



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:30 PM GMT

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

This is a full wwPDB validation 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/ValidationPDFNotes.html>

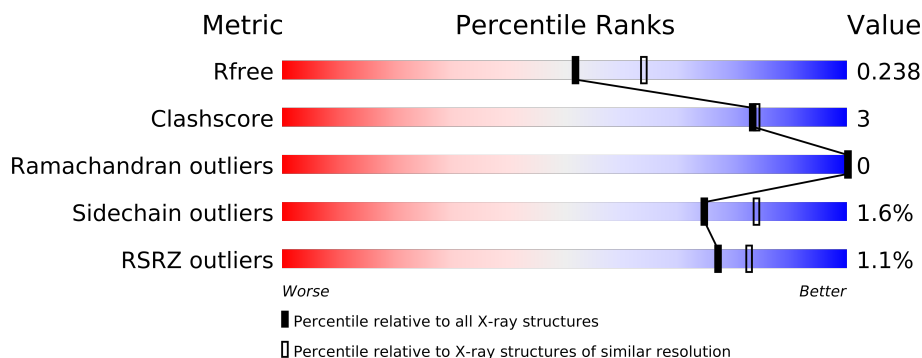
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. 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	297	
1	B	297	
1	C	297	
1	D	297	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8688 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 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	-	LEADER SEQUENCE	UNP Q9PIP7
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9PIP7
A	-9	SER	-	LEADER SEQUENCE	UNP Q9PIP7
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9PIP7
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9PIP7
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9PIP7
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
A	0	HIS	-	LEADER SEQUENCE	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	-	LEADER SEQUENCE	UNP Q9PIP7
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9PIP7
B	-9	SER	-	LEADER SEQUENCE	UNP Q9PIP7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9PIP7
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9PIP7
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9PIP7
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
B	0	HIS	-	LEADER SEQUENCE	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	-	LEADER SEQUENCE	UNP Q9PIP7
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9PIP7
C	-9	SER	-	LEADER SEQUENCE	UNP Q9PIP7
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9PIP7
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9PIP7
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9PIP7
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
C	0	HIS	-	LEADER SEQUENCE	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	-	LEADER SEQUENCE	UNP Q9PIP7
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9PIP7
D	-9	SER	-	LEADER SEQUENCE	UNP Q9PIP7
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9PIP7
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9PIP7
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9PIP7
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9PIP7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9PIP7
D	0	HIS	-	LEADER SEQUENCE	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.

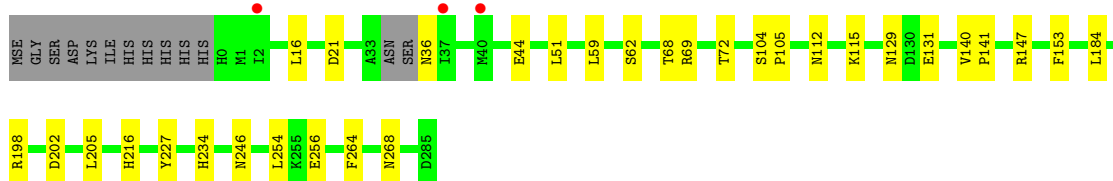
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	68	Total O 68 68	0	0
2	B	47	Total O 47 47	0	0
2	C	36	Total O 36 36	0	0
2	D	42	Total O 42 42	0	0

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.

