WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 17, 2023 – 01:56 AM EST

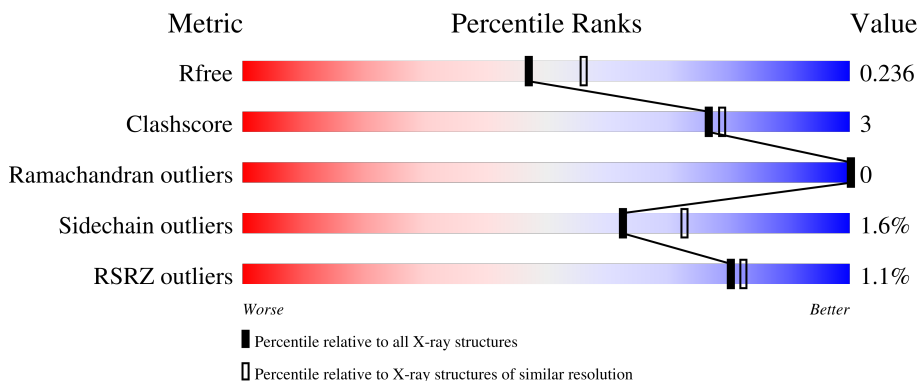|		
PDB ID	:	1VQR
Title	:	Crystal structure of a virulence factor (cj0248) from campylobacter jejuni subsp. jejuni at 2.25 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2004-12-17
Resolution	:	2.25 Å(reported)

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 2.25 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		1.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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% 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	297	85% — 11% ·
1	B	297	82% — 8% 9%
1	C	297	2% / 88% — 6% · 5%
1	D	297	2% / 84% — 5% · 10%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8688 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 Cj0248.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	Se	0	1	0
			2210	1424	362	415	3	6			
1	B	269	Total	C	N	O	S	Se	0	1	0
			2076	1351	338	379	3	5			
1	C	281	Total	C	N	O	S	Se	0	0	0
			2149	1392	350	398	3	6			
1	D	267	Total	C	N	O	S	Se	0	2	0
			2060	1339	337	377	3	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q9PIP7
A	-10	GLY	-	expression tag	UNP Q9PIP7
A	-9	SER	-	expression tag	UNP Q9PIP7
A	-8	ASP	-	expression tag	UNP Q9PIP7
A	-7	LYS	-	expression tag	UNP Q9PIP7
A	-6	ILE	-	expression tag	UNP Q9PIP7
A	-5	HIS	-	expression tag	UNP Q9PIP7
A	-4	HIS	-	expression tag	UNP Q9PIP7
A	-3	HIS	-	expression tag	UNP Q9PIP7
A	-2	HIS	-	expression tag	UNP Q9PIP7
A	-1	HIS	-	expression tag	UNP Q9PIP7
A	0	HIS	-	expression tag	UNP Q9PIP7
A	1	MSE	MET	modified residue	UNP Q9PIP7
A	5	MSE	MET	modified residue	UNP Q9PIP7
A	40	MSE	MET	modified residue	UNP Q9PIP7
A	52	MSE	MET	modified residue	UNP Q9PIP7
A	91	MSE	MET	modified residue	UNP Q9PIP7
A	144	MSE	MET	modified residue	UNP Q9PIP7
B	-11	MSE	-	expression tag	UNP Q9PIP7
B	-10	GLY	-	expression tag	UNP Q9PIP7
B	-9	SER	-	expression tag	UNP Q9PIP7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	expression tag	UNP Q9PIP7
B	-7	LYS	-	expression tag	UNP Q9PIP7
B	-6	ILE	-	expression tag	UNP Q9PIP7
B	-5	HIS	-	expression tag	UNP Q9PIP7
B	-4	HIS	-	expression tag	UNP Q9PIP7
B	-3	HIS	-	expression tag	UNP Q9PIP7
B	-2	HIS	-	expression tag	UNP Q9PIP7
B	-1	HIS	-	expression tag	UNP Q9PIP7
B	0	HIS	-	expression tag	UNP Q9PIP7
B	1	MSE	MET	modified residue	UNP Q9PIP7
B	5	MSE	MET	modified residue	UNP Q9PIP7
B	40	MSE	MET	modified residue	UNP Q9PIP7
B	52	MSE	MET	modified residue	UNP Q9PIP7
B	91	MSE	MET	modified residue	UNP Q9PIP7
B	144	MSE	MET	modified residue	UNP Q9PIP7
C	-11	MSE	-	expression tag	UNP Q9PIP7
C	-10	GLY	-	expression tag	UNP Q9PIP7
C	-9	SER	-	expression tag	UNP Q9PIP7
C	-8	ASP	-	expression tag	UNP Q9PIP7
C	-7	LYS	-	expression tag	UNP Q9PIP7
C	-6	ILE	-	expression tag	UNP Q9PIP7
C	-5	HIS	-	expression tag	UNP Q9PIP7
C	-4	HIS	-	expression tag	UNP Q9PIP7
C	-3	HIS	-	expression tag	UNP Q9PIP7
C	-2	HIS	-	expression tag	UNP Q9PIP7
C	-1	HIS	-	expression tag	UNP Q9PIP7
C	0	HIS	-	expression tag	UNP Q9PIP7
C	1	MSE	MET	modified residue	UNP Q9PIP7
C	5	MSE	MET	modified residue	UNP Q9PIP7
C	40	MSE	MET	modified residue	UNP Q9PIP7
C	52	MSE	MET	modified residue	UNP Q9PIP7
C	91	MSE	MET	modified residue	UNP Q9PIP7
C	144	MSE	MET	modified residue	UNP Q9PIP7
D	-11	MSE	-	expression tag	UNP Q9PIP7
D	-10	GLY	-	expression tag	UNP Q9PIP7
D	-9	SER	-	expression tag	UNP Q9PIP7
D	-8	ASP	-	expression tag	UNP Q9PIP7
D	-7	LYS	-	expression tag	UNP Q9PIP7
D	-6	ILE	-	expression tag	UNP Q9PIP7
D	-5	HIS	-	expression tag	UNP Q9PIP7
D	-4	HIS	-	expression tag	UNP Q9PIP7
D	-3	HIS	-	expression tag	UNP Q9PIP7

