



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 01:49 AM EDT

PDB ID : 2O9T  
Title : beta-glucosidase B from Bacillus polymyxa complexed with glucose  
Authors : Isorna, P.; Polaina, J.; Sanz-Aparicio, J.  
Deposited on : 2006-12-14  
Resolution : 2.15 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 : 2.23.2  
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) : 2.23.2

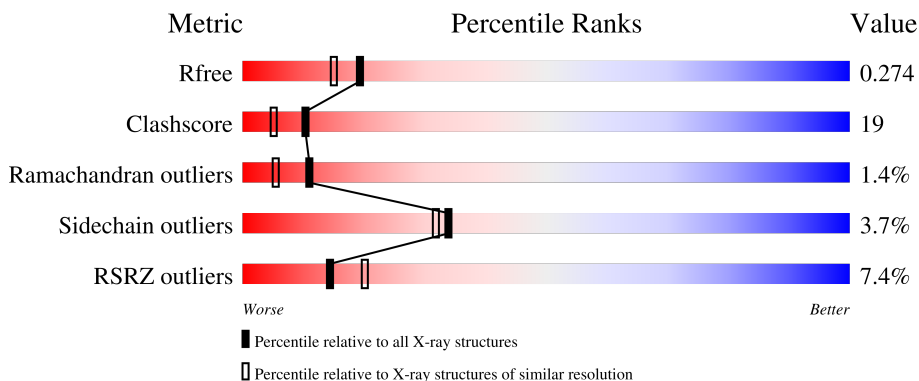
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	454	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3764 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.

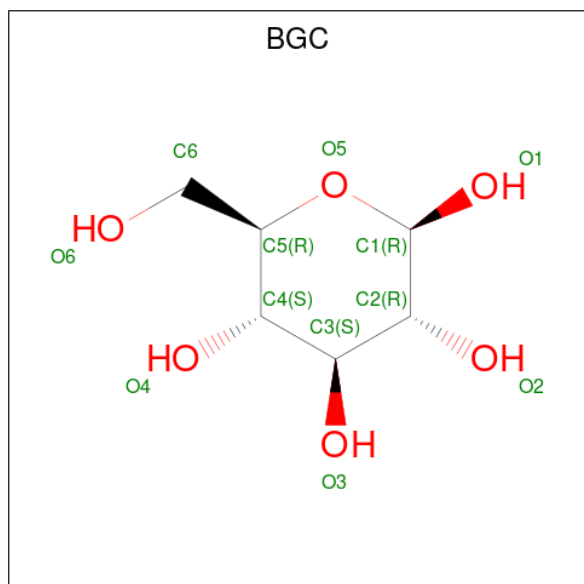
- Molecule 1 is a protein called Beta-glucosidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3625	2327	612	666	20	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P22505
A	-4	HIS	-	expression tag	UNP P22505
A	-3	HIS	-	expression tag	UNP P22505
A	-2	HIS	-	expression tag	UNP P22505
A	-1	HIS	-	expression tag	UNP P22505
A	0	HIS	-	expression tag	UNP P22505
A	1	HIS	-	expression tag	UNP P22505
A	376	GLN	HIS	engineered mutation	UNP P22505
A	377	ARG	GLY	engineered mutation	UNP P22505

