



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 PM GMT

PDB ID : 4R27
Title : Crystal structure of beta-glycosidase BGL167
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Deposited on : 2014-08-09
Resolution : 2.03 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

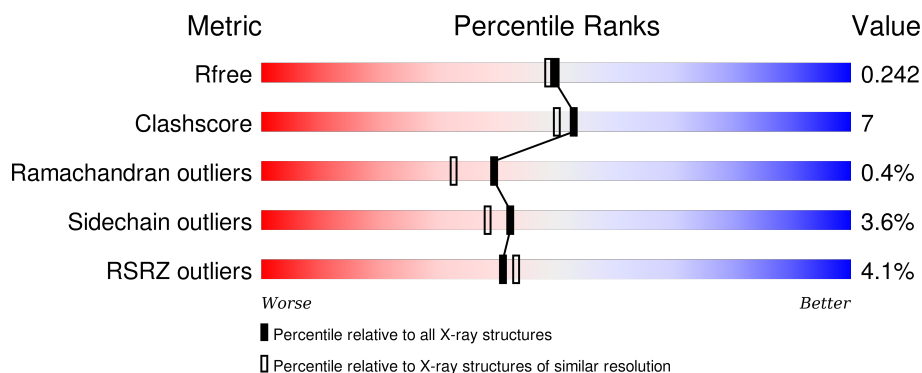
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.03 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}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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. 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	434	 4% 80% 14% • •
1	B	434	 4% 82% 9% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6482 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 Glycoside hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3241	2055	574	603	9			
1	B	407	Total	C	N	O	S	0	0	0
			3173	2013	562	589	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	LYS	-	EXPRESSION TAG	UNP L0ELG0
A	435	LEU	-	EXPRESSION TAG	UNP L0ELG0
A	436	ALA	-	EXPRESSION TAG	UNP L0ELG0
A	437	ALA	-	EXPRESSION TAG	UNP L0ELG0
A	438	ALA	-	EXPRESSION TAG	UNP L0ELG0
A	439	LEU	-	EXPRESSION TAG	UNP L0ELG0
A	440	GLU	-	EXPRESSION TAG	UNP L0ELG0
A	441	HIS	-	EXPRESSION TAG	UNP L0ELG0
A	442	HIS	-	EXPRESSION TAG	UNP L0ELG0
A	443	HIS	-	EXPRESSION TAG	UNP L0ELG0
A	444	HIS	-	EXPRESSION TAG	UNP L0ELG0
A	445	HIS	-	EXPRESSION TAG	UNP L0ELG0
A	446	HIS	-	EXPRESSION TAG	UNP L0ELG0
B	434	LYS	-	EXPRESSION TAG	UNP L0ELG0
B	435	LEU	-	EXPRESSION TAG	UNP L0ELG0
B	436	ALA	-	EXPRESSION TAG	UNP L0ELG0
B	437	ALA	-	EXPRESSION TAG	UNP L0ELG0
B	438	ALA	-	EXPRESSION TAG	UNP L0ELG0
B	439	LEU	-	EXPRESSION TAG	UNP L0ELG0
B	440	GLU	-	EXPRESSION TAG	UNP L0ELG0
B	441	HIS	-	EXPRESSION TAG	UNP L0ELG0
B	442	HIS	-	EXPRESSION TAG	UNP L0ELG0
B	443	HIS	-	EXPRESSION TAG	UNP L0ELG0
B	444	HIS	-	EXPRESSION TAG	UNP L0ELG0
B	445	HIS	-	EXPRESSION TAG	UNP L0ELG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	HIS	-	EXPRESSION TAG	UNP L0ELG0

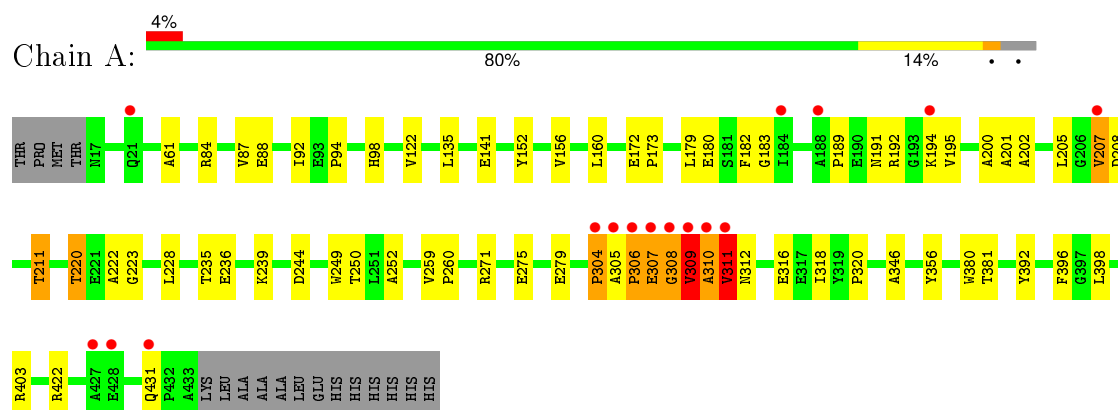
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	18	Total O 18 18	0	0

