



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:46 am BST

PDB ID : 5WZP  
Title : Alpha-N-acetylgalactosaminidase NagBb from Bifidobacterium bifidum -  
ligand free  
Authors : Sato, M.; Arakawa, T.; Ashida, H.; Fushinobu, S.  
Deposited on : 2017-01-18  
Resolution : 2.64 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

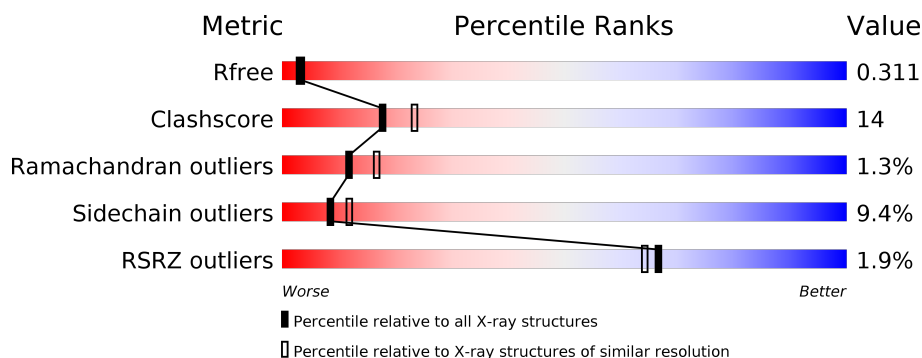
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	640	<div> <div> <div></div> <div>68%</div> <div>24%</div> <div>6%</div> </div> <div> <div>2%</div> <div>64%</div> <div>27%</div> <div>6%</div> </div> </div>
1	B	640	<div> <div> <div></div> <div>68%</div> <div>24%</div> <div>6%</div> </div> <div> <div>2%</div> <div>64%</div> <div>27%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	701	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9667 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-N-acetylgalactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4801	3023	853	890	35			
1	B	602	Total	C	N	O	S	0	0	0
			4786	3015	852	884	35			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	635	HIS	-	expression tag	UNP G5ELM1
A	636	HIS	-	expression tag	UNP G5ELM1
A	637	HIS	-	expression tag	UNP G5ELM1
A	638	HIS	-	expression tag	UNP G5ELM1
A	639	HIS	-	expression tag	UNP G5ELM1
A	640	HIS	-	expression tag	UNP G5ELM1
B	635	HIS	-	expression tag	UNP G5ELM1
B	636	HIS	-	expression tag	UNP G5ELM1
B	637	HIS	-	expression tag	UNP G5ELM1
B	638	HIS	-	expression tag	UNP G5ELM1
B	639	HIS	-	expression tag	UNP G5ELM1
B	640	HIS	-	expression tag	UNP G5ELM1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0

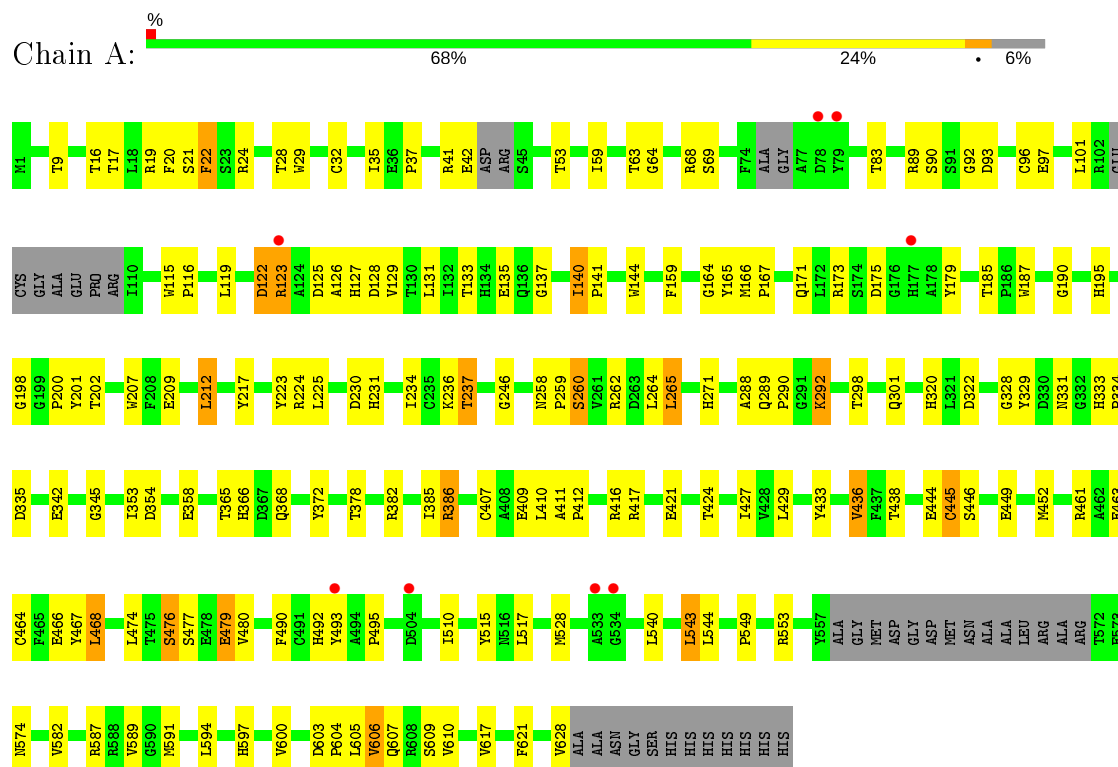
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total 37	O 37	0	0
4	B	39	Total 39	O 39	0	0