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

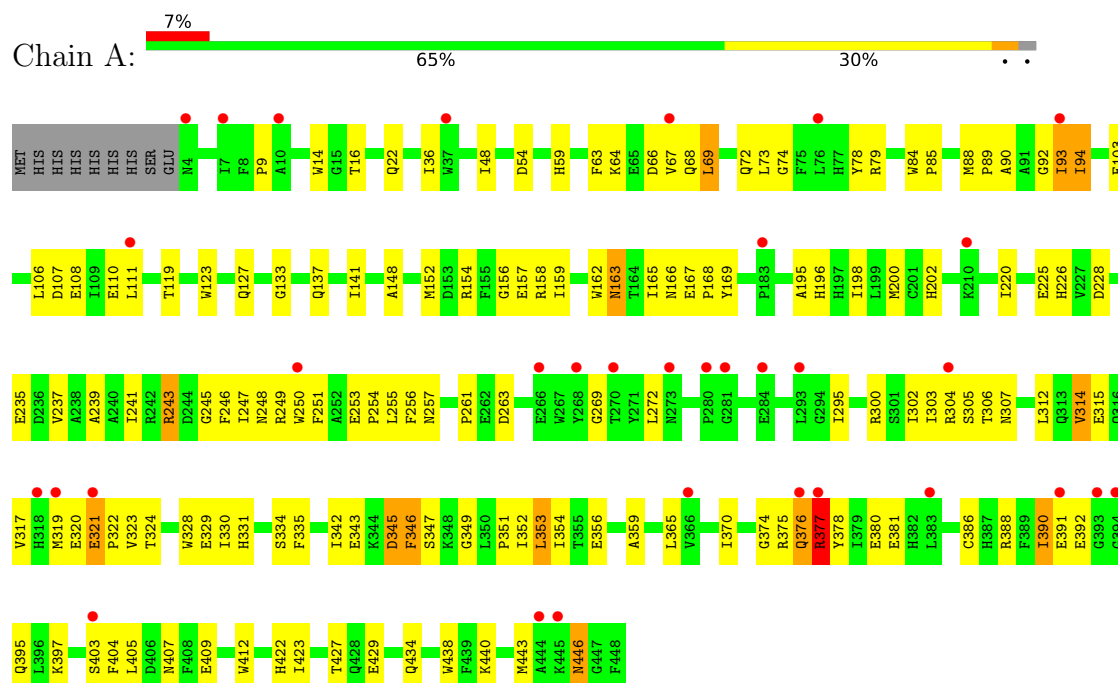
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		

### 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: Beta-glucosidase B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.33Å 75.58Å 88.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.33 – 2.15 18.33 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.6 (18.33-2.15) 97.1 (18.33-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.15Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.245 , 0.275 0.238 , 0.274	Depositor DCC
$R_{free}$ test set	1769 reflections (6.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

### 5.1 Standard geometry

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

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	0.45	1/3736 (0.0%)	0.66	3/5066 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	ARG	C-N	6.94	1.50	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	CA-C-N	-7.57	100.56	117.20
1	A	377	ARG	C-N-CA	-6.87	104.53	121.70
1	A	390	ILE	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	ARG	Mainchain

## 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	3625	0	3423	132	0
2	A	12	0	12	4	0
3	A	127	0	0	3	0
All	All	3764	0	3435	132	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 19.

