Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 03:14 PM EST

PDB ID	:	4FML
Title	:	Catalytic domain of VahC from Aeromonas hydrophila
Authors	:	Ravulapalli, R.; Kimber, M.S.; Merrill, A.R.
Deposited on	:	2012-06-18
Resolution	:	1.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

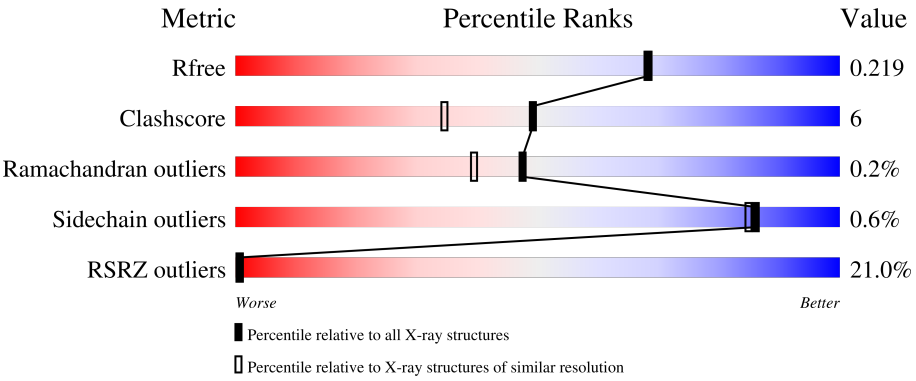
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.93 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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	223	8% 84% 7% 9%
1	B	223	3% 80% 8% 12%
1	C	223	42% 53% 17% 29%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9215 atoms, of which 4419 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 VsdC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	204	Total	C	H	N	O	S	0	1	0
			3189	1001	1596	280	308	4			
1	B	196	Total	C	H	N	O	S	0	2	0
			3118	979	1570	273	292	4			
1	C	158	Total	C	H	N	O	S	0	0	0
			2496	789	1253	215	237	2			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	expression tag	UNP Q49TP5
A	45	GLY	-	expression tag	UNP Q49TP5
A	46	SER	-	expression tag	UNP Q49TP5
A	47	SER	-	expression tag	UNP Q49TP5
A	48	HIS	-	expression tag	UNP Q49TP5
A	49	HIS	-	expression tag	UNP Q49TP5
A	50	HIS	-	expression tag	UNP Q49TP5
A	51	HIS	-	expression tag	UNP Q49TP5
A	52	HIS	-	expression tag	UNP Q49TP5
A	53	HIS	-	expression tag	UNP Q49TP5
A	54	SER	-	expression tag	UNP Q49TP5
A	55	SER	-	expression tag	UNP Q49TP5
A	56	GLY	-	expression tag	UNP Q49TP5
A	57	GLU	-	expression tag	UNP Q49TP5
A	58	ASN	-	expression tag	UNP Q49TP5
A	59	LEU	-	expression tag	UNP Q49TP5
A	60	TYR	-	expression tag	UNP Q49TP5
A	61	PHE	-	expression tag	UNP Q49TP5
A	62	GLN	-	expression tag	UNP Q49TP5
A	63	GLY	-	expression tag	UNP Q49TP5
A	64	SER	-	expression tag	UNP Q49TP5
A	65	HIS	-	expression tag	UNP Q49TP5
A	66	MET	-	expression tag	UNP Q49TP5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	44	MET	-	expression tag	UNP Q49TP5
B	45	GLY	-	expression tag	UNP Q49TP5
B	46	SER	-	expression tag	UNP Q49TP5
B	47	SER	-	expression tag	UNP Q49TP5
B	48	HIS	-	expression tag	UNP Q49TP5
B	49	HIS	-	expression tag	UNP Q49TP5
B	50	HIS	-	expression tag	UNP Q49TP5
B	51	HIS	-	expression tag	UNP Q49TP5
B	52	HIS	-	expression tag	UNP Q49TP5
B	53	HIS	-	expression tag	UNP Q49TP5
B	54	SER	-	expression tag	UNP Q49TP5
B	55	SER	-	expression tag	UNP Q49TP5
B	56	GLY	-	expression tag	UNP Q49TP5
B	57	GLU	-	expression tag	UNP Q49TP5
B	58	ASN	-	expression tag	UNP Q49TP5
B	59	LEU	-	expression tag	UNP Q49TP5
B	60	TYR	-	expression tag	UNP Q49TP5
B	61	PHE	-	expression tag	UNP Q49TP5
B	62	GLN	-	expression tag	UNP Q49TP5
B	63	GLY	-	expression tag	UNP Q49TP5
B	64	SER	-	expression tag	UNP Q49TP5
B	65	HIS	-	expression tag	UNP Q49TP5
B	66	MET	-	expression tag	UNP Q49TP5
C	44	MET	-	expression tag	UNP Q49TP5
C	45	GLY	-	expression tag	UNP Q49TP5
C	46	SER	-	expression tag	UNP Q49TP5
C	47	SER	-	expression tag	UNP Q49TP5
C	48	HIS	-	expression tag	UNP Q49TP5
C	49	HIS	-	expression tag	UNP Q49TP5
C	50	HIS	-	expression tag	UNP Q49TP5
C	51	HIS	-	expression tag	UNP Q49TP5
C	52	HIS	-	expression tag	UNP Q49TP5
C	53	HIS	-	expression tag	UNP Q49TP5
C	54	SER	-	expression tag	UNP Q49TP5
C	55	SER	-	expression tag	UNP Q49TP5
C	56	GLY	-	expression tag	UNP Q49TP5
C	57	GLU	-	expression tag	UNP Q49TP5
C	58	ASN	-	expression tag	UNP Q49TP5
C	59	LEU	-	expression tag	UNP Q49TP5
C	60	TYR	-	expression tag	UNP Q49TP5
C	61	PHE	-	expression tag	UNP Q49TP5
C	62	GLN	-	expression tag	UNP Q49TP5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	GLY	-	expression tag	UNP Q49TP5
C	64	SER	-	expression tag	UNP Q49TP5
C	65	HIS	-	expression tag	UNP Q49TP5
C	66	MET	-	expression tag	UNP Q49TP5

