



wwPDB X-ray Structure Validation Summary Report

Jun 12, 2024 – 07:43 AM EDT

PDB ID : 2I00
Title : Crystal structure of acetyltransferase (GNAT family) from *Enterococcus faecalis*
Authors : Zhang, R.; Zhou, M.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-08-09
Resolution : 2.30 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  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) : 1.20.1
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

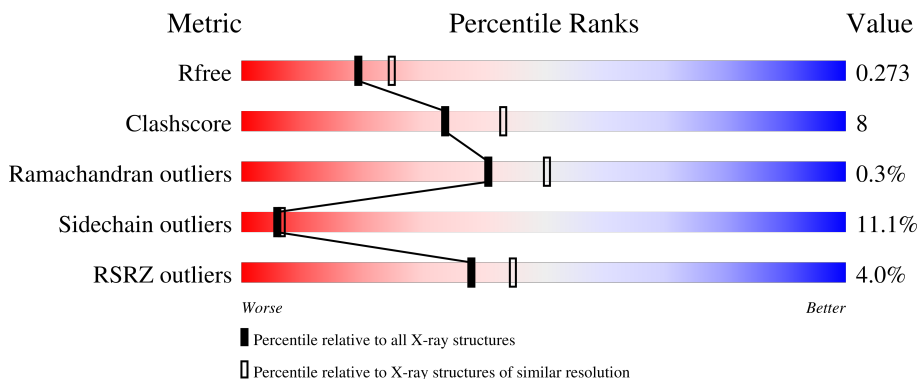
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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	406	 3% (poor fit), 74% (0 outliers), 19% (1 outlier), 2% (2 outliers), 2% (3+ outliers)
1	B	406	 7% (poor fit), 75% (0 outliers), 19% (1 outlier), 2% (2 outliers), 2% (3+ outliers)
1	C	406	 2% (poor fit), 73% (0 outliers), 20% (1 outlier), 5% (2 outliers), 2% (3+ outliers)
1	D	406	 2% (poor fit), 72% (0 outliers), 21% (1 outlier), 2% (2 outliers), 2% (3+ outliers)
1	E	406	 % (poor fit), 77% (0 outliers), 17% (1 outlier), 2% (2 outliers), 2% (3+ outliers)

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Mol	Chain	Length	Quality of chain
1	F	406	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into segments: a small red segment at the beginning labeled '7%', a large green segment labeled '76%', and a yellow segment at the end labeled '18%'. There are two small black dots at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20278 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 Acetyltransferase, GNAT family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3318	2157	539	611	11	0	0	0
1	B	396	3310	2151	538	610	11	0	0	0
1	C	398	3327	2162	541	613	11	0	0	0
1	D	396	3310	2151	538	610	11	0	0	0
1	E	396	3310	2151	538	610	11	0	0	0
1	F	398	3327	2162	541	613	11	0	0	0

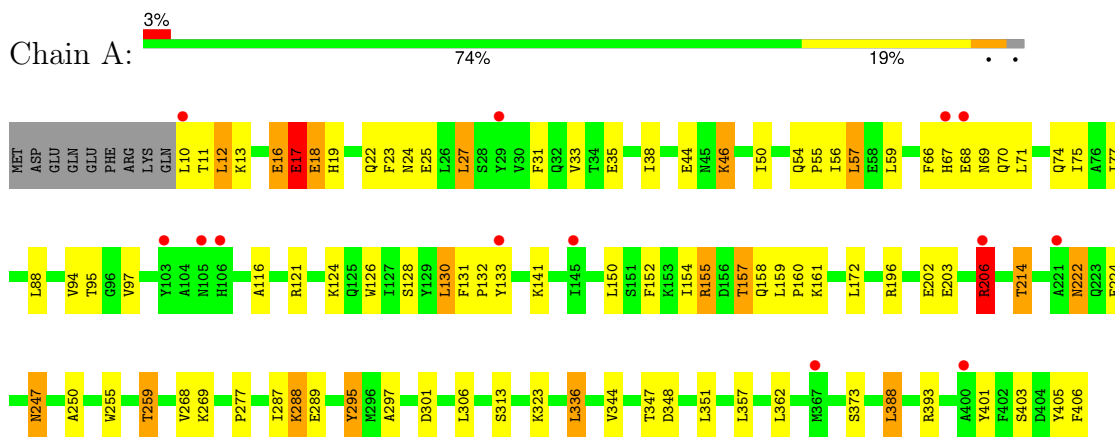
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	80	Total	O	0	0
			80	80		
2	C	48	Total	O	0	0
			48	48		
2	D	59	Total	O	0	0
			59	59		
2	E	57	Total	O	0	0
			57	57		
2	F	42	Total	O	0	0
			42	42		