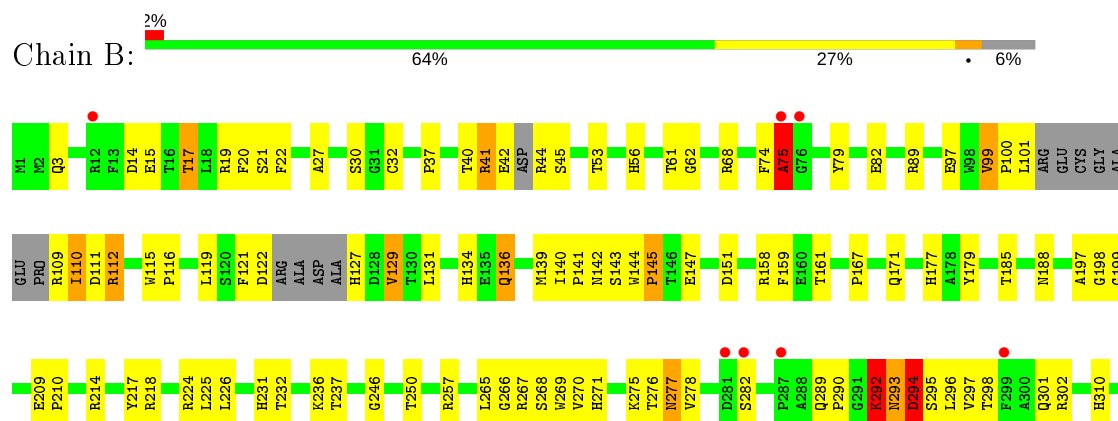
### 3 Residue-property plots

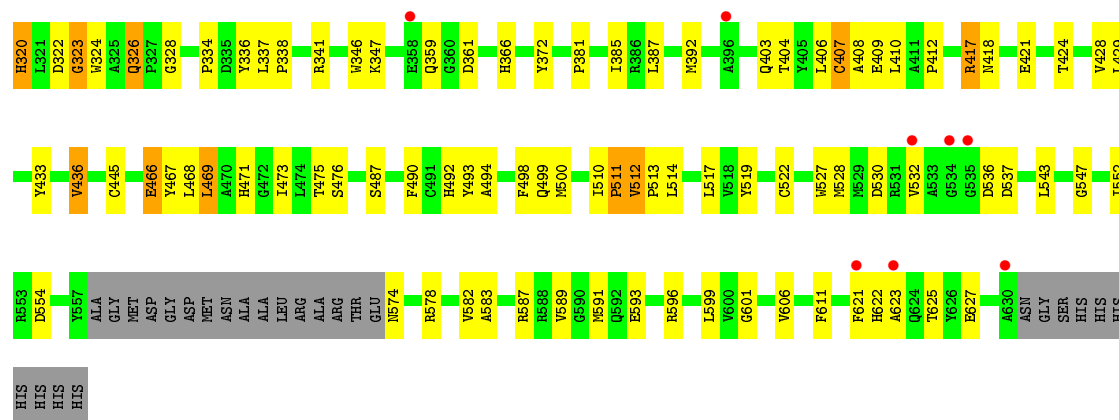
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