- Molecule 2 is water.

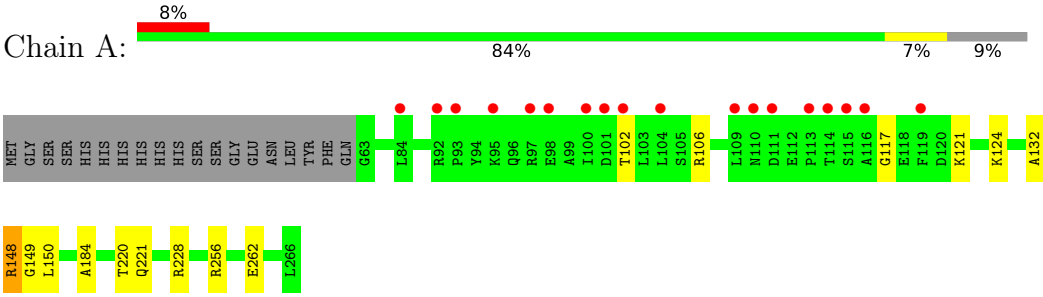
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	174	Total O 174 174	0	0
2	B	215	Total O 215 215	0	0
2	C	23	Total O 23 23	0	0

3 Residue-property plots (i)

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.

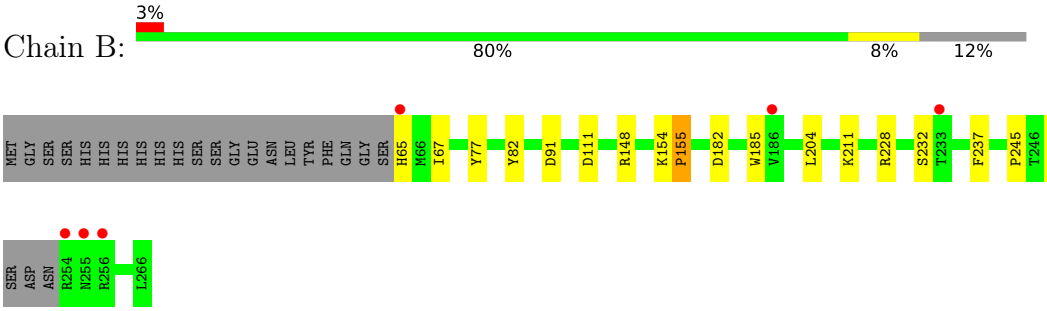
• Molecule 1: VsdC

Chain A:



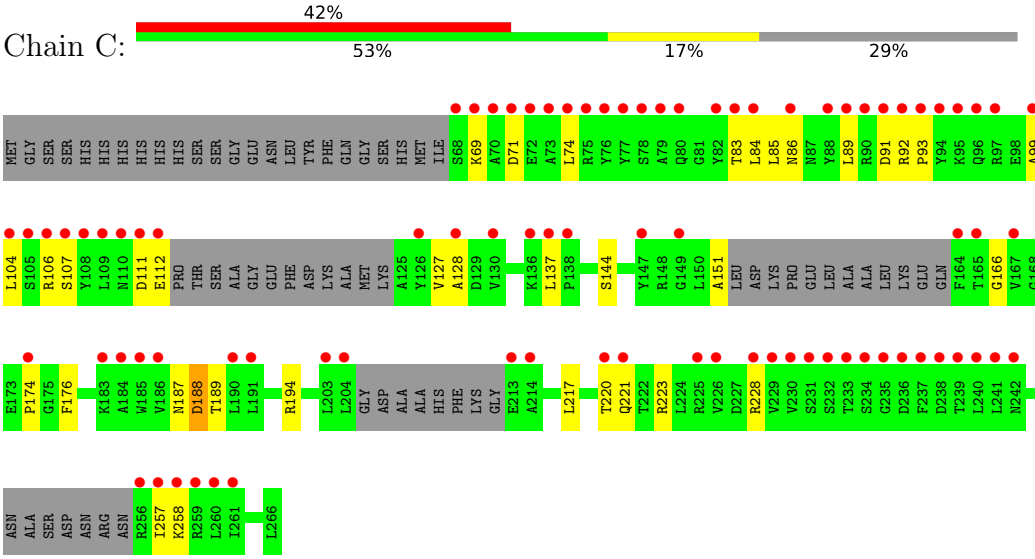
• Molecule 1: VsdC

Chain B:



• Molecule 1: VsdC

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.10Å 91.10Å 303.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.55 – 1.93 48.10 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.55-1.93) 99.9 (48.10-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 1.92Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.191 , 0.217 0.196 , 0.219	Depositor DCC
R_{free} test set	2852 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9215	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 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	1.00	2/1625 (0.1%)	0.77	0/2198
1	B	1.14	0/1582	0.85	2/2138 (0.1%)
1	C	0.56	0/1262	0.61	0/1706
All	All	0.95	2/4469 (0.0%)	0.76	2/6042 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLU	CG-CD	5.29	1.59	1.51
1	A	132	ALA	CA-CB	5.01	1.62	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	111	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	228	ARG	NE-CZ-NH2	-5.06	117.77	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	1593	1596	1593	9	0
1	B	1548	1570	1567	9	1
1	C	1243	1253	1252	34	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	174	0	0	1	1
2	B	215	0	0	1	2
2	C	23	0	0	6	0
All	All	4796	4419	4412	52	6

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 6.

