



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:47 PM BST

PDB ID : 6MOY  
Title : Crystal structure of the E257A mutant of B1Man5B in complex with GlcNAc (co-crystallization)  
Authors : Lorigzolla-Cordeiro, R.; Giuseppe, P.O.; Murakami, M.T.  
Deposited on : 2018-10-05  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

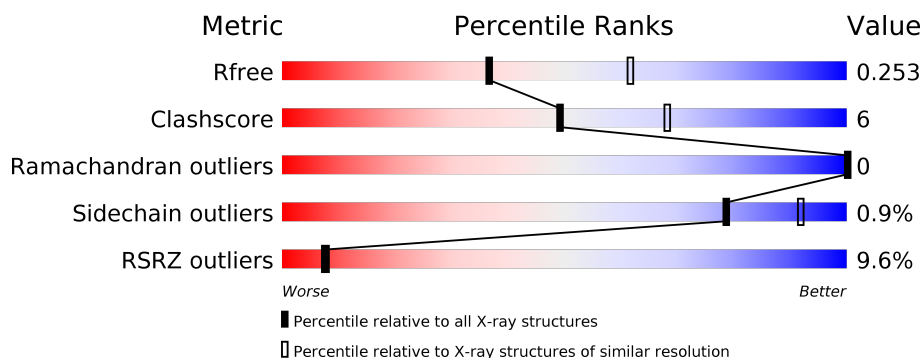
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	449	<div> <div>11%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>6%</div> </div> </div>
1	B	449	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6702 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 B1Man5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	1	0
			3313	2106	585	607	15			
1	B	426	Total	C	N	O	S	0	0	0
			3324	2112	586	611	15			

There are 42 discrepancies between the modelled and reference sequences:

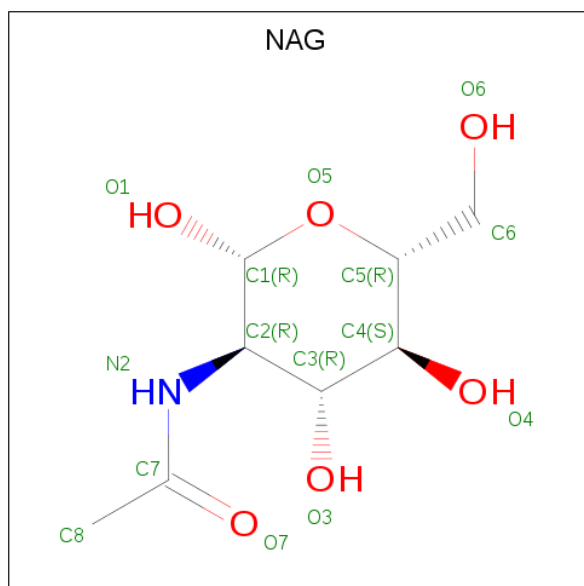
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B3DQP5
A	-18	GLY	-	expression tag	UNP B3DQP5
A	-17	SER	-	expression tag	UNP B3DQP5
A	-16	SER	-	expression tag	UNP B3DQP5
A	-15	HIS	-	expression tag	UNP B3DQP5
A	-14	HIS	-	expression tag	UNP B3DQP5
A	-13	HIS	-	expression tag	UNP B3DQP5
A	-12	HIS	-	expression tag	UNP B3DQP5
A	-11	HIS	-	expression tag	UNP B3DQP5
A	-10	HIS	-	expression tag	UNP B3DQP5
A	-9	SER	-	expression tag	UNP B3DQP5
A	-8	SER	-	expression tag	UNP B3DQP5
A	-7	GLY	-	expression tag	UNP B3DQP5
A	-6	LEU	-	expression tag	UNP B3DQP5
A	-5	VAL	-	expression tag	UNP B3DQP5
A	-4	PRO	-	expression tag	UNP B3DQP5
A	-3	ARG	-	expression tag	UNP B3DQP5
A	-2	GLY	-	expression tag	UNP B3DQP5
A	-1	SER	-	expression tag	UNP B3DQP5
A	0	HIS	-	expression tag	UNP B3DQP5
A	257	ALA	GLU	engineered mutation	UNP B3DQP5
B	-19	MET	-	initiating methionine	UNP B3DQP5
B	-18	GLY	-	expression tag	UNP B3DQP5
B	-17	SER	-	expression tag	UNP B3DQP5
B	-16	SER	-	expression tag	UNP B3DQP5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP B3DQP5
B	-14	HIS	-	expression tag	UNP B3DQP5
B	-13	HIS	-	expression tag	UNP B3DQP5
B	-12	HIS	-	expression tag	UNP B3DQP5
B	-11	HIS	-	expression tag	UNP B3DQP5
B	-10	HIS	-	expression tag	UNP B3DQP5
B	-9	SER	-	expression tag	UNP B3DQP5
B	-8	SER	-	expression tag	UNP B3DQP5
B	-7	GLY	-	expression tag	UNP B3DQP5
B	-6	LEU	-	expression tag	UNP B3DQP5
B	-5	VAL	-	expression tag	UNP B3DQP5
B	-4	PRO	-	expression tag	UNP B3DQP5
B	-3	ARG	-	expression tag	UNP B3DQP5
B	-2	GLY	-	expression tag	UNP B3DQP5
B	-1	SER	-	expression tag	UNP B3DQP5
B	0	HIS	-	expression tag	UNP B3DQP5
B	257	ALA	GLU	engineered mutation	UNP B3DQP5