All (132) 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:324:THR:HG23	1:A:330:ILE:HD11	1.55	0.87
1:A:321:GLU:HB3	1:A:322:PRO:CD	2.06	0.84
1:A:253:GLU:HB3	1:A:254:PRO:HD3	1.66	0.77
1:A:90:ALA:O	1:A:93:ILE:HD12	1.84	0.76
1:A:89:PRO:HD2	1:A:93:ILE:HD11	1.68	0.76
1:A:166:ASN:OD1	1:A:167:GLU:HG3	1.85	0.76
1:A:321:GLU:HB3	1:A:322:PRO:HD2	1.67	0.74
1:A:427:THR:OG1	1:A:429:GLU:HG2	1.87	0.74
1:A:376:GLN:C	1:A:378:TYR:H	1.91	0.73
1:A:168:PRO:HA	1:A:198:ILE:HD13	1.71	0.71
1:A:321:GLU:O	1:A:323:VAL:HG13	1.90	0.71
1:A:376:GLN:C	1:A:378:TYR:N	2.43	0.71
1:A:156:GLY:HA2	1:A:162:TRP:HZ2	1.60	0.67
1:A:148:ALA:O	1:A:152:MET:HG3	1.96	0.66
1:A:93:ILE:H	1:A:93:ILE:HD13	1.59	0.66
1:A:93:ILE:HD13	1:A:94:ILE:H	1.60	0.65
1:A:343:GLU:HA	1:A:347:SER:HB3	1.79	0.64
1:A:84:TRP:HB3	1:A:85:PRO:HD3	1.78	0.64
1:A:107:ASP:O	1:A:111:LEU:HD13	1.97	0.64
1:A:165:ILE:HG21	1:A:198:ILE:HD11	1.81	0.63
1:A:165:ILE:CG2	1:A:198:ILE:HD11	2.28	0.62
1:A:14:TRP:HE1	1:A:446:ASN:ND2	1.96	0.62
1:A:249:ARG:NH2	1:A:263:ASP:OD1	2.32	0.62
1:A:256:PHE:CD1	1:A:346:PHE:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:C	1:A:392:GLU:H	2.04	0.61
1:A:249:ARG:HH22	1:A:263:ASP:CG	2.04	0.61
1:A:342:ILE:O	1:A:345:ASP:O	2.18	0.61
1:A:48:ILE:HD12	1:A:412:TRP:HA	1.82	0.61
1:A:89:PRO:CD	1:A:93:ILE:HD11	2.30	0.61
1:A:320:GLU:O	1:A:321:GLU:O	2.19	0.60
1:A:324:THR:CG2	1:A:330:ILE:HD11	2.30	0.59
1:A:235:GLU:OE2	3:A:504:HOH:O	2.17	0.59
1:A:351:PRO:HB3	1:A:397:LYS:HG3	1.84	0.59
1:A:390:ILE:O	1:A:391:GLU:HB3	2.03	0.58
1:A:377:ARG:O	1:A:381:GLU:HG2	2.05	0.57
1:A:64:LYS:O	1:A:68:GLN:HG3	2.04	0.57
1:A:245:GLY:HA2	1:A:249:ARG:HB2	1.87	0.56
1:A:255:LEU:HD23	1:A:256:PHE:CE1	2.40	0.56
1:A:323:VAL:HG12	1:A:329:GLU:HA	1.86	0.56
1:A:106:LEU:O	1:A:110:GLU:HG3	2.05	0.55
1:A:36:ILE:HA	1:A:127:GLN:NE2	2.22	0.55
1:A:74:GLY:O	1:A:443:MET:HE1	2.07	0.54
1:A:295:ILE:HD12	1:A:352:ILE:HG23	1.90	0.54
1:A:141:ILE:HD11	1:A:200:MET:HE3	1.89	0.54
1:A:304:ARG:HD2	1:A:315:GLU:OE2	2.08	0.53
1:A:380:GLU:HG3	1:A:438:TRP:CZ2	2.44	0.53
1:A:335:PHE:HZ	1:A:354:ILE:HD13	1.74	0.53
1:A:328:TRP:HH2	2:A:500:BGC:H6	1.57	0.52
1:A:249:ARG:O	1:A:253:GLU:HB2	2.10	0.52
1:A:253:GLU:CB	1:A:254:PRO:HD3	2.37	0.51
1:A:93:ILE:HD13	1:A:93:ILE:N	2.24	0.51
1:A:328:TRP:HH2	2:A:500:BGC:O6	1.93	0.51
1:A:306:THR:CG2	1:A:315:GLU:HB2	2.41	0.51
1:A:169:TYR:CE1	1:A:247:ILE:HG12	2.45	0.51
1:A:349:GLY:O	1:A:395:GLN:HG3	2.11	0.51
1:A:376:GLN:O	1:A:378:TYR:N	2.44	0.50
1:A:246:PHE:HB2	1:A:312:LEU:HD11	1.92	0.50
1:A:353:LEU:CD1	1:A:397:LYS:HB2	2.42	0.50
1:A:370:ILE:O	1:A:434:GLN:HG2	2.12	0.50
1:A:63:PHE:O	1:A:67:VAL:HG22	2.12	0.50
1:A:250:TRP:CE3	1:A:261:PRO:HD2	2.47	0.50
1:A:374:GLY:C	1:A:376:GLN:N	2.64	0.50
1:A:226:HIS:HE1	1:A:228:ASP:OD1	1.95	0.50
1:A:427:THR:HG1	1:A:429:GLU:HG2	1.77	0.50
1:A:89:PRO:HG2	1:A:93:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:TYR:CD1	1:A:378:TYR:C	2.85	0.49