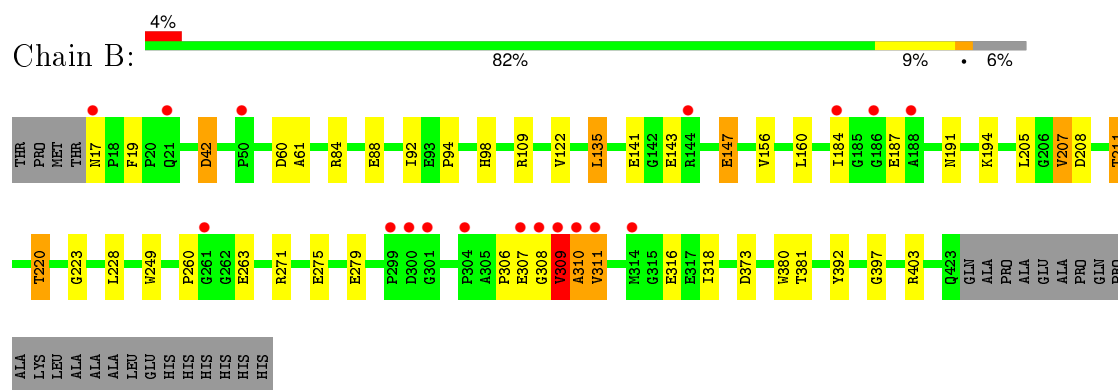
3 Residue-property plots [i](#)

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: Glycoside hydrolase



• Molecule 1: Glycoside hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.50 Å 146.94 Å 53.04 Å 90.00° 101.99° 90.00°	Depositor
Resolution (Å)	23.20 – 2.03 23.20 – 2.03	Depositor EDS
% Data completeness (in resolution range)	97.3 (23.20-2.03) 97.3 (23.20-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.03 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.239 0.200 , 0.242	Depositor DCC
R_{free} test set	2295 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 45460 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6482	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.88	0/3334	0.95	8/4547 (0.2%)
1	B	0.89	0/3263	1.00	15/4447 (0.3%)
All	All	0.89	0/6597	0.98	23/8994 (0.3%)

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	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	VAL	CB-CA-C	-13.15	86.42	111.40
1	B	403	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	B	309	VAL	CB-CA-C	9.01	128.52	111.40
1	B	310	ALA	CB-CA-C	7.52	121.39	110.10
1	A	304	PRO	N-CA-C	-7.33	93.05	112.10
1	B	309	VAL	C-N-CA	7.24	139.80	121.70
1	A	310	ALA	N-CA-C	-7.06	91.94	111.00
1	A	310	ALA	N-CA-CB	6.40	119.06	110.10
1	B	310	ALA	N-CA-CB	6.30	118.92	110.10
1	B	403	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	403	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	307	GLU	N-CA-C	-5.65	95.74	111.00
1	B	109	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	147	GLU	OE1-CD-OE2	-5.53	116.67	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	VAL	CB-CA-C	5.50	121.85	111.40
1	B	373	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	304	PRO	CB-CA-C	5.32	125.29	112.00
1	A	244	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	60	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	109	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	311	VAL	N-CA-C	-5.11	97.21	111.00
1	B	42	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	422	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	PRO	Peptide
1	A	306	PRO	Peptide
1	A	308	GLY	Peptide
1	A	311	VAL	Peptide
1	B	309	VAL	Peptide

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	3241	0	3079	56	0
1	B	3173	0	3016	26	0
2	A	50	0	0	1	0
2	B	18	0	0	0	0
All	All	6482	0	6095	82	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 7.