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

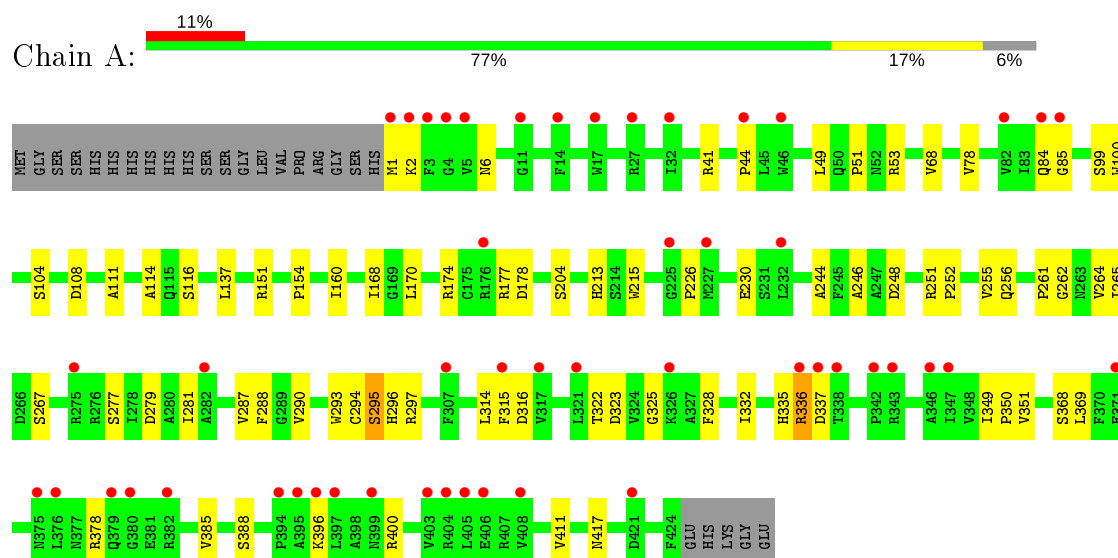
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	14	Total 14	O 14	0	0

