molecule 1: hypothetical protein SO0799

Chain D:

4%

47% | 36% | 9% | • | 7%

Chain D residue blocks:

MSE GLY HIS HIS HIS HIS SER HIS | M1 Q2 N3 A4 D5 D6 F7 I8 K9 L13 H16 G19 G20 F21 Y22 R23 R27 S28 F32 D33 P34 S35 R36 W39 S40 S41 F44 L45 L46 R47 T48 F54 L57 T58 A59 M62 W63 Y64 F65 H66

A67 L71 L82 T83 Q86 L87 G88 L89 D90 L91 G94 E95 R96 P97 V101 P102 K103 F107 M111 N112 D114 F116 S117 L118 V119 G120 C121 M122 V123 S124 P125 G126 F127 T128 F129 D130 D131 S136 Q137 E138 A139 L140 L141 Y144 P145 Q146 H147 K148 A149

V150 V151 Q152 K153 L154 S155 R156 P157 E158 VAL ASN

• Molecule 1: hypothetical protein SO0799

Chain E:

7%

47% | 35% | 11% | • | 7%

Chain E residue blocks:

MSE GLY HIS HIS HIS HIS SER HIS | M1 Q2 N3 A4 D5 D6 F7 I8 L13 H16 V17 E18 G19 Y22 R23 S24 S25 Y26 R27 S28 E29 T30 D33 P34 S35 Q37 L38 W39 Y43 F44 L45 L46 R47 F54 H55 R56 L57 T58 A59 M62 F65

H66 A67 G68 Q69 S70 L71 Y74 M75 L89 D90 L91 E95 R96 P97 L100 V101 P102 I106 F107 A110 M111 N112 Q113 D114 G115 F116 S117 L118 V119 G120 C121 M122 V123 S124 P125 G126 F127 T128 F129 D130 D131 Q137 L140 L141 Y144 P145 Q146 H147 V150 V151

L154 S155 E158 VAL ASN

• Molecule 1: hypothetical protein SO0799

Chain F:

8%

38% | 45% | 10% | 7%

Chain F residue blocks:

MSE GLY HIS HIS HIS HIS SER HIS | M1 Q2 N3 A4 D5 D6 F7 I8 K9 F10 L11 E12 L13 E14 Q15 H16 V17 E18 Y22 R23 S24 S25 Y26 R27 S28 E29 T30 A31 F32 D33 P34 S35 R36 Q37 L38 W39 Y43 F44 L45 L46 E50 V51 S52 R56 L57 T58

A59 D60 E61 M62 W63 Y64 F65 H66 Q69 S70 L71 T72 I73 Y74 M75 I76 S77 P78 E79 T84 L89 D90 L91 A92 E95 R96 P97 Q98 F99 L100 V101 P102 C105 I106 S109 A110 M111 N112 Q113 D114 G115 V119 G120 C121 M122 V123 S124 P125 G126 F127 T128 D131

F135 E138 A139 L140 L141 A142 M143 Y144 P145 Q146 H147 V150 V151 Q152 K153 L154 S155 R156 P157 E158 VAL ASN

• Molecule 1: hypothetical protein SO0799

Chain G:

11%

41% | 44% | 8% | 7%

Chain G residue blocks:

MSE GLY HIS HIS HIS HIS SER HIS | M1 A4 D5 D6 F7 I8 K9 F10 L11 E12 L13 H16 V17 E18 Y22 R23 S24 S25 Y26 R27 S28 E29 T30 A31 F32 D33 P34 S35 R36 Q37 L38 W39 I42 Y43 F44 L45 L46 R47 E50 H53 F54 H55 R56 L57

T58 A59 D60 E61 M62 W63 Y64 Q69 S70 L71 T72 M75 I76 S77 P78 E79 T83 T84 D90 L91 A92 A93 G94 E95 R96 L100 V101 P102 K103 C104 C105 I106 F107 M111 N112 Q113 D114 S117 L118 V119 G120 C121 M122 V123 S124 P125 G126 F127 D130 E133 L134

• Molecule 1: hypothetical protein SO0799

Chain H:

• Molecule 1: hypothetical protein SO0799
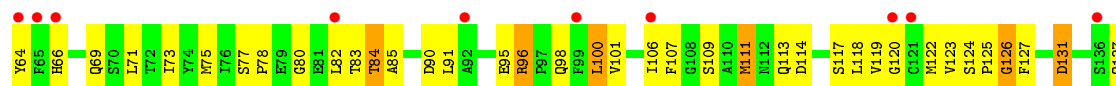
Chain I:

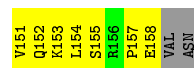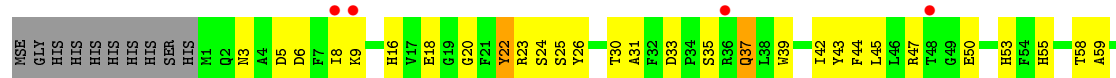• Molecule 1: hypothetical protein SO0799

Chain J:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.52 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.292 0.256 , 0.313	Depositor DCC
R_{free} test set	2583 reflections (4.83%)	DCC
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.42	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(^{o})	Ideal(^{o})
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 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	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

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 33.

The worst 5 of 811 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: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 (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	156/170 (92%)	134 (86%)	17 (11%)	5 (3%)	5	12
1	B	156/170 (92%)	139 (89%)	11 (7%)	6 (4%)	4	9
1	C	156/170 (92%)	136 (87%)	14 (9%)	6 (4%)	4	9
1	D	156/170 (92%)	132 (85%)	18 (12%)	6 (4%)	4	9
1	E	156/170 (92%)	134 (86%)	15 (10%)	7 (4%)	3	6
1	F	156/170 (92%)	123 (79%)	24 (15%)	9 (6%)	2	3
1	G	156/170 (92%)	117 (75%)	30 (19%)	9 (6%)	2	3
1	H	156/170 (92%)	137 (88%)	18 (12%)	1 (1%)	30	59
1	I	156/170 (92%)	129 (83%)	22 (14%)	5 (3%)	5	12
1	J	156/170 (92%)	140 (90%)	12 (8%)	4 (3%)	7	16
All	All	1560/1700 (92%)	1321 (85%)	181 (12%)	58 (4%)	4	9

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 (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	135/139 (97%)	125 (93%)	10 (7%)	17	39
1	B	135/139 (97%)	121 (90%)	14 (10%)	9	20
1	C	135/139 (97%)	120 (89%)	15 (11%)	8	17
1	D	135/139 (97%)	119 (88%)	16 (12%)	6	15
1	E	135/139 (97%)	120 (89%)	15 (11%)	8	17
1	F	135/139 (97%)	123 (91%)	12 (9%)	12	27
1	G	135/139 (97%)	124 (92%)	11 (8%)	15	33
1	H	135/139 (97%)	123 (91%)	12 (9%)	12	27
1	I	135/139 (97%)	127 (94%)	8 (6%)	24	51
1	J	135/139 (97%)	122 (90%)	13 (10%)	10	24
All	All	1350/1390 (97%)	1224 (91%)	126 (9%)	11	25

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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	152/170 (89%)	0.25	3 (1%)	68 69	24, 62, 87, 120	0
1	B	152/170 (89%)	-0.21	1 (0%)	89 90	16, 39, 72, 110	0
1	C	152/170 (89%)	-0.02	3 (1%)	68 69	27, 55, 86, 118	0
1	D	152/170 (89%)	0.29	7 (4%)	36 35	36, 60, 84, 115	0
1	E	152/170 (89%)	0.59	12 (7%)	15 13	39, 72, 98, 122	0
1	F	152/170 (89%)	0.60	13 (8%)	13 10	43, 77, 112, 132	0
1	G	152/170 (89%)	0.87	18 (11%)	6 5	65, 89, 115, 137	0
1	H	152/170 (89%)	0.03	0	100 100	23, 47, 79, 115	0
1	I	152/170 (89%)	0.92	20 (13%)	4 4	53, 86, 116, 132	0
1	J	152/170 (89%)	0.34	6 (3%)	43 43	33, 59, 85, 127	0
All	All	1520/1700 (89%)	0.36	83 (5%)	29 27	16, 66, 106, 137	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	PRO	6.7
1	F	33	ASP	6.1
1	I	157	PRO	5.4
1	I	144	TYR	5.1
1	A	121	CYS	4.6

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.