wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 09:50 PM EDT

PDB ID	:	3EGC
Title	:	Crystal structure of a putative ribose operon repressor from Burkholderia thailandensis
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Deposited on	:	2008-09-10
Resolution	:	2.35 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

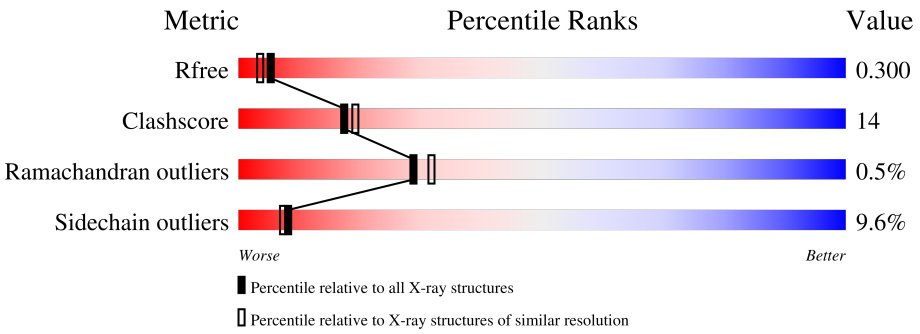
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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%

Mol	Chain	Length	Quality of chain
1	A	291	66% 20% • 10%
1	B	291	66% 20% • 10%
1	C	291	66% 19% • • 10%
1	D	291	69% 18% • 10%
1	E	291	65% 21% • 10%
1	F	291	67% 20% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12302 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 putative ribose operon repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	2006	1257	372	368	9	0	0	0
1	B	261	2013	1262	374	368	9	0	1	0
1	C	261	2006	1257	372	368	9	0	0	0
1	D	262	2011	1260	373	369	9	0	0	0
1	E	261	2006	1257	372	368	9	0	0	0
1	F	262	2011	1260	373	369	9	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	expression tag	UNP Q2T0D1
A	344	GLY	-	expression tag	UNP Q2T0D1
A	345	HIS	-	expression tag	UNP Q2T0D1
A	346	HIS	-	expression tag	UNP Q2T0D1
A	347	HIS	-	expression tag	UNP Q2T0D1
A	348	HIS	-	expression tag	UNP Q2T0D1
A	349	HIS	-	expression tag	UNP Q2T0D1
A	350	HIS	-	expression tag	UNP Q2T0D1
B	60	MET	-	expression tag	UNP Q2T0D1
B	344	GLY	-	expression tag	UNP Q2T0D1
B	345	HIS	-	expression tag	UNP Q2T0D1
B	346	HIS	-	expression tag	UNP Q2T0D1
B	347	HIS	-	expression tag	UNP Q2T0D1
B	348	HIS	-	expression tag	UNP Q2T0D1
B	349	HIS	-	expression tag	UNP Q2T0D1
B	350	HIS	-	expression tag	UNP Q2T0D1
C	60	MET	-	expression tag	UNP Q2T0D1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	344	GLY	-	expression tag	UNP Q2T0D1
C	345	HIS	-	expression tag	UNP Q2T0D1
C	346	HIS	-	expression tag	UNP Q2T0D1
C	347	HIS	-	expression tag	UNP Q2T0D1
C	348	HIS	-	expression tag	UNP Q2T0D1
C	349	HIS	-	expression tag	UNP Q2T0D1
C	350	HIS	-	expression tag	UNP Q2T0D1
D	60	MET	-	expression tag	UNP Q2T0D1
D	344	GLY	-	expression tag	UNP Q2T0D1
D	345	HIS	-	expression tag	UNP Q2T0D1
D	346	HIS	-	expression tag	UNP Q2T0D1
D	347	HIS	-	expression tag	UNP Q2T0D1
D	348	HIS	-	expression tag	UNP Q2T0D1
D	349	HIS	-	expression tag	UNP Q2T0D1
D	350	HIS	-	expression tag	UNP Q2T0D1
E	60	MET	-	expression tag	UNP Q2T0D1
E	344	GLY	-	expression tag	UNP Q2T0D1
E	345	HIS	-	expression tag	UNP Q2T0D1
E	346	HIS	-	expression tag	UNP Q2T0D1
E	347	HIS	-	expression tag	UNP Q2T0D1
E	348	HIS	-	expression tag	UNP Q2T0D1
E	349	HIS	-	expression tag	UNP Q2T0D1
E	350	HIS	-	expression tag	UNP Q2T0D1
F	60	MET	-	expression tag	UNP Q2T0D1
F	344	GLY	-	expression tag	UNP Q2T0D1
F	345	HIS	-	expression tag	UNP Q2T0D1
F	346	HIS	-	expression tag	UNP Q2T0D1
F	347	HIS	-	expression tag	UNP Q2T0D1
F	348	HIS	-	expression tag	UNP Q2T0D1
F	349	HIS	-	expression tag	UNP Q2T0D1
F	350	HIS	-	expression tag	UNP Q2T0D1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	47	47	47	0	0
			Total	O		
2	B	52	52	52	0	0
			Total	O		
2	C	56	56	56	0	0
			Total	O		
2	D	46	46	46	0	0