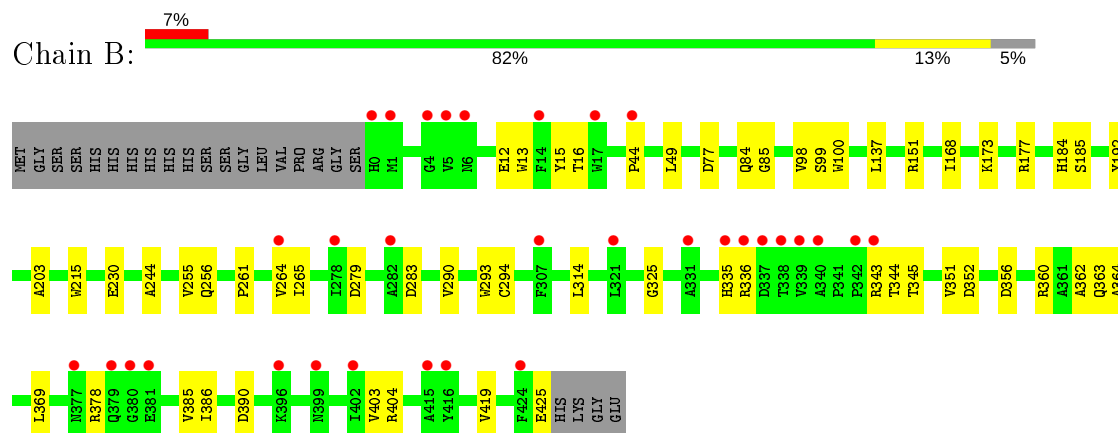
### 3 Residue-property plots [i](#)

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: B1Man5B



#### • Molecule 1: B1Man5B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.83Å 100.88Å 171.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.49 – 2.50 43.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.49-2.50) 96.3 (43.49-2.50)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.226 , 0.254 0.226 , 0.253	Depositor DCC
$R_{free}$ test set	2186 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.26	0/3413	0.47	0/4659
1	B	0.26	0/3422	0.48	0/4672
All	All	0.26	0/6835	0.47	0/9331

There are no bond length outliers.

There are no bond angle outliers.

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	3313	0	3179	47	0
1	B	3324	0	3179	34	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	21	0	0	0	0
3	B	14	0	0	0	0
All	All	6702	0	6388	77	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 6.

