



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:01 AM UTC

PDB ID : 5DJW / pdb_00005djw
Title : Crystal structure of Family 31 alpha-glucosidase (BT_3299) from Bacteroides
thetaiotaomicron
Authors : Chaudet, M.M.; Rose, D.R.
Deposited on : 2015-09-02
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

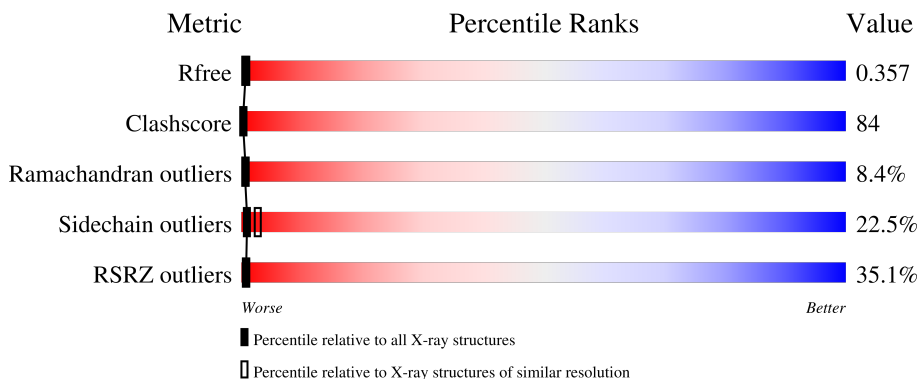
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	697	
1	B	697	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9139 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 Alpha-glucosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4569	2924	782	843	20			
1	B	587	Total	C	N	O	S	0	0	0
			4547	2913	783	831	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8A2K6
A	685	HIS	-	expression tag	UNP Q8A2K6
A	686	HIS	-	expression tag	UNP Q8A2K6
A	687	HIS	-	expression tag	UNP Q8A2K6
A	688	HIS	-	expression tag	UNP Q8A2K6
A	689	HIS	-	expression tag	UNP Q8A2K6
A	690	HIS	-	expression tag	UNP Q8A2K6
A	691	LEU	-	expression tag	UNP Q8A2K6
A	692	ARG	-	expression tag	UNP Q8A2K6
A	693	VAL	-	expression tag	UNP Q8A2K6
A	694	PRO	-	expression tag	UNP Q8A2K6
A	695	ARG	-	expression tag	UNP Q8A2K6
A	696	GLY	-	expression tag	UNP Q8A2K6
A	697	SER	-	expression tag	UNP Q8A2K6
B	1	MET	-	initiating methionine	UNP Q8A2K6
B	685	HIS	-	expression tag	UNP Q8A2K6
B	686	HIS	-	expression tag	UNP Q8A2K6
B	687	HIS	-	expression tag	UNP Q8A2K6
B	688	HIS	-	expression tag	UNP Q8A2K6
B	689	HIS	-	expression tag	UNP Q8A2K6
B	690	HIS	-	expression tag	UNP Q8A2K6
B	691	LEU	-	expression tag	UNP Q8A2K6
B	692	ARG	-	expression tag	UNP Q8A2K6
B	693	VAL	-	expression tag	UNP Q8A2K6
B	694	PRO	-	expression tag	UNP Q8A2K6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	695	ARG	-	expression tag	UNP Q8A2K6
B	696	GLY	-	expression tag	UNP Q8A2K6
B	697	SER	-	expression tag	UNP Q8A2K6