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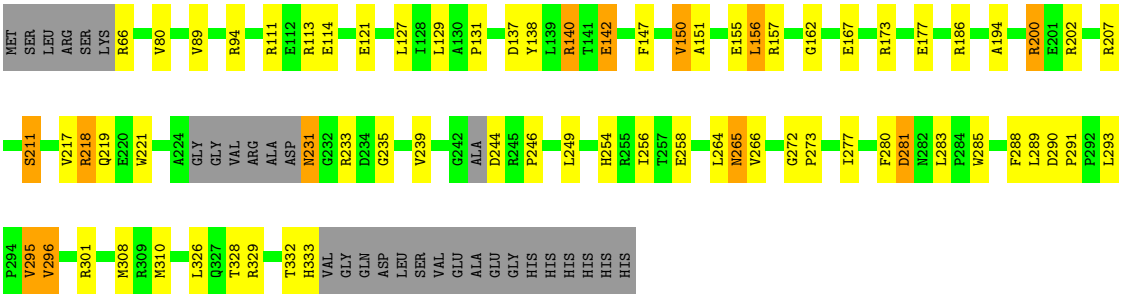
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	E	29	29	29	0	0
			Total	O		
2	F	19	19	19	0	0

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. 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. 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.

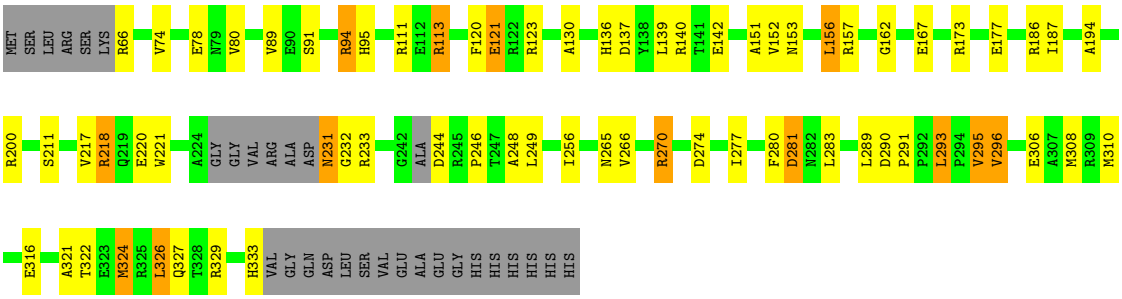
- Molecule 1: putative ribose operon repressor

Chain A:



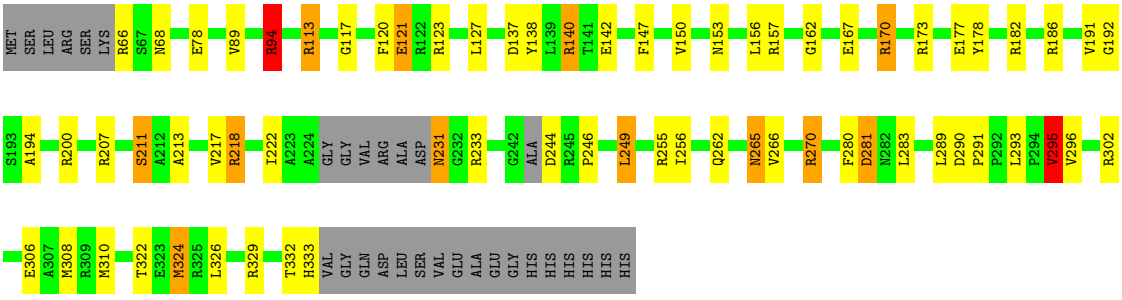
- Molecule 1: putative ribose operon repressor