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| Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP Q9PIP7
D	-1	HIS	-	expression tag	UNP Q9PIP7
D	0	HIS	-	expression tag	UNP Q9PIP7
D	1	MSE	MET	modified residue	UNP Q9PIP7
D	5	MSE	MET	modified residue	UNP Q9PIP7
D	40	MSE	MET	modified residue	UNP Q9PIP7
D	52	MSE	MET	modified residue	UNP Q9PIP7
D	91	MSE	MET	modified residue	UNP Q9PIP7
D	144	MSE	MET	modified residue	UNP Q9PIP7

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	68	Total	O	0	0
			68	68		
2	B	47	Total	O	0	0
			47	47		
2	C	36	Total	O	0	0
			36	36		
2	D	42	Total	O	0	0
			42	42		

3 Residue-property plots ⓘ

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 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.
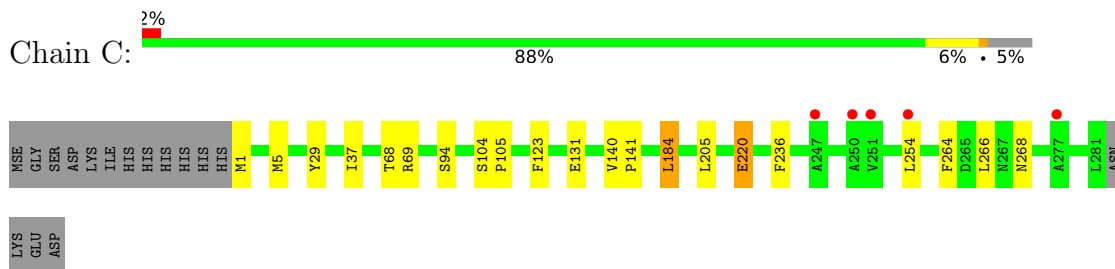
- Molecule 1: hypothetical protein Cj0248
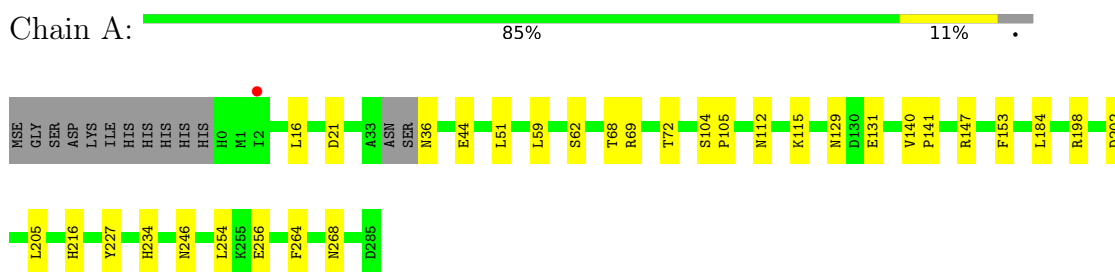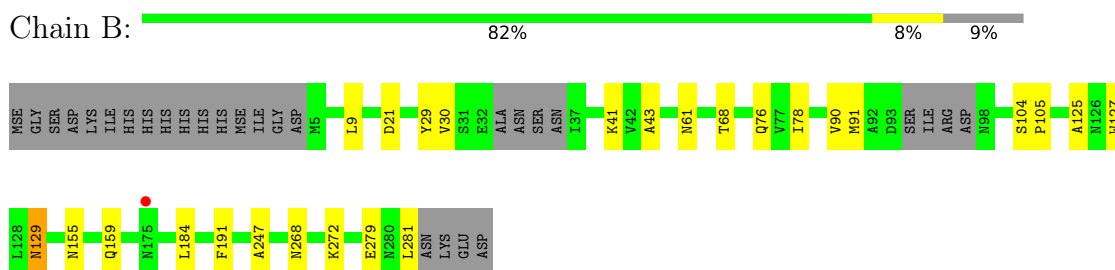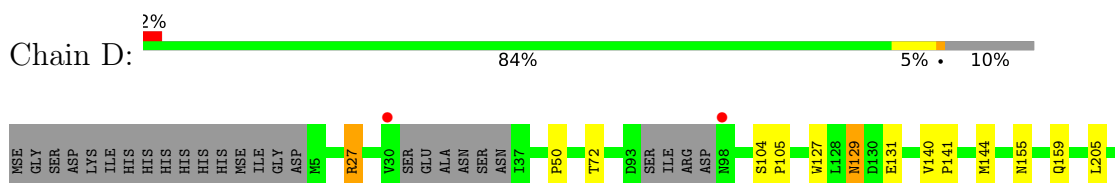
Chain A:

- Molecule 1: hypothetical protein Cj0248

Chain B:

- Molecule 1: hypothetical protein Cj0248

Chain C:

- Molecule 1: hypothetical protein Cj0248

Chain D:

H234 N246 V251 N268 K272 L273 P274 A277 L281 ASN LYS GLU ASP

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.14Å 122.09Å 96.90Å 90.00° 120.58° 90.00°	Depositor
Resolution (Å)	61.04 – 2.25 61.05 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.3 (61.04-2.25) 97.3 (61.05-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.233 0.199 , 0.236	Depositor DCC
R_{free} test set	2850 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.3	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8688	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, 0.333 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	0.71	0/2249	0.73	2/3044 (0.1%)
1	B	0.69	0/2117	0.68	0/2873
1	C	0.70	2/2186 (0.1%)	0.65	0/2970
1	D	0.64	0/2105	0.65	0/2859
All	All	0.69	2/8657 (0.0%)	0.68	2/11746 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	220	GLU	CD-OE2	9.32	1.35	1.25
1	C	220	GLU	CD-OE1	6.15	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	198	ARG	NE-CZ-NH2	-5.27	117.66	120.30

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	2210	0	2187	14	0
1	B	2076	0	2048	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2149	0	2110	12	0
1	D	2060	0	2021	12	0
2	A	68	0	0	1	0
2	B	47	0	0	1	0
2	C	36	0	0	1	0
2	D	42	0	0	2	0
All	All	8688	0	8366	51	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 3.

The worst 5 of 51 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:C:5:MSE:CE	1:C:5:MSE:SE	2.16	1.44
1:D:129[B]:ASN:ND2	2:D:325:HOH:O	2.25	0.70
1:A:216:HIS:ND1	2:A:343:HOH:O	2.28	0.65
1:C:5:MSE:HG2	1:C:184:LEU:O	2.03	0.59
1:D:155:ASN:O	1:D:159:GLN:HG2	2.04	0.58

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	281/297 (95%)	279 (99%)	2 (1%)	0	100	100
1	B	264/297 (89%)	258 (98%)	6 (2%)	0	100	100
1	C	279/297 (94%)	273 (98%)	6 (2%)	0	100	100
1	D	263/297 (89%)	259 (98%)	4 (2%)	0	100	100
All	All	1087/1188 (92%)	1069 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	237/256 (93%)	232 (98%)	5 (2%)	53	62
1	B	218/256 (85%)	215 (99%)	3 (1%)	67	76
1	C	224/256 (88%)	220 (98%)	4 (2%)	59	68
1	D	216/256 (84%)	213 (99%)	3 (1%)	67	76
All	All	895/1024 (87%)	880 (98%)	15 (2%)	62	71

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	279	GLU
1	D	129[A]	ASN
1	C	1	MSE
1	D	129[B]	ASN
1	C	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	C	118	ASN
1	C	173	ASN
1	C	216	HIS
1	C	246	ASN

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 monosaccharides 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	278/297 (93%)	-0.23	1 (0%)	92	93	38, 47, 60, 72	0
1	B	264/297 (88%)	-0.20	1 (0%)	92	93	37, 47, 60, 69	0
1	C	275/297 (92%)	0.01	5 (1%)	68	71	37, 47, 60, 70	0
1	D	262/297 (88%)	-0.02	5 (1%)	66	69	37, 47, 58, 66	0
All	All	1079/1188 (90%)	-0.11	12 (1%)	80	82	37, 47, 60, 72	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	4.5
1	C	251	VAL	3.2
1	D	98	ASN	3.1
1	C	247	ALA	2.9
1	D	277	ALA	2.5

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 monosaccharides 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.