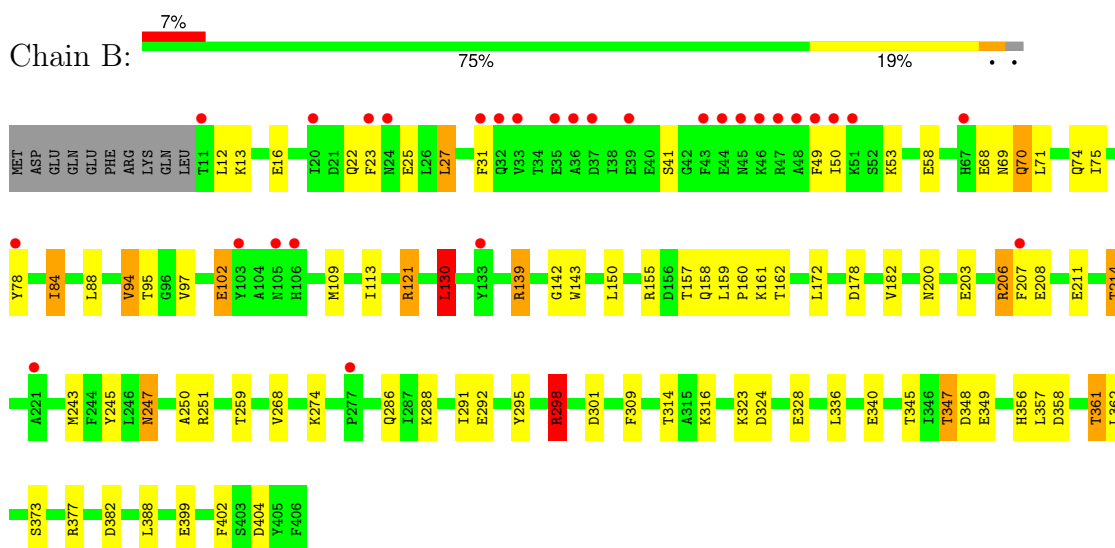
3 Residue-property plots [i](#)

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.

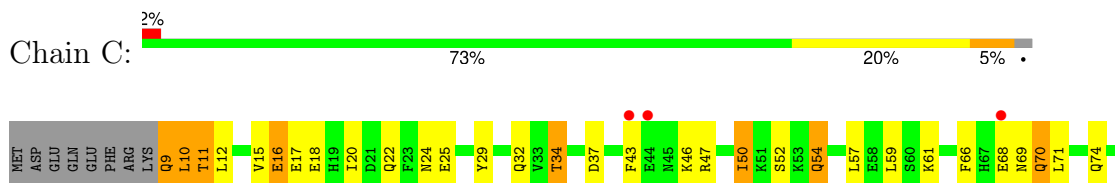
- Molecule 1: Acetyltransferase, GNAT family