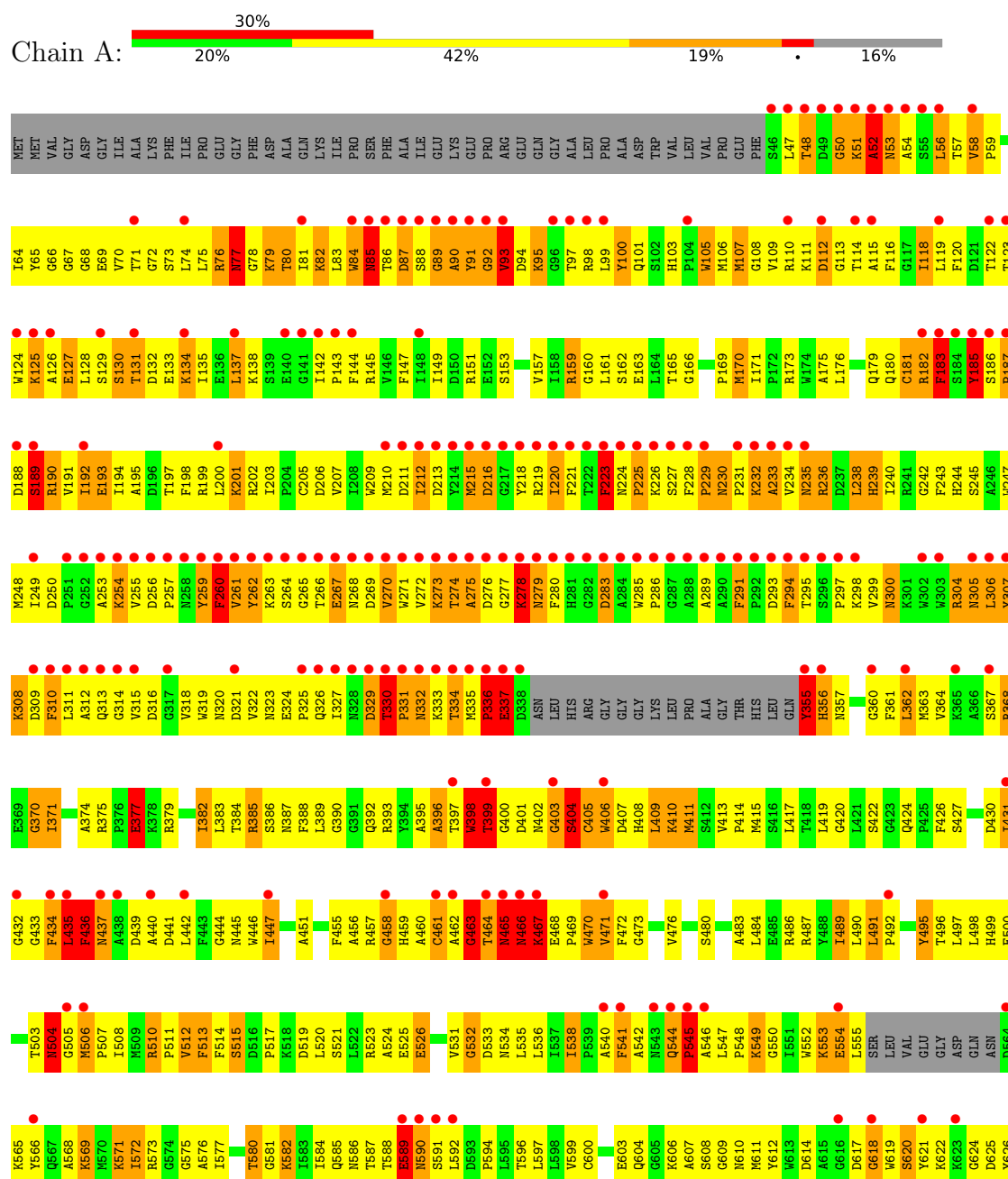
- Molecule 2 is water.

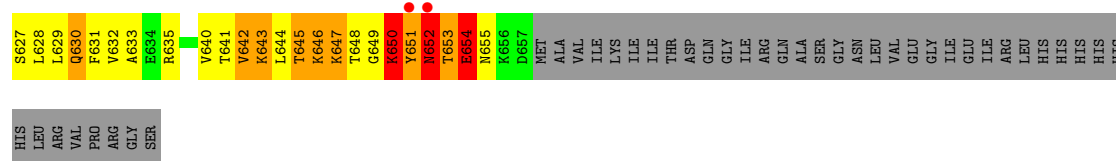
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	8	Total	O	0	0
			8	8		