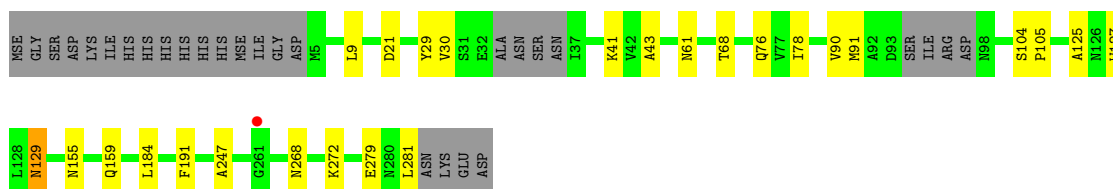
- Molecule 1: hypothetical protein Cj0248

Chain A: 



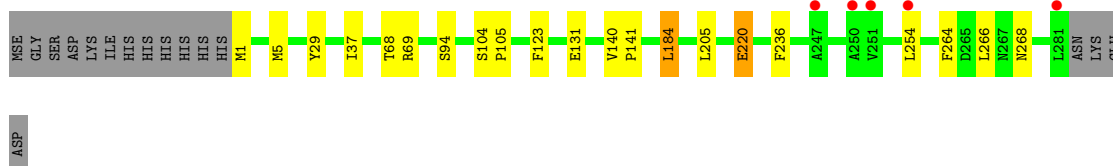
- Molecule 1: hypothetical protein Cj0248

Chain B: 



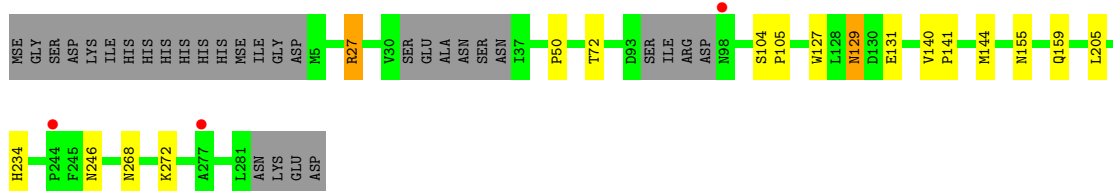
- Molecule 1: hypothetical protein Cj0248

Chain C: 



- Molecule 1: hypothetical protein Cj0248

Chain D: 



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
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.193 , 0.233 0.201 , 0.238	Depositor DCC
R_{free} test set	2850 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 56899 reflections (0.002%)	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.*

¹Intensities 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	0.71	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(°)	Ideal(°)
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 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	2210	0	2187	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2076	0	2048	14	0
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

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 3.