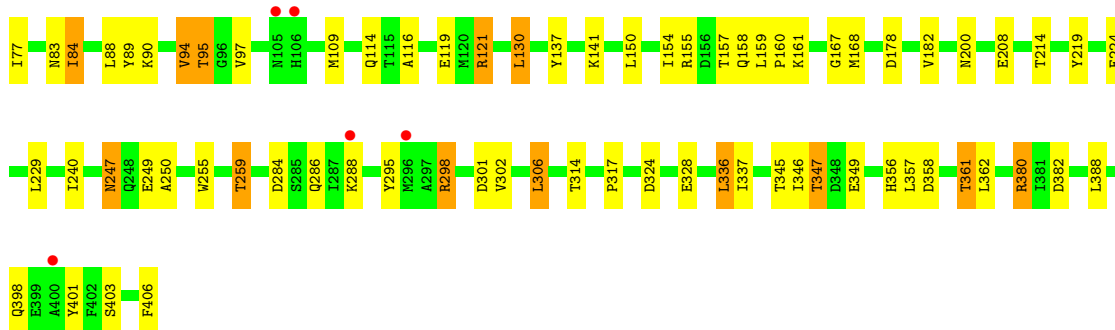


- Molecule 1: Acetyltransferase, GNAT family

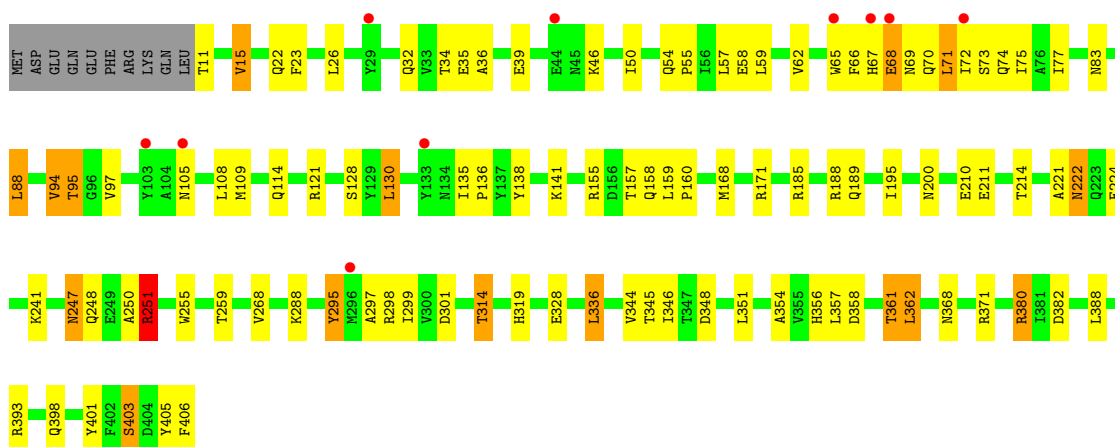


- Molecule 1: Acetyltransferase, GNAT family

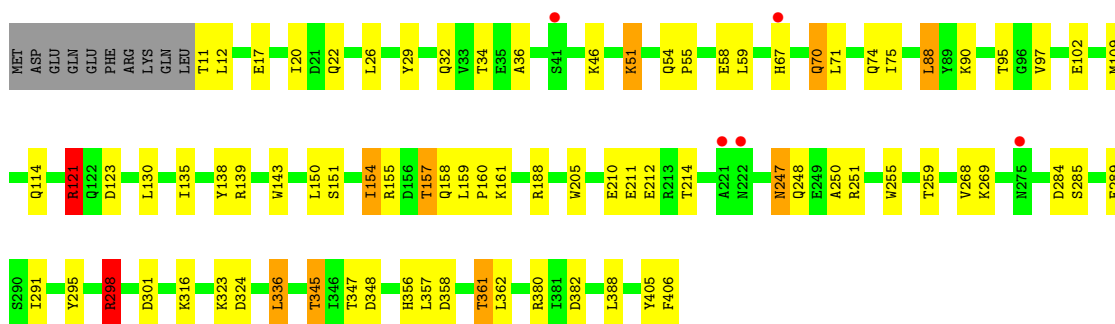
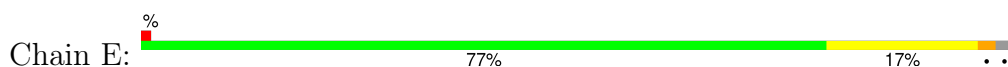




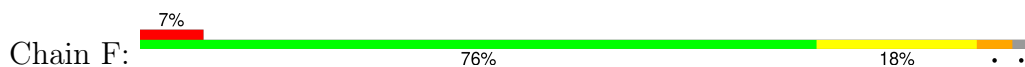
• Molecule 1: Acetyltransferase, GNAT family