All (52) 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:228:ARG:NH1	2:C:322:HOH:O	1.99	0.86
1:C:220:THR:O	1:C:221:GLN:HG2	1.85	0.76
1:C:84:LEU:HD21	1:C:99:ALA:HA	1.71	0.73
1:C:92:ARG:HB3	1:C:93:PRO:HD2	1.73	0.69
1:B:91:ASP:OD1	2:B:462:HOH:O	2.12	0.66
1:C:71:ASP:OD1	2:C:320:HOH:O	2.16	0.63
1:C:220:THR:O	1:C:221:GLN:CG	2.50	0.58
1:A:228:ARG:NH1	1:A:262:GLU:OE2	2.36	0.57
1:C:172:VAL:HG12	1:C:223:ARG:HG2	1.86	0.57
1:C:106:ARG:O	1:C:107:SER:HB2	2.06	0.54
1:C:111:ASP:O	1:C:112:GLU:C	2.44	0.54
1:A:117:GLY:O	1:A:121:LYS:HB2	2.07	0.54
1:C:166:GLY:HA3	1:C:169:ASN:ND2	2.22	0.53
1:B:204:LEU:HD12	1:B:211:LYS:HE2	1.91	0.53
1:A:121:LYS:HA	1:A:124:LYS:HE3	1.90	0.52
1:C:221:GLN:HG3	1:C:221:GLN:O	2.10	0.52
1:A:256:ARG:HG3	2:A:356:HOH:O	2.10	0.51
1:A:147:TYR:HB3	1:A:184:ALA:HB2	1.93	0.50
1:C:151:ALA:C	1:C:188:ASP:OD2	2.51	0.50
1:A:148[A]:ARG:HD2	1:A:149:GLY:O	2.12	0.49
1:B:185:TRP:CE3	1:B:247:SER:CB	2.95	0.49
1:B:232:SER:HA	1:B:237:PHE:CD1	2.48	0.48
1:C:74:LEU:HD21	1:C:137:LEU:HD11	1.95	0.48
1:A:220:THR:O	1:A:221:GLN:HB2	2.14	0.48
1:C:220:THR:O	1:C:221:GLN:CB	2.61	0.48
1:C:85:LEU:HD21	1:C:127:VAL:HG22	1.96	0.47
1:C:84:LEU:HD21	1:C:99:ALA:CA	2.43	0.47
1:C:69:LYS:HZ1	1:C:107:SER:HB2	1.80	0.46
1:A:102:THR:O	1:A:106:ARG:HG3	2.15	0.46
1:A:150:LEU:HD23	1:A:150:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:TRP:CE3	1:B:247:SER:HB3	2.52	0.45
1:B:182:ASP:O	1:B:245:PRO:HG2	2.15	0.45
1:C:127:VAL:O	1:C:128:ALA:C	2.53	0.45
1:C:176:PHE:HB3	1:C:217:LEU:HD11	1.99	0.44
1:C:86:ASN:HD21	1:C:176:PHE:H	1.67	0.43
1:C:187:ASN:O	1:C:257:ILE:HA	2.19	0.43
1:C:69:LYS:NZ	1:C:107:SER:HB2	2.34	0.43
1:C:84:LEU:N	2:C:313:HOH:O	2.26	0.43
1:C:194:ARG:NH2	2:C:318:HOH:O	2.51	0.43
1:B:77:TYR:CE1	1:B:82:TYR:HA	2.54	0.43
1:C:74:LEU:HD12	1:C:74:LEU:O	2.19	0.42
1:C:89:LEU:C	1:C:91:ASP:H	2.23	0.42
1:C:221:GLN:CG	1:C:221:GLN:O	2.66	0.42
1:C:144:SER:OG	2:C:314:HOH:O	1.96	0.42
1:C:174:PRO:O	1:C:220:THR:HB	2.20	0.41
1:C:83:THR:HB	2:C:313:HOH:O	2.21	0.41
1:C:100:ILE:O	1:C:104:LEU:HD13	2.21	0.41
1:C:188:ASP:HB2	1:C:258:LYS:HE3	2.03	0.41
1:B:154:LYS:HA	1:B:155:PRO:HD3	1.86	0.40
1:C:151:ALA:HA	1:C:187:ASN:OD1	2.20	0.40
1:B:65:HIS:ND1	1:B:65:HIS:N	2.69	0.40
1:C:188:ASP:OD1	1:C:189:THR:OG1	2.35	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:VAL:HB	1:C:172:VAL:HB[11_654]	0.65	0.95
1:B:67:ILE:HD11	1:B:67:ILE:HD11[12_564]	0.91	0.69
2:A:449:HOH:O	2:B:490:HOH:O[7_554]	1.98	0.22
2:B:446:HOH:O	2:B:451:HOH:O[12_564]	2.07	0.13
1:C:172:VAL:CB	1:C:172:VAL:HB[11_654]	1.50	0.10
1:C:170:ILE:O	1:C:221:GLN:HB2[11_654]	1.56	0.04

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	203/223 (91%)	201 (99%)	2 (1%)	0	100 100
1	B	194/223 (87%)	189 (97%)	4 (2%)	1 (0%)	29 17
1	C	148/223 (66%)	141 (95%)	7 (5%)	0	100 100
All	All	545/669 (82%)	531 (97%)	13 (2%)	1 (0%)	47 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155	PRO

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	171/187 (91%)	169 (99%)	2 (1%)	71 64
1	B	166/187 (89%)	164 (99%)	2 (1%)	71 64
1	C	135/187 (72%)	134 (99%)	1 (1%)	84 81
All	All	472/561 (84%)	467 (99%)	5 (1%)	86 67