3 Residue-property plots

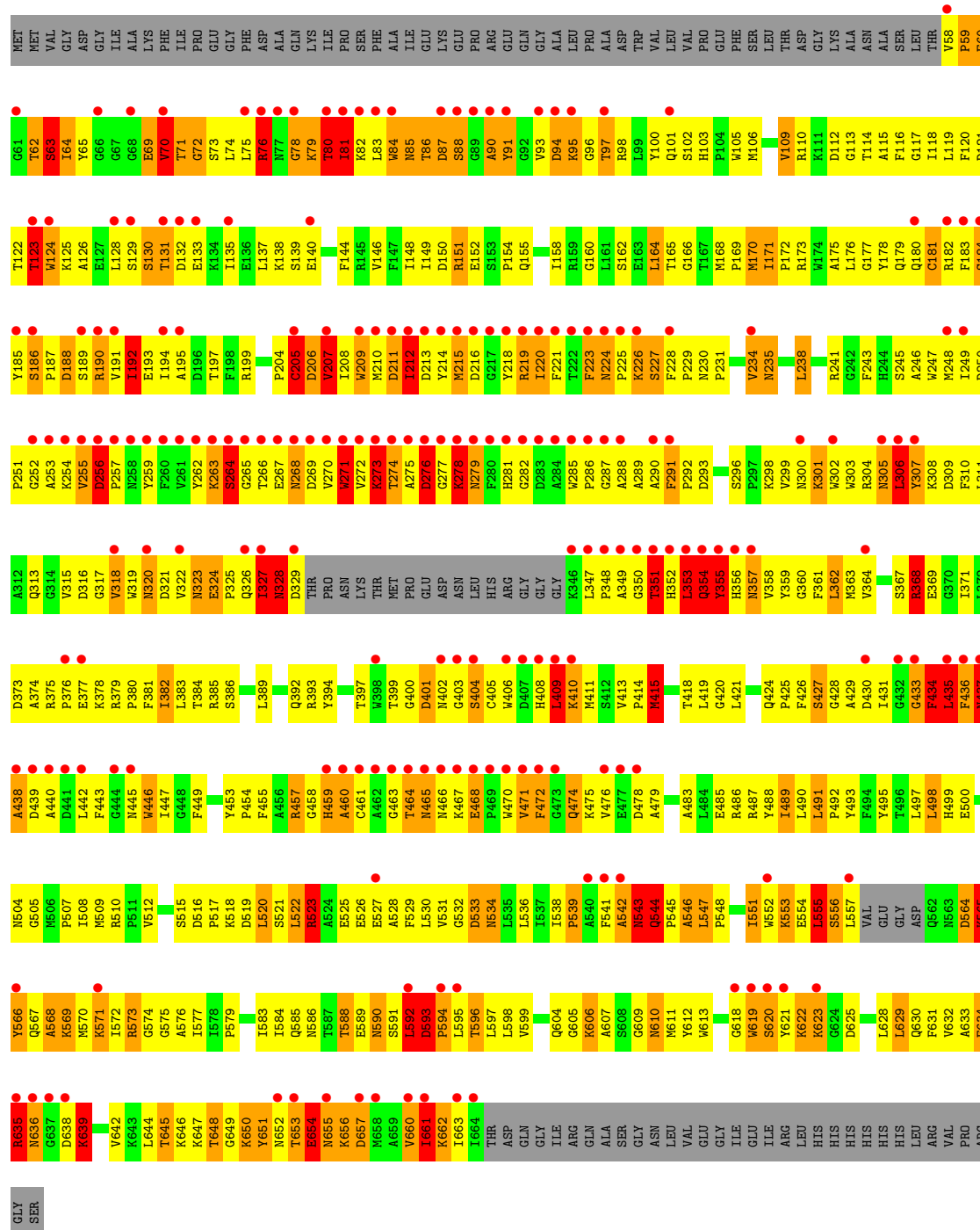
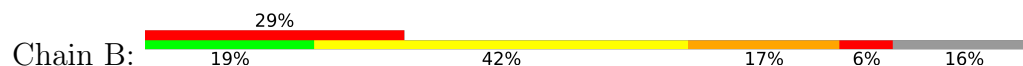
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-glucosidase II