Chain B:



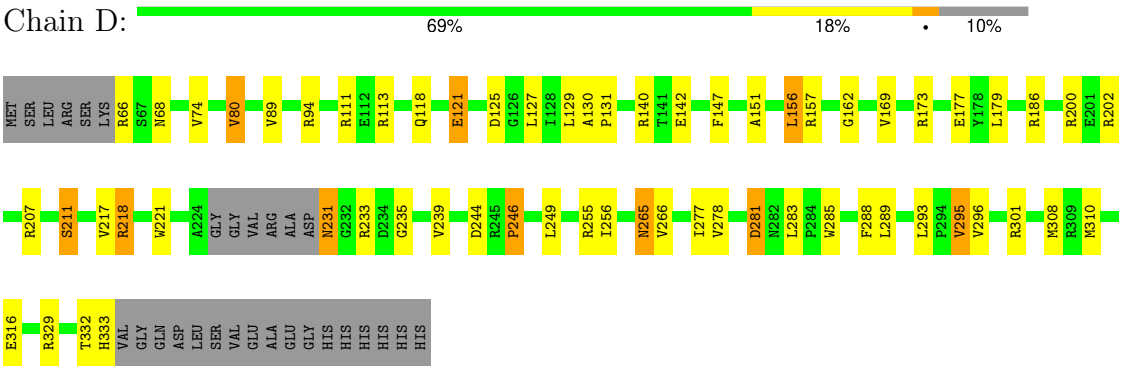
- Molecule 1: putative ribose operon repressor

Chain C:



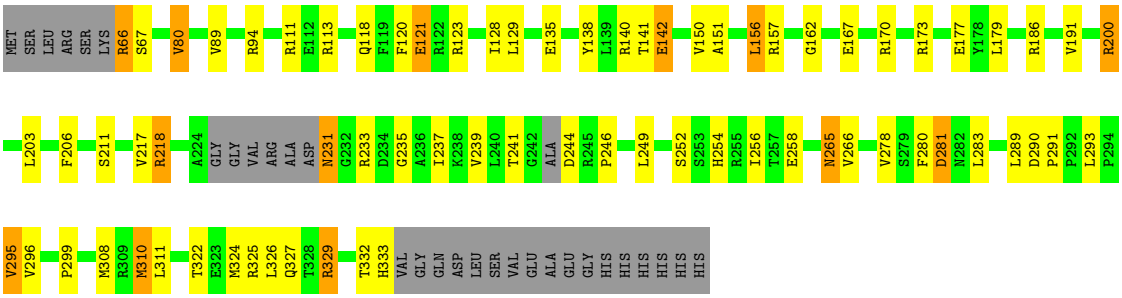
- Molecule 1: putative ribose operon repressor

Chain D:



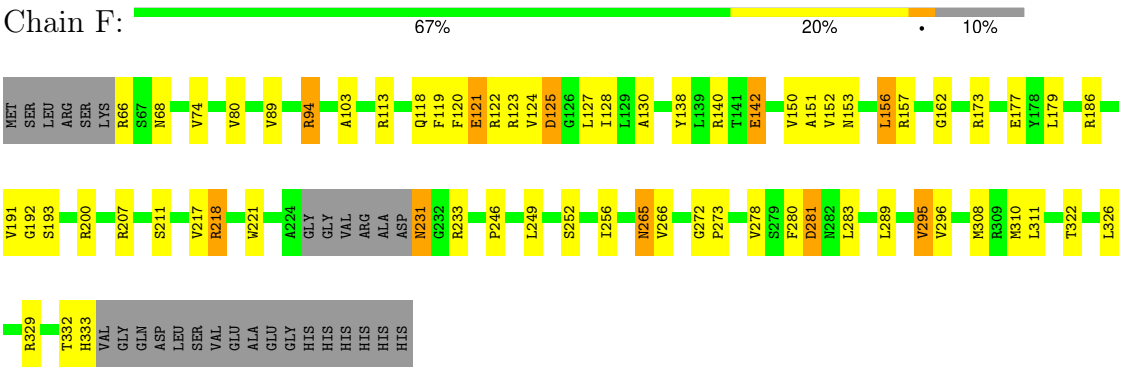
- Molecule 1: putative ribose operon repressor

Chain E:



- Molecule 1: putative ribose operon repressor

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.71Å 288.65Å 63.35Å 90.00° 113.59° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 46.47 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.35) 98.0 (46.47-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	7.95 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.299 0.259 , 0.300	Depositor DCC
R_{free} test set	3379 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.397 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12302	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 (i)