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148[A]	ARG
1	A	148[B]	ARG
1	B	148[A]	ARG
1	B	148[B]	ARG
1	C	188	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	C	86	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, 95^{th} 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	204/223 (91%)	0.50	18 (8%) 10 15	22, 39, 93, 136	0
1	B	196/223 (87%)	0.34	6 (3%) 49 56	20, 31, 74, 111	0
1	C	158/223 (70%)	3.11	93 (58%) 0 0	65, 107, 152, 231	0
All	All	558/669 (83%)	1.19	117 (20%) 1 1	20, 48, 131, 231	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	LEU	13.0
1	C	233	THR	9.3
1	C	111	ASP	9.1
1	C	234	SER	8.3
1	C	109	LEU	8.2
1	C	110	ASN	8.1
1	C	100	ILE	8.0
1	C	236	ASP	8.0
1	C	232	SER	7.6
1	C	185	TRP	7.6
1	C	237	PHE	7.6
1	C	75	ARG	7.4
1	A	111	ASP	7.1
1	C	88	TYR	7.1
1	C	235	GLY	6.7
1	C	89	LEU	6.6
1	C	107	SER	6.3
1	C	213	GLU	6.2
1	C	68	SER	6.0
1	C	72	GLU	5.8
1	A	109	LEU	5.7
1	C	74	LEU	5.7
1	C	102	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	79	ALA	5.7
1	C	97	ARG	5.6
1	C	76	TYR	5.6
1	C	229	VAL	5.6
1	C	239	THR	5.5
1	C	96	GLN	5.5
1	C	230	VAL	5.5
1	C	108	TYR	5.4
1	C	221	GLN	5.3
1	C	80	GLN	5.3
1	C	167	VAL	5.2
1	A	93	PRO	5.0
1	C	174	PRO	5.0
1	C	70	ALA	5.0
1	C	186	VAL	5.0
1	C	103	LEU	4.9
1	C	184	ALA	4.9
1	C	164	PHE	4.9
1	C	231	SER	4.7
1	C	90	ARG	4.7
1	C	238	ASP	4.6
1	C	240	LEU	4.6
1	C	246	THR	4.5
1	C	260	LEU	4.5
1	C	225	ARG	4.5
1	A	100	ILE	4.5
1	C	137	LEU	4.4
1	C	71	ASP	4.3
1	B	255	ASN	4.2
1	C	112	GLU	4.1
1	C	204	LEU	4.1
1	C	106	ARG	4.1
1	C	82	TYR	4.0
1	C	172	VAL	4.0
1	C	241	LEU	3.9
1	C	73	ALA	3.9
1	C	214	ALA	3.8
1	C	242	ASN	3.8
1	A	97	ARG	3.8
1	C	69	LYS	3.8
1	C	95	LYS	3.7
1	C	261	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	257	ILE	3.7
1	C	256	ARG	3.6
1	C	93	PRO	3.6
1	C	83	THR	3.5
1	A	102	THR	3.5
1	C	92	ARG	3.5
1	A	95	LYS	3.5
1	A	104	LEU	3.4
1	B	254	ARG	3.4
1	C	183	LYS	3.4
1	C	171	VAL	3.4
1	C	149	GLY	3.3
1	C	99	ALA	3.2
1	C	226	VAL	3.1
1	A	113	PRO	3.1
1	A	101	ASP	3.0
1	C	203	LEU	3.0
1	A	84	LEU	3.0
1	C	86	ASN	3.0
1	C	136	LYS	3.0
1	A	116	ALA	2.9
1	B	186	VAL	2.9
1	C	258	LYS	2.9
1	C	105	SER	2.8
1	C	84	LEU	2.7
1	C	138	PRO	2.6
1	C	130	VAL	2.6
1	C	94	TYR	2.6
1	C	190	LEU	2.6
1	C	147	TYR	2.6
1	A	98	GLU	2.6
1	C	259	ARG	2.5
1	B	65	HIS	2.5
1	C	101	ASP	2.5
1	C	220	THR	2.4
1	A	115	SER	2.4
1	C	191	LEU	2.4
1	A	92	ARG	2.3
1	C	170	ILE	2.3
1	B	256	ARG	2.3
1	A	119	PHE	2.3
1	A	114	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	78	SER	2.2
1	C	77	TYR	2.2
1	B	233	THR	2.2
1	C	126	TYR	2.1
1	A	110	ASN	2.1
1	C	165	THR	2.1
1	C	228	ARG	2.1
1	C	91	ASP	2.1
1	C	128	ALA	2.0
1	C	245	PRO	2.0

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.