1:A:405:LEU:HD22	1:A:423:ILE:HD11	1.95	0.49
1:A:69:LEU:O	1:A:69:LEU:HD23	2.13	0.48
1:A:239:ALA:HB2	1:A:305:SER:HB3	1.96	0.48
1:A:119:THR:HA	1:A:163:ASN:O	2.12	0.48
1:A:390:ILE:HG22	1:A:391:GLU:H	1.79	0.48
1:A:403:SER:OG	1:A:405:LEU:O	2.30	0.48
1:A:246:PHE:CB	1:A:312:LEU:HD11	2.44	0.48
1:A:409:GLU:OE2	2:A:500:BGC:H6C2	2.13	0.48
1:A:202:HIS:CD2	1:A:220:ILE:HB	2.49	0.48
1:A:324:THR:HG23	1:A:330:ILE:CD1	2.35	0.48
1:A:79:ARG:NH1	1:A:356:GLU:OE1	2.39	0.47
1:A:84:TRP:HB2	3:A:552:HOH:O	2.14	0.47
1:A:239:ALA:HB1	1:A:314:VAL:HG22	1.95	0.47
1:A:330:ILE:HD12	1:A:378:TYR:CD2	2.49	0.47
1:A:67:VAL:HG21	1:A:108:GLU:CG	2.44	0.47
1:A:330:ILE:HD12	1:A:378:TYR:CE2	2.49	0.47
1:A:345:ASP:O	1:A:347:SER:N	2.47	0.47
1:A:16:THR:OG1	1:A:404:PHE:HB2	2.15	0.47
1:A:225:GLU:H	1:A:248:ASN:HD21	1.63	0.47
1:A:300:ARG:HD3	1:A:334:SER:OG	2.15	0.47
1:A:321:GLU:O	1:A:322:PRO:C	2.53	0.47
1:A:123:TRP:N	1:A:123:TRP:CD1	2.83	0.46
1:A:14:TRP:HB3	1:A:443:MET:CE	2.44	0.46
1:A:165:ILE:HG21	1:A:198:ILE:CD1	2.46	0.46
1:A:84:TRP:N	1:A:85:PRO:CD	2.79	0.46
1:A:59:HIS:HD2	1:A:66:ASP:OD2	1.99	0.46
1:A:243:ARG:CZ	1:A:247:ILE:HD11	2.46	0.46
1:A:295:ILE:HD12	1:A:352:ILE:CG2	2.46	0.46
1:A:22:GLN:O	1:A:407:ASN:HB2	2.15	0.45
1:A:168:PRO:HA	1:A:198:ILE:CD1	2.44	0.45
1:A:195:ALA:HA	1:A:198:ILE:HG22	1.97	0.45
1:A:303:ILE:HG23	1:A:314:VAL:HG13	1.97	0.45
1:A:295:ILE:HD13	1:A:342:ILE:HD13	1.99	0.45
1:A:168:PRO:HB2	1:A:251:PHE:CD1	2.52	0.45
1:A:141:ILE:CD1	1:A:200:MET:HE3	2.46	0.45
1:A:253:GLU:HB3	1:A:254:PRO:CD	2.43	0.44
1:A:67:VAL:HG21	1:A:108:GLU:HG3	1.99	0.44
1:A:237:VAL:O	1:A:241:ILE:HG12	2.18	0.44
1:A:246:PHE:CG	1:A:312:LEU:HD11	2.52	0.44
1:A:374:GLY:C	1:A:376:GLN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD13	1:A:94:ILE:N	2.29	0.43
1:A:156:GLY:HA2	1:A:162:TRP:CZ2	2.46	0.43
1:A:302:ILE:HD12	1:A:319:MET:HG2	1.99	0.43
1:A:335:PHE:CZ	1:A:354:ILE:HD13	2.53	0.43
1:A:359:ALA:O	1:A:375:ARG:HD3	2.19	0.43
1:A:168:PRO:HD2	3:A:600:HOH:O	2.17	0.43
1:A:88:MET:HA	1:A:93:ILE:HD11	2.01	0.42
1:A:93:ILE:N	1:A:93:ILE:CD1	2.82	0.42
1:A:133:GLY:HA3	1:A:137:GLN:HG2	2.01	0.42
1:A:390:ILE:O	1:A:392:GLU:N	2.51	0.42
1:A:323:VAL:HA	1:A:328:TRP:O	2.19	0.42
1:A:103:GLU:HG3	1:A:158:ARG:NH2	2.34	0.42
1:A:302:ILE:HB	1:A:317:VAL:HB	2.01	0.42
1:A:390:ILE:C	1:A:392:GLU:N	2.70	0.42
1:A:328:TRP:CH2	2:A:500:BGC:O6	2.72	0.42
1:A:386:CYS:O	1:A:390:ILE:HG13	2.20	0.42
1:A:72:GLN:O	1:A:440:LYS:HE2	2.19	0.41
1:A:156:GLY:H	1:A:159:ILE:HG12	1.85	0.41
1:A:16:THR:HG23	1:A:78:TYR:HD1	1.86	0.41
1:A:370:ILE:N	1:A:370:ILE:HD12	2.35	0.41
1:A:365:LEU:HD11	1:A:422:HIS:CE1	2.56	0.41
1:A:388:ARG:O	1:A:390:ILE:O	2.39	0.40
1:A:103:GLU:CD	1:A:154:ARG:HH11	2.25	0.40
1:A:196:HIS:CD2	1:A:200:MET:CE	3.04	0.40
1:A:331:HIS:HD2	1:A:334:SER:OG	2.04	0.40
1:A:253:GLU:OE1	1:A:257:ASN:OD1	2.40	0.40