All (77) 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:B:12:GLU:HB2	1:B:16:THR:HG22	1.45	0.94
1:A:99:SER:OG	1:A:100:TRP:N	2.21	0.74
1:B:99:SER:OG	1:B:100:TRP:N	2.22	0.71
1:A:368:SER:HB3	1:A:411:VAL:HG22	1.72	0.69
1:A:68:VAL:HG22	1:A:78:VAL:HG21	1.78	0.66
1:B:283:ASP:O	1:B:343:ARG:NH1	2.30	0.64
1:B:230:GLU:OE2	1:B:378:ARG:NH2	2.31	0.63
1:B:344:THR:HB	1:B:403:VAL:HG22	1.82	0.60
1:A:264:VAL:HG23	1:A:265:ILE:HG12	1.85	0.59
1:A:230:GLU:OE1	1:A:378:ARG:NH2	2.36	0.59
1:A:295:SER:OG	1:A:296:HIS:ND1	2.36	0.58
1:B:314:LEU:HD22	1:B:325:GLY:HA2	1.86	0.58
1:B:13:TRP:O	1:B:16:THR:HG23	2.03	0.58
1:A:174:ARG:CZ	1:A:177:ARG:HH12	2.18	0.57
1:B:215:TRP:HE3	1:B:261:PRO:HG3	1.69	0.56
1:B:244:ALA:HB2	1:B:385:VAL:HG12	1.88	0.55
1:B:351:VAL:HG12	1:B:352:ASP:O	2.08	0.53
1:A:350:PRO:HA	1:A:388:SER:HB3	1.89	0.53
1:B:279:ASP:OD1	1:B:335:HIS:NE2	2.40	0.52
1:B:255:VAL:HG23	1:B:290:VAL:HA	1.92	0.52
1:A:137:LEU:HD11	1:A:168:ILE:HG13	1.90	0.52
1:A:151:ARG:NH2	1:B:151:ARG:HG2	2.24	0.52
1:A:226:PRO:HB3	1:A:264:VAL:O	2.10	0.52
1:A:279:ASP:OD1	1:A:335:HIS:NE2	2.42	0.51
1:A:297:ARG:HD2	1:A:316:ASP:HA	1.92	0.51
1:A:396:LYS:HE2	1:A:400:ARG:HD2	1.94	0.50
1:A:244:ALA:HB2	1:A:385:VAL:HG12	1.94	0.50
1:A:252:PRO:HB2	1:A:288:PHE:HB2	1.94	0.49
1:B:137:LEU:HD11	1:B:168:ILE:HG13	1.95	0.48
1:B:44:PRO:HB2	1:B:49:LEU:HD11	1.95	0.48
1:A:215:TRP:HE3	1:A:261:PRO:HG3	1.79	0.48
1:B:84:GLN:HA	1:B:85:GLY:HA3	1.62	0.48
1:A:204:SER:HB3	1:A:246:ALA:HB2	1.96	0.47
1:A:349:ILE:O	1:A:351:VAL:HG13	2.13	0.47
1:A:104:SER:HB2	1:A:154:PRO:HD2	1.97	0.47
1:A:116:SER:HB3	1:A:170:LEU:HD11	1.97	0.47
1:A:255:VAL:HG23	1:A:290:VAL:HA	1.97	0.46
1:A:328:PHE:O	1:A:332:ILE:HG13	2.16	0.46
1:B:352:ASP:OD2	1:B:356:ASP:HB2	2.16	0.46
1:B:264:VAL:HG23	1:B:265:ILE:HG13	1.97	0.46
1:A:296:HIS:CD2	1:A:315:PHE:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ALA:HB1	1:B:369:LEU:HD23	1.98	0.46
1:A:277:SER:O	1:A:281:ILE:HG13	2.15	0.45
1:B:184:HIS:CE1	1:B:203:ALA:HA	2.51	0.45
1:A:314:LEU:HD22	1:A:325:GLY:HA2	1.99	0.45
1:A:84:GLN:HA	1:A:85:GLY:HA3	1.64	0.45
1:B:192:TYR:CD1	1:B:364:ALA:HA	2.51	0.45
1:B:419:VAL:HG21	1:B:425:GLU:HG2	1.99	0.45
1:A:177:ARG:NH1	1:A:178:ASP:OD1	2.49	0.44
1:A:293:TRP:HA	1:A:294:CYS:HA	1.63	0.44
1:A:2:LYS:HE3	1:A:288:PHE:CE1	2.52	0.44
1:A:53:ARG:HG3	1:A:114:ALA:HB2	1.99	0.44
1:A:336:ARG:NH1	1:A:337:ASP:OD1	2.50	0.44
1:A:349:ILE:HG12	1:A:369:LEU:HD13	1.99	0.44
1:A:151:ARG:HG3	1:B:151:ARG:HH21	1.82	0.43
1:B:255:VAL:HG23	1:B:255:VAL:O	2.19	0.43
1:B:98:VAL:HG13	1:B:151:ARG:HH22	1.84	0.43
1:A:248:ASP:HB3	1:A:251:ARG:HB2	2.01	0.43
1:A:322:THR:HG22	1:A:323:ASP:N	2.34	0.42
1:B:293:TRP:HA	1:B:294:CYS:HA	1.69	0.42
1:B:386:ILE:HG12	1:B:390:ASP:HB2	2.00	0.42
1:A:108:ASP:HB3	1:A:111:ALA:HB3	2.01	0.42
1:A:262:GLY:HA2	1:A:265:ILE:O	2.20	0.42
1:A:293:TRP:CD1	1:A:294:CYS:HB3	2.55	0.42
1:A:51:PRO:HB2	1:B:15:TYR:CD1	2.54	0.42
1:A:44:PRO:HB2	1:A:49:LEU:HD11	2.00	0.41
1:A:160:ILE:HA	1:A:160:ILE:HD13	1.88	0.41