• Molecule 1: Alpha-glucosidase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.26Å 74.86Å 94.43Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	47.55 – 2.70 47.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.55-2.70) 100.0 (47.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.330 , 0.390 0.314 , 0.357	Depositor DCC
R_{free} test set	1716 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 101.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	9139	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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	1.15	6/4694 (0.1%)	1.49	84/6370 (1.3%)
1	B	1.67	8/4672 (0.2%)	1.51	88/6342 (1.4%)
All	All	1.43	14/9366 (0.1%)	1.50	172/12712 (1.4%)

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	A	0	18
1	B	0	20
All	All	0	38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	PHE	C-N	-81.29	0.19	1.33
1	B	594	PRO	C-N	22.21	1.64	1.33
1	A	50	GLY	C-N	16.85	1.55	1.33
1	B	91	TYR	CA-C	-7.58	1.42	1.52
1	B	597	LEU	C-O	-6.85	1.15	1.24

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	GLY	N-CA-C	-22.86	87.19	112.33
1	A	50	GLY	O-C-N	-22.62	93.30	122.70
1	B	326	GLN	CA-C-N	19.44	156.97	121.97
1	B	326	GLN	C-N-CA	19.44	156.97	121.97
1	A	309	ASP	CB-CA-C	-18.14	82.94	111.06

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	TYR	Peptide
1	A	235	ASN	Peptide
1	A	259	TYR	Peptide
1	A	50	GLY	Mainchain
1	A	77	ASN	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	4569	0	4348	758	5
1	B	4547	0	4344	734	1
2	A	15	0	0	8	1
2	B	8	0	0	3	0
All	All	9139	0	8692	1488	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 84.

The worst 5 of 1488 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:84:TRP:CD1	1:A:85:ASN:H	1.12	1.64
1:A:272:VAL:CG1	1:A:336:PRO:HG2	1.40	1.51
1:B:553:LYS:CB	1:B:572:ILE:HG22	1.36	1.50
1:B:256:ASP:O	1:B:259:TYR:CD2	1.73	1.40
1:B:552:TRP:CB	1:B:571:LYS:HE2	1.49	1.39

The worst 5 of 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:A:554:GLU:OE1	1:A:653:THR:OG1[2_557]	0.80	1.40
1:A:521:SER:OG	1:B:377:GLU:CB[2_557]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLU:CD	1:A:653:THR:OG1[2_557]	1.72	0.48
1:A:554:GLU:OE2	1:A:652:ASN:O[2_557]	1.90	0.30
1:A:554:GLU:OE1	1:A:653:THR:CB[2_557]	1.98	0.22

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	582/697 (84%)	471 (81%)	66 (11%)	45 (8%)	1	1
1	B	581/697 (83%)	464 (80%)	64 (11%)	53 (9%)	0	0
All	All	1163/1394 (83%)	935 (80%)	130 (11%)	98 (8%)	0	1

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	TRP
1	A	87	ASP
1	A	90	ALA
1	A	93	VAL
1	A	112	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	464/579 (80%)	360 (78%)	104 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	462/579 (80%)	358 (78%)	104 (22%)	1	3
All	All	926/1158 (80%)	718 (78%)	208 (22%)	1	3

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	ASP
1	B	306	LEU
1	B	646	LYS
1	B	123	THR
1	B	219	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	352	HIS
1	B	474	GLN
1	B	466	ASN
1	B	543	ASN
1	A	328	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	594:PRO	C	595:LEU	N	1.64
1	B	434:PHE	C	435:LEU	N	0.19

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	588/697 (84%)	1.66	211 (35%) 1 0	10, 42, 120, 162	0
1	B	587/697 (84%)	1.59	202 (34%) 1 1	11, 43, 110, 166	0
All	All	1175/1394 (84%)	1.62	413 (35%) 1 1	10, 42, 117, 166	0

The worst 5 of 413 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	8.4
1	A	264	SER	7.5
1	A	261	VAL	7.5
1	B	265	GLY	7.0
1	A	544	GLN	6.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.