#### • Molecule 1: Alpha-N-acetylgalactosaminidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.64Å 127.76Å 176.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.55 – 2.64 36.34 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.1 (103.55-2.64) 99.1 (36.34-2.64)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.231 , 0.311 0.231 , 0.311	Depositor DCC
$R_{free}$ test set	2114 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: ZN, CA

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	0.66	0/4937	0.85	0/6708
1	B	0.62	0/4922	0.82	0/6687
All	All	0.64	0/9859	0.83	0/13395

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	75	ALA	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	4801	0	4507	112	0
1	B	4786	0	4498	149	0
2	A	1	0	0	2	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	37	0	0	3	0
4	B	39	0	0	2	0
All	All	9667	0	9005	253	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 14.

All (253) 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:407:CYS:SG	1:B:409:GLU:HB2	2.09	0.92
1:A:407:CYS:HG	2:A:701:ZN:ZN	0.79	0.89
1:A:125:ASP:O	1:A:127:HIS:N	2.07	0.86
1:A:378:THR:HG21	1:B:62:GLY:HA3	1.56	0.86
1:B:298:THR:HG23	1:B:301:GLN:HB2	1.60	0.82
1:B:267:ARG:HH12	1:B:361:ASP:HA	1.45	0.80
1:B:334:PRO:HD3	1:B:372:TYR:HD1	1.43	0.80
1:B:392:MET:HE2	1:B:404:THR:HG21	1.62	0.79
1:B:298:THR:CG2	1:B:301:GLN:HB2	2.13	0.78
1:A:353:ILE:HD13	1:A:427:ILE:HG23	1.66	0.78
1:A:605:LEU:HD12	1:A:605:LEU:H	1.48	0.77
1:A:122:ASP:HB3	1:A:201:TYR:HB3	1.66	0.77
1:B:417:ARG:HG2	1:B:417:ARG:HH11	1.50	0.76
1:A:165:TYR:OH	1:A:479:GLU:HG2	1.83	0.76
1:B:136:GLN:HG2	1:B:494:ALA:O	1.86	0.76
1:A:605:LEU:HD12	1:A:605:LEU:N	2.01	0.76
1:A:246:GLY:HA3	1:B:466:GLU:HG2	1.69	0.74
1:A:123:ARG:HB2	1:A:200:PRO:HB2	1.71	0.73
1:B:267:ARG:NH1	1:B:361:ASP:HA	2.03	0.72
1:B:326:GLN:NE2	1:B:341:ARG:HH12	1.87	0.72
1:B:42:GLU:HA	1:B:44:ARG:N	2.05	0.72
1:B:334:PRO:HD3	1:B:372:TYR:CD1	2.24	0.71
1:A:212:LEU:N	1:A:444:GLU:OE2	2.21	0.71
1:B:297:VAL:HG12	1:B:298:THR:H	1.55	0.70
1:B:269:TRP:HH2	1:B:490:PHE:CD2	2.10	0.70
1:B:144:TRP:O	1:B:198:GLY:CA	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:TRP:HH2	1:B:490:PHE:CE2	2.09	0.69
1:A:258:ASN:HA	4:A:823:HOH:O	1.92	0.69
1:A:41:ARG:HE	1:A:42:GLU:HG2	1.57	0.69
1:A:335:ASP:OD2	1:A:378:THR:HB	1.93	0.69
1:A:466:GLU:HG2	1:B:246:GLY:CA	2.23	0.69