All (82) 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:310:ALA:HB1	1:A:312:ASN:N	1.52	1.23
1:A:310:ALA:HB2	1:A:318:ILE:HG13	1.29	1.11
1:A:310:ALA:HB1	1:A:312:ASN:H	1.20	0.96
1:A:220:THR:HG22	1:A:223:GLY:H	1.33	0.92
1:A:310:ALA:CB	1:A:318:ILE:HG13	2.04	0.88
1:A:309:VAL:O	1:A:309:VAL:HG22	1.74	0.86
1:A:180:GLU:O	1:A:183:GLY:HA3	1.76	0.85
1:A:310:ALA:HB2	1:A:318:ILE:CG1	2.07	0.85
1:A:179:LEU:O	1:A:183:GLY:HA2	1.76	0.85
1:B:220:THR:HG22	1:B:223:GLY:H	1.49	0.78
1:A:310:ALA:HB3	1:A:316:GLU:O	1.88	0.74
1:A:310:ALA:HB1	1:A:311:VAL:C	2.11	0.71
1:A:208:ASP:O	1:A:211:THR:HG22	1.94	0.67
1:A:308:GLY:O	1:A:309:VAL:HG12	1.96	0.65
1:A:211:THR:HG23	2:A:529:HOH:O	1.96	0.64
1:B:310:ALA:HB3	1:B:318:ILE:HD12	1.79	0.63
1:A:84:ARG:HA	1:A:122:VAL:O	1.99	0.63
1:A:191:ASN:HB3	1:A:194:LYS:CE	2.29	0.63
1:B:141:GLU:OE2	1:B:220:THR:HG21	1.98	0.62
1:B:156:VAL:HG23	1:B:160:LEU:HD11	1.82	0.61
1:A:310:ALA:CB	1:A:316:GLU:O	2.50	0.60
1:B:310:ALA:CB	1:B:318:ILE:HD12	2.33	0.58
1:B:61:ALA:HA	1:B:392:TYR:OH	2.05	0.57
1:A:94:PRO:HD2	1:A:98:HIS:O	2.04	0.57
1:A:311:VAL:O	1:A:311:VAL:HG23	2.06	0.56
1:A:220:THR:HG22	1:A:223:GLY:N	2.14	0.56
1:A:310:ALA:CB	1:A:312:ASN:H	2.07	0.56
1:A:202:ALA:HB1	1:A:207:VAL:O	2.06	0.56
1:B:17:ASN:HB3	1:B:19:PHE:H	1.71	0.56
1:A:275:GLU:O	1:A:279:GLU:HG3	2.06	0.55
1:A:191:ASN:HB3	1:A:194:LYS:HE2	1.89	0.54
1:A:309:VAL:O	1:A:318:ILE:HB	2.07	0.54
1:A:309:VAL:HG13	1:A:318:ILE:H	1.73	0.53
1:A:307:GLU:O	1:A:308:GLY:C	2.44	0.53
1:A:309:VAL:HG11	1:A:318:ILE:O	2.09	0.52
1:A:207:VAL:HG22	1:A:211:THR:HG21	1.91	0.52
1:A:380:TRP:CD2	1:A:381:THR:HB	2.44	0.52
1:A:160:LEU:C	1:A:160:LEU:HD12	2.30	0.51
1:A:172:GLU:HG2	1:A:252:ALA:HB2	1.93	0.51
1:B:94:PRO:HD2	1:B:98:HIS:O	2.11	0.50
1:B:271:ARG:HD2	1:B:275:GLU:HB2	1.92	0.50
1:B:208:ASP:O	1:B:211:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ALA:HB2	1:A:318:ILE:N	2.27	0.50
1:A:310:ALA:HB2	1:A:318:ILE:CB	2.43	0.49
1:B:84:ARG:HA	1:B:122:VAL:O	2.12	0.49
1:A:172:GLU:CG	1:A:252:ALA:HB2	2.43	0.49
1:A:141:GLU:OE2	1:A:220:THR:HG21	2.13	0.48
1:B:306:PRO:C	1:B:308:GLY:N	2.66	0.48
1:B:220:THR:HG22	1:B:223:GLY:N	2.24	0.47
1:A:173:PRO:HD2	1:A:250:THR:O	2.15	0.47
1:A:309:VAL:HG13	1:A:309:VAL:O	2.05	0.46
1:A:200:ALA:O	1:A:201:ALA:C	2.53	0.46
1:A:87:VAL:HG23	1:A:152:TYR:OH	2.15	0.46
1:B:42:ASP:HB2	1:B:135:LEU:HD22	1.97	0.46
1:B:311:VAL:HG22	1:B:316:GLU:O	2.15	0.46
1:B:271:ARG:NH2	1:B:279:GLU:OE1	2.49	0.45
1:B:260:PRO:HA	1:B:263:GLU:OE2	2.16	0.45
1:B:306:PRO:O	1:B:308:GLY:N	2.49	0.45
1:A:380:TRP:CE2	1:A:381:THR:HB	2.51	0.45
1:A:235:THR:O	1:A:239:LYS:HG2	2.17	0.45
1:A:189:PRO:HA	1:A:192:ARG:HD2	1.99	0.45
1:A:182:PHE:N	1:A:183:GLY:HA2	2.31	0.45
1:B:187:GLU:CD	1:B:187:GLU:H	2.20	0.45
1:A:320:PRO:HB3	1:A:356:TYR:CE1	2.53	0.44
1:A:61:ALA:HA	1:A:392:TYR:OH	2.17	0.44
1:B:191:ASN:O	1:B:194:LYS:HG2	2.17	0.44
1:B:381:THR:O	1:B:397:GLY:HA2	2.18	0.43
1:A:398:LEU:HD12	1:A:398:LEU:N	2.34	0.43
1:A:88:GLU:O	1:A:92:ILE:HG12	2.20	0.42
1:A:220:THR:CG2	1:A:223:GLY:H	2.17	0.42
1:A:346:ALA:HB2	1:A:396:PHE:CZ	2.55	0.42
1:A:180:GLU:C	1:A:183:GLY:HA3	2.40	0.42
1:B:207:VAL:HG22	1:B:211:THR:HG21	2.02	0.42
1:B:380:TRP:CD2	1:B:381:THR:HB	2.55	0.41
1:A:191:ASN:HB3	1:A:194:LYS:HE3	2.01	0.41
1:B:184:ILE:CG2	1:B:184:ILE:O	2.68	0.41
1:B:147:GLU:OE2	1:B:147:GLU:N	2.48	0.41
1:A:259:VAL:HB	1:A:260:PRO:CD	2.51	0.41
1:A:220:THR:CG2	1:A:222:ALA:HB3	2.51	0.41
1:B:88:GLU:O	1:B:92:ILE:HG12	2.21	0.40
1:A:156:VAL:HG23	1:A:160:LEU:HD11	2.04	0.40
1:A:182:PHE:N	1:A:183:GLY:CA	2.83	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	415/434 (96%)	401 (97%)	12 (3%)	2 (0%)	34	26
1	B	405/434 (93%)	391 (96%)	13 (3%)	1 (0%)	52	47
All	All	820/868 (94%)	792 (97%)	25 (3%)	3 (0%)	39	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	VAL
1	B	309	VAL
1	A	305	ALA