5.1 Standard geometry (i)

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	1.05	3/2038 (0.1%)	0.92	3/2756 (0.1%)
1	B	0.95	0/2049	0.99	6/2771 (0.2%)
1	C	0.91	1/2038 (0.0%)	0.96	10/2756 (0.4%)
1	D	0.94	1/2044 (0.0%)	0.89	3/2766 (0.1%)
1	E	0.92	0/2038	0.91	4/2756 (0.1%)
1	F	0.95	0/2044	0.89	2/2766 (0.1%)
All	All	0.95	5/12251 (0.0%)	0.93	28/16571 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLU	CD-OE1	-12.01	1.12	1.25
1	A	155	GLU	CD-OE2	-11.95	1.12	1.25
1	D	80	VAL	CB-CG2	-7.82	1.36	1.52
1	A	150	VAL	CB-CG2	-5.52	1.41	1.52
1	C	140	ARG	CG-CD	-5.09	1.39	1.51

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	ARG	NE-CZ-NH1	-16.66	111.97	120.30
1	A	155	GLU	OE1-CD-OE2	-16.62	103.35	123.30
1	B	113	ARG	NE-CZ-NH2	16.02	128.31	120.30
1	C	94	ARG	NE-CZ-NH1	-13.33	113.63	120.30
1	C	94	ARG	NE-CZ-NH2	12.34	126.47	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2006	0	2028	81	0
1	B	2013	0	2035	76	1
1	C	2006	0	2028	61	2
1	D	2011	0	2034	40	0
1	E	2006	0	2028	85	1
1	F	2011	0	2034	49	1
2	A	47	0	0	3	0
2	B	52	0	0	8	0
2	C	56	0	0	9	0
2	D	46	0	0	3	1
2	E	29	0	0	4	0
2	F	19	0	0	4	0
All	All	12302	0	12187	335	4

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 14.

The worst 5 of 335 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:E:162:GLY:HA3	1:E:310:MET:CE	1.24	1.63
1:F:162:GLY:HA3	1:F:310:MET:CE	1.49	1.43
1:D:162:GLY:HA3	1:D:310:MET:CE	1.55	1.35
1:C:162:GLY:HA3	1:C:310:MET:CE	1.52	1.35
1:A:162:GLY:HA3	1:A:310:MET:CE	1.54	1.35

All (4) 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:E:218:ARG:NH2	1:F:207:ARG:NH2[1_556]	1.77	0.43
1:B:123:ARG:CG	1:B:270:ARG:NH1[1_454]	2.00	0.20
1:C:302:ARG:NH1	2:D:352:HOH:O[1_455]	2.09	0.11
1:C:123:ARG:CG	1:C:270:ARG:NH1[1_556]	2.11	0.09

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	255/291 (88%)	248 (97%)	6 (2%)	1 (0%)	34	38
1	B	256/291 (88%)	251 (98%)	4 (2%)	1 (0%)	34	38
1	C	255/291 (88%)	248 (97%)	5 (2%)	2 (1%)	19	20
1	D	258/291 (89%)	248 (96%)	9 (4%)	1 (0%)	34	38
1	E	255/291 (88%)	247 (97%)	7 (3%)	1 (0%)	34	38
1	F	258/291 (89%)	250 (97%)	7 (3%)	1 (0%)	34	38
All	All	1537/1746 (88%)	1492 (97%)	38 (2%)	7 (0%)	29	32

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	ASP
1	A	281	ASP
1	C	281	ASP
1	D	281	ASP
1	E	281	ASP

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	209/233 (90%)	190 (91%)	19 (9%)	9	8
1	B	210/233 (90%)	190 (90%)	20 (10%)	8	7
1	C	209/233 (90%)	189 (90%)	20 (10%)	8	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	209/233 (90%)	189 (90%)	20 (10%)	8 7
1	E	209/233 (90%)	187 (90%)	22 (10%)	7 6
1	F	209/233 (90%)	189 (90%)	20 (10%)	8 7
All	All	1255/1398 (90%)	1134 (90%)	121 (10%)	8 7

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	324	MET
1	F	217	VAL
1	D	246	PRO
1	F	211	SER
1	F	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	333	HIS
1	D	265	ASN
1	F	262	GLN
1	D	262	GLN
1	E	153	ASN

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 monosaccharides 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.