All (51) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:5:MSE:SE	1:C:5:MSE:CE	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
1:C:5:MSE:HA	1:C:5:MSE:HE2	1.88	0.56
1:D:72:THR:HG21	2:D:318:HOH:O	2.06	0.55
1:A:36:ASN:ND2	1:B:76:GLN:HE21	2.03	0.55
1:B:125:ALA:O	1:B:129:ASN:HB2	2.08	0.53
1:D:27:ARG:HG3	1:D:27:ARG:NH1	2.22	0.52
1:C:104:SER:N	1:C:105:PRO:CD	2.73	0.52
1:A:227:TYR:OH	1:A:256:GLU:OE2	2.21	0.52
1:B:61:ASN:O	1:B:68:THR:HG23	2.11	0.51
1:C:220:GLU:HG2	2:C:310:HOH:O	2.11	0.50
1:A:59:LEU:O	1:A:62:SER:HB3	2.10	0.50
1:D:131:GLU:OE1	1:D:268:ASN:ND2	2.45	0.50
1:B:127:TRP:O	1:B:268:ASN:ND2	2.37	0.50
1:D:140:VAL:HB	1:D:141:PRO:HD3	1.95	0.48
1:A:140:VAL:HB	1:A:141:PRO:HD3	1.96	0.47
1:C:254:LEU:HG	1:C:264:PHE:HB2	1.97	0.47
1:A:254:LEU:HG	1:A:264:PHE:HB2	1.97	0.46
1:D:127:TRP:HA	1:D:272:LYS:HD3	1.97	0.46
1:B:29:TYR:CZ	1:B:41:LYS:CB	2.98	0.46
1:A:131:GLU:OE1	1:A:268:ASN:ND2	2.48	0.46
1:A:72:THR:HG22	1:A:202:ASP:HB3	1.99	0.45
1:D:27:ARG:HH11	1:D:27:ARG:HG3	1.82	0.45
1:C:68:THR:HG22	1:C:69:ARG:HG3	1.98	0.45
1:B:90:VAL:HG12	1:B:91:MSE:HE2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:PHE:CD2	1:A:184:LEU:HD12	2.52	0.44
1:C:29:TYR:HE2	1:C:37:ILE:HG23	1.83	0.44
1:A:205:LEU:HD23	1:A:205:LEU:C	2.38	0.43
1:A:234:HIS:O	1:A:246:ASN:HB3	2.18	0.43
1:D:50:PRO:HB3	1:D:144:MSE:O	2.18	0.43
1:B:30:VAL:HG12	1:B:30:VAL:O	2.19	0.43
1:C:131:GLU:OE1	1:C:268:ASN:ND2	2.50	0.43
1:B:43:ALA:HB2	1:B:78:ILE:CD1	2.47	0.43
1:A:68:THR:HG22	1:A:69:ARG:HG3	2.01	0.42
1:C:205:LEU:C	1:C:205:LEU:HD23	2.39	0.42
1:D:234:HIS:O	1:D:246:ASN:HB3	2.18	0.42
1:B:155:ASN:O	1:B:159:GLN:HG2	2.20	0.42
1:B:247:ALA:HB1	1:B:281:LEU:HD13	2.01	0.42
1:C:140:VAL:HB	1:C:141:PRO:HD3	2.02	0.41
1:A:104:SER:N	1:A:105:PRO:CD	2.83	0.41
1:D:205:LEU:HD23	1:D:205:LEU:C	2.40	0.41
1:C:123:PHE:CD2	1:C:236:PHE:HE2	2.39	0.41
1:B:104:SER:N	1:B:105:PRO:CD	2.84	0.41
1:B:9:LEU:HB3	1:B:191:PHE:CZ	2.56	0.41
1:A:16:LEU:HD22	1:A:51:LEU:HD23	2.03	0.41
1:D:104:SER:N	1:D:105:PRO:CD	2.85	0.40
1:B:127:TRP:HA	1:B:272:LYS:HD3	2.04	0.40
1:B:21:ASP:HB2	2:B:293:HOH:O	2.22	0.40

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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	66	75
1	B	218/256 (85%)	215 (99%)	3 (1%)	78	87
1	C	224/256 (88%)	220 (98%)	4 (2%)	71	80
1	D	216/256 (84%)	213 (99%)	3 (1%)	78	87
All	All	895/1024 (87%)	880 (98%)	15 (2%)	75	82

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	44	GLU
1	A	112	ASN
1	A	115	LYS
1	A	129	ASN
1	B	129	ASN
1	B	184	LEU
1	B	279	GLU
1	C	1	MSE
1	C	94	SER
1	C	184	LEU
1	C	266	LEU
1	D	27	ARG
1	D	129[A]	ASN
1	D	129[B]	ASN

Some 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 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, 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	284/297 (95%)	-0.33	3 (1%) 77 83	38, 48, 61, 73	0
1	B	269/297 (90%)	-0.32	1 (0%) 90 93	37, 47, 60, 75	0
1	C	281/297 (94%)	-0.11	5 (1%) 65 72	37, 47, 60, 75	0
1	D	267/297 (89%)	-0.13	3 (1%) 77 83	37, 47, 58, 66	0
All	All	1101/1188 (92%)	-0.22	12 (1%) 77 83	37, 47, 60, 75	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	MSE	3.5
1	C	254	LEU	3.1
1	C	247	ALA	2.9
1	C	251	VAL	2.7
1	C	281	LEU	2.5
1	D	98	ASN	2.5
1	D	277	ALA	2.3
1	C	250	ALA	2.2
1	A	2	ILE	2.1
1	D	244	PRO	2.1
1	B	261	GLY	2.1
1	A	37	ILE	2.1

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.