1:A:255:VAL:HG23	1:A:255:VAL:O	2.20	0.41
1:A:1:MET:HE2	1:A:287:VAL:HB	2.01	0.41
1:B:173:LYS:O	1:B:177:ARG:HG2	2.20	0.41
1:A:213:HIS:CD2	1:A:256:GLN:HB3	2.56	0.41
1:B:137:LEU:HD12	1:B:184:HIS:HB3	2.01	0.41
1:B:185:SER:HB2	1:B:256:GLN:HE22	1.86	0.41
1:B:360:ARG:O	1:B:363:GLN:HG2	2.21	0.41
1:B:345:THR:HG23	1:B:404:ARG:HD2	2.03	0.41
1:A:151:ARG:HD2	1:B:151:ARG:HE	1.86	0.40
1:A:6:ASN:OD1	1:A:41:ARG:NH1	2.50	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	423/449 (94%)	409 (97%)	14 (3%)	0	100	100
1	B	424/449 (94%)	414 (98%)	10 (2%)	0	100	100
All	All	847/898 (94%)	823 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	342/362 (94%)	338 (99%)	4 (1%)	71	88
1	B	343/362 (95%)	341 (99%)	2 (1%)	86	95
All	All	685/724 (95%)	679 (99%)	6 (1%)	78	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	A	295	SER
1	A	336	ARG
1	A	417	ASN
1	B	77	ASP
1	B	336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	501	-	15,15,15	0.10	0	21,21,21	0.15	0
2	NAG	B	481	-	15,15,15	0.08	0	21,21,21	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	-	-	0/6/26/26	0/1/1/1
2	NAG	B	481	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	424/449 (94%)	0.72	50 (11%) <b>4</b> <b>4</b>	38, 66, 93, 117	0
1	B	426/449 (94%)	0.53	32 (7%) <b>14</b> <b>14</b>	35, 59, 82, 119	0
All	All	850/898 (94%)	0.62	82 (9%) <b>8</b> <b>7</b>	35, 62, 90, 119	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	ALA	5.1
1	A	282	ALA	4.7
1	A	337	ASP	4.1
1	A	403	VAL	4.0
1	A	394	PRO	4.0
1	A	343	ARG	4.0
1	A	396	LYS	3.9
1	A	307	PHE	3.8
1	A	395	ALA	3.6
1	B	338	THR	3.6
1	B	339	VAL	3.6
1	B	307	PHE	3.5
1	A	336	ARG	3.5
1	A	421	ASP	3.3
1	A	326	LYS	3.3
1	B	340	ALA	3.3
1	B	337	ASP	3.2
1	A	376	LEU	3.2
1	B	264	VAL	3.1
1	A	375	ASN	3.1
1	B	379	GLN	3.0
1	A	404	ARG	3.0
1	A	315	PHE	3.0
1	B	282	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	278	ILE	2.9
1	A	44	PRO	2.9
1	B	396	LYS	2.8
1	A	227	MET	2.8
1	B	343	ARG	2.8
1	B	415	ALA	2.8
1	B	321	LEU	2.7
1	B	336	ARG	2.7
1	A	85	GLY	2.7
1	A	27	ARG	2.7
1	A	4	GLY	2.7
1	B	399	ASN	2.7
1	A	5	VAL	2.7
1	A	317	VAL	2.6
1	B	5	VAL	2.6
1	A	408	VAL	2.6
1	B	380	GLY	2.6
1	B	14	PHE	2.5
1	A	380	GLY	2.5
1	A	1	MET	2.5
1	A	379	GLN	2.5
1	B	342	PRO	2.5
1	B	335	HIS	2.5
1	A	32	ILE	2.5
1	A	176	ARG	2.5
1	B	402	ILE	2.5
1	A	371	GLU	2.4
1	A	397	LEU	2.4
1	B	424	PHE	2.4
1	B	381	GLU	2.4
1	A	321	LEU	2.4
1	A	225	GLY	2.4
1	A	406	GLU	2.4
1	A	17	TRP	2.3
1	B	377	ASN	2.3
1	B	4	GLY	2.3
1	B	44	PRO	2.3
1	A	14	PHE	2.3
1	B	331	ALA	2.3
1	A	3	PHE	2.3
1	B	416	TYR	2.3
1	A	405	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	PRO	2.2
1	A	46	TRP	2.2
1	A	2	LYS	2.2
1	A	347	ILE	2.1
1	A	82	VAL	2.1
1	A	84	GLN	2.1
1	A	382	ARG	2.1
1	A	232	LEU	2.1
1	B	0	HIS	2.1
1	A	275	ARG	2.1
1	B	17	TRP	2.1
1	B	1	MET	2.0
1	A	338	THR	2.0
1	A	11	GLY	2.0
1	A	399	ASN	2.0
1	B	6	ASN	2.0

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	501	15/15	0.91	0.25	70,75,80,83	0
2	NAG	B	481	15/15	0.92	0.19	69,73,78,82	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.