1:B:385:ILE:HD13	1:B:445:CYS:HB2	1.76	0.68
1:A:510:ILE:HG12	1:A:604:PRO:HB3	1.75	0.68
1:A:128:ASP:HB3	1:A:173:ARG:HA	1.74	0.68
1:B:498:PHE:HE2	1:B:511:PRO:HB3	1.58	0.67
1:B:417:ARG:CG	1:B:417:ARG:HH11	2.06	0.67
1:A:438:THR:CG2	1:A:477:SER:HB3	2.23	0.67
1:A:246:GLY:CA	1:B:466:GLU:HG2	2.25	0.66
1:A:334:PRO:HD3	1:A:372:TYR:CD1	2.30	0.66
1:B:417:ARG:NH1	1:B:418:ASN:OD1	2.29	0.66
1:A:9:THR:HG22	1:A:24:ARG:HD2	1.76	0.66
1:A:433:TYR:HE2	1:A:492:HIS:HB2	1.61	0.66
1:A:438:THR:OG1	1:A:477:SER:HB3	1.96	0.65
1:A:96:CYS:HB3	1:A:115:TRP:CH2	2.32	0.65
1:B:289:GLN:N	1:B:290:PRO:CD	2.59	0.64
1:B:292:LYS:O	1:B:293:ASN:C	2.35	0.64
1:A:260:SER:HB2	1:A:474:LEU:HD21	1.80	0.64
1:B:275:LYS:HB2	1:B:296:LEU:HD12	1.79	0.64
1:B:188:ASN:HB3	1:B:209:GLU:HG3	1.80	0.63
1:B:417:ARG:NH1	1:B:417:ARG:HG2	2.11	0.63
1:A:159:PHE:CD1	1:A:167:PRO:HA	2.33	0.63
1:B:129:VAL:CG2	1:B:139:MET:HG2	2.28	0.63
1:A:116:PRO:HG2	1:A:223:TYR:OH	1.98	0.63
1:A:265:LEU:HD21	1:A:591:MET:HG3	1.81	0.62
1:B:278:VAL:HB	1:B:293:ASN:HB2	1.80	0.62
1:A:466:GLU:HG2	1:B:246:GLY:HA3	1.81	0.62
1:B:185:THR:HG22	1:B:217:TYR:HE2	1.64	0.62
1:B:14:ASP:HB3	1:B:17:THR:HG22	1.80	0.61
1:A:438:THR:HG21	1:A:477:SER:HB3	1.83	0.61
1:B:99:VAL:HB	1:B:218:ARG:HG2	1.83	0.61
1:B:185:THR:CG2	1:B:217:TYR:HE2	2.13	0.61
1:A:334:PRO:HD3	1:A:372:TYR:HD1	1.64	0.61
1:B:278:VAL:HB	1:B:293:ASN:CB	2.30	0.61
1:B:112:ARG:HH11	1:B:112:ARG:HG2	1.66	0.61
1:A:133:THR:HG21	1:A:166:MET:O	2.02	0.59
1:A:32:CYS:HB2	1:A:35:ILE:CG1	2.32	0.59
1:A:433:TYR:CE2	1:A:492:HIS:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:CYS:SG	1:A:409:GLU:HB2	2.43	0.59
1:B:131:LEU:HD21	1:B:231:HIS:HB2	1.85	0.59
1:B:392:MET:CE	1:B:404:THR:HG21	2.32	0.59
1:A:407:CYS:SG	2:A:701:ZN:ZN	1.86	0.58
1:A:385:ILE:O	1:A:386:ARG:HD3	2.04	0.57
1:A:467:TYR:HD1	1:A:468:LEU:HD13	1.70	0.57
1:A:603:ASP:O	1:A:605:LEU:O	2.23	0.57
1:A:195:HIS:HB2	1:A:202:THR:HG23	1.87	0.56
1:A:411:ALA:HB3	1:A:412:PRO:HD3	1.88	0.56
1:A:378:THR:O	1:A:378:THR:HG22	2.05	0.56
1:B:589:VAL:HG11	1:B:611:PHE:CD2	2.41	0.55
1:B:22:PHE:HD1	1:B:225:LEU:HD21	1.72	0.55
1:B:499:GLN:HB3	1:B:528:MET:SD	2.47	0.55
1:A:259:PRO:HD2	4:A:823:HOH:O	2.05	0.55
1:A:378:THR:HG21	1:B:62:GLY:CA	2.32	0.55
1:A:544:LEU:HD21	1:A:607:GLN:HB2	1.89	0.55
1:A:9:THR:HG21	1:A:92:GLY:O	2.07	0.55
1:B:574:ASN:O	1:B:578:ARG:HG3	2.07	0.55
1:B:469:LEU:HD13	1:B:475:THR:HG23	1.89	