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	443/454 (98%)	413 (93%)	24 (5%)	6 (1%)	11 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLU
1	A	346	PHE
1	A	9	PRO
1	A	269	GLY
1	A	94	ILE
1	A	92	GLY

### 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	377/386 (98%)	363 (96%)	14 (4%)	34 32

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	69	LEU
1	A	73	LEU
1	A	93	ILE
1	A	157	GLU
1	A	163	ASN
1	A	243	ARG
1	A	272	LEU
1	A	307	ASN
1	A	314	VAL
1	A	345	ASP
1	A	353	LEU
1	A	376	GLN
1	A	446	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	95	ASN
1	A	122	HIS
1	A	127	GLN
1	A	202	HIS
1	A	207	ASN
1	A	226	HIS
1	A	248	ASN
1	A	257	ASN
1	A	287	GLN
1	A	288	GLN
1	A	307	ASN
1	A	313	GLN
1	A	331	HIS
1	A	395	GLN
1	A	441	GLN
1	A	446	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](#)

1 ligand is 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	BGC	A	500	-	12,12,12	1.35	3 (25%)	17,17,17	2.07	4 (23%)

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	BGC	A	500	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	BGC	O2-C2	2.69	1.49	1.43
2	A	500	BGC	O3-C3	2.17	1.48	1.43
2	A	500	BGC	O5-C1	2.12	1.48	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BGC	O5-C1-C2	-6.18	99.25	110.28
2	A	500	BGC	C1-O5-C5	2.93	119.19	113.66
2	A	500	BGC	C4-C3-C2	-2.53	106.41	110.82
2	A	500	BGC	O2-C2-C3	-2.01	105.69	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	BGC	4	0

## 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	445/454 (98%)	0.46	33 (7%) <span style="border: 1px solid red; padding: 0 2px;">14</span> <span style="border: 1px solid red; padding: 0 2px;">20</span>	22, 35, 48, 56	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ASN	7.0
1	A	377	ARG	4.5
1	A	76	LEU	4.2
1	A	321	GLU	3.7
1	A	280	PRO	3.7
1	A	393	GLY	3.7
1	A	383	LEU	3.6
1	A	403	SER	3.5
1	A	270	THR	3.3
1	A	10	ALA	3.3
1	A	391	GLU	2.9
1	A	444	ALA	2.7
1	A	93	ILE	2.6
1	A	273	ASN	2.6
1	A	394	GLY	2.6
1	A	366	VAL	2.6
1	A	376	GLN	2.5
1	A	445	LYS	2.5
1	A	7	ILE	2.5
1	A	210	LYS	2.4
1	A	37	TRP	2.4
1	A	284	GLU	2.4
1	A	111	LEU	2.3
1	A	67	VAL	2.3
1	A	281	GLY	2.2
1	A	319	MET	2.2
1	A	304	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	250	TRP	2.1
1	A	266	GLU	2.1
1	A	183	PRO	2.1
1	A	268	TYR	2.1
1	A	318	HIS	2.1
1	A	293	LEU	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(Å <sup>2</sup> )	Q<0.9
2	BGC	A	500	12/12	0.81	0.18	28,38,46,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.