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	324/338 (96%)	310 (96%)	14 (4%)	35	30
1	B	318/338 (94%)	309 (97%)	9 (3%)	51	49
All	All	642/676 (95%)	619 (96%)	23 (4%)	42	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	195	VAL
1	A	205	LEU

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Mol	Chain	Res	Type
1	A	207	VAL
1	A	211	THR
1	A	220	THR
1	A	228	LEU
1	A	236	GLU
1	A	249	TRP
1	A	271	ARG
1	A	306	PRO
1	A	307	GLU
1	A	311	VAL
1	A	431	GLN
1	B	135	LEU
1	B	143	GLU
1	B	205	LEU
1	B	207	VAL
1	B	211	THR
1	B	220	THR
1	B	228	LEU
1	B	249	TRP
1	B	309	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	127	HIS
1	A	225	ASN
1	A	268	GLN
1	A	302	HIS
1	B	203	GLN
1	B	268	GLN

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 [i](#)

There are no carbohydrates 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

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	417/434 (96%)	0.07	16 (3%) 44 46	13, 22, 45, 83	0
1	B	407/434 (93%)	-0.08	18 (4%) 38 40	13, 19, 39, 72	0
All	All	824/868 (94%)	-0.01	34 (4%) 41 43	13, 21, 41, 83	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	VAL	14.7
1	A	310	ALA	7.3
1	B	310	ALA	6.8
1	B	309	VAL	5.9
1	A	308	GLY	5.4
1	B	17	ASN	4.8
1	B	308	GLY	4.8
1	A	311	VAL	4.2
1	B	311	VAL	4.0
1	B	307	GLU	4.0
1	A	184	ILE	3.8
1	A	305	ALA	3.6
1	B	50	PRO	3.3
1	B	184	ILE	3.0
1	A	427	ALA	3.0
1	A	188	ALA	2.9
1	A	428	GLU	2.8
1	B	301	GLY	2.7
1	B	144	ARG	2.6
1	B	299	PRO	2.5
1	B	300	ASP	2.5
1	A	306	PRO	2.4
1	B	314	MET	2.4
1	B	21	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	304	PRO	2.4
1	B	304	PRO	2.3
1	A	194	LYS	2.3
1	A	21	GLN	2.3
1	A	207	VAL	2.2
1	A	431	GLN	2.1
1	A	307	GLU	2.1
1	B	186	GLY	2.1
1	B	261	GLY	2.1
1	B	188	ALA	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 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.