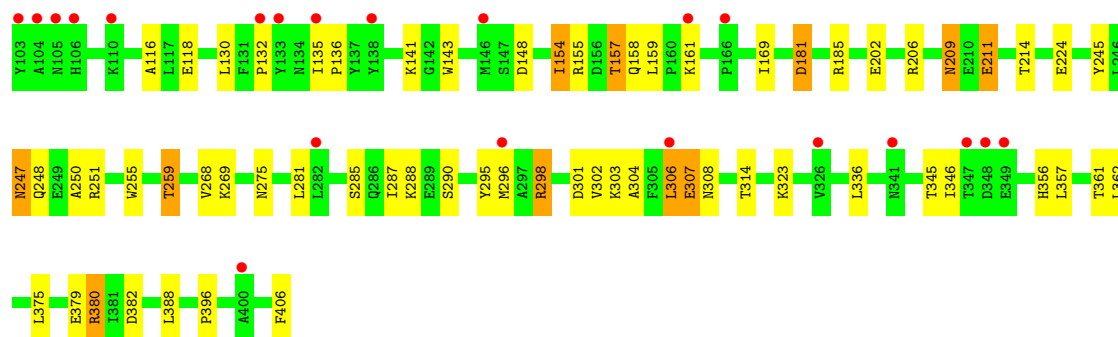


• Molecule 1: Acetyltransferase, GNAT family



• Molecule 1: Acetyltransferase, GNAT family





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.41Å 177.09Å 104.43Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	41.92 – 2.30 41.93 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.92-2.30) 92.3 (41.93-2.17)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.270 0.218 , 0.273	Depositor DCC
R_{free} test set	6834 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20278	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.74	0/3417	0.76	2/4642 (0.0%)
1	B	0.69	0/3409	0.76	4/4631 (0.1%)
1	C	0.66	0/3426	0.73	2/4654 (0.0%)
1	D	0.68	0/3409	0.73	2/4631 (0.0%)
1	E	0.68	0/3409	0.77	4/4631 (0.1%)
1	F	0.62	0/3426	0.68	0/4654
All	All	0.68	0/20496	0.74	14/27843 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	F	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	298	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	139	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	B	130	LEU	CA-CB-CG	7.16	131.76	115.30
1	E	298	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	298	ARG	NE-CZ-NH1	6.84	123.72	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	9	GLN	Peptide
1	E	67	HIS	Peptide
1	F	67	HIS	Peptide
1	F	68	GLU	Peptide

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	3318	0	3181	65	0
1	B	3310	0	3170	44	0
1	C	3327	0	3189	60	0
1	D	3310	0	3170	58	0
1	E	3310	0	3170	50	0
1	F	3327	0	3189	64	0
2	A	90	0	0	6	0
2	B	80	0	0	2	0
2	C	48	0	0	4	0
2	D	59	0	0	8	0
2	E	57	0	0	4	0
2	F	42	0	0	7	0
All	All	20278	0	19069	330	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 8.

The worst 5 of 330 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:18:GLU:HG2	2:A:487:HOH:O	1.41	1.18
1:F:13:LYS:NZ	1:F:68:GLU:OE1	1.85	1.09
1:F:11:THR:CG2	1:F:68:GLU:HG3	1.87	1.03
2:C:446:HOH:O	1:D:371:ARG:HG3	1.68	0.93
1:F:379:GLU:OE2	2:F:420:HOH:O	1.88	0.92

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	395/406 (97%)	382 (97%)	12 (3%)	1 (0%)	41	50
1	B	394/406 (97%)	377 (96%)	17 (4%)	0	100	100
1	C	396/406 (98%)	382 (96%)	13 (3%)	1 (0%)	41	50
1	D	394/406 (97%)	378 (96%)	13 (3%)	3 (1%)	19	23
1	E	394/406 (97%)	379 (96%)	14 (4%)	1 (0%)	41	50
1	F	396/406 (98%)	369 (93%)	27 (7%)	0	100	100
All	All	2369/2436 (97%)	2267 (96%)	96 (4%)	6 (0%)	41	50

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	D	222	ASN
1	C	10	LEU
1	D	68	GLU
1	D	210	GLU

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	355/364 (98%)	318 (90%)	37 (10%)	7	8
1	B	354/364 (97%)	311 (88%)	43 (12%)	5	5
1	C	356/364 (98%)	313 (88%)	43 (12%)	5	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	354/364 (97%)	316 (89%)	38 (11%)	6	7
1	E	354/364 (97%)	323 (91%)	31 (9%)	10	12
1	F	356/364 (98%)	312 (88%)	44 (12%)	4	5
All	All	2129/2184 (98%)	1893 (89%)	236 (11%)	6	7

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	336	LEU
1	F	288	LYS
1	D	211	GLU
1	F	259	THR
1	F	50	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	247	ASN
1	F	247	ASN
1	D	74	GLN
1	F	209	ASN
1	F	24	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](#)

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	397/406 (97%)	0.10	13 (3%) 46 53	22, 44, 79, 87	0
1	B	396/406 (97%)	0.23	29 (7%) 15 20	22, 47, 101, 116	0
1	C	398/406 (98%)	0.08	8 (2%) 65 71	23, 52, 69, 75	0
1	D	396/406 (97%)	0.11	10 (2%) 57 64	22, 51, 83, 88	0
1	E	396/406 (97%)	0.00	5 (1%) 77 81	23, 51, 68, 71	0
1	F	398/406 (98%)	0.49	30 (7%) 14 19	25, 62, 86, 96	0
All	All	2381/2436 (97%)	0.17	95 (3%) 38 45	22, 51, 82, 116	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ALA	6.2
1	B	44	GLU	5.7
1	B	50	ILE	5.4
1	B	49	PHE	5.2
1	B	33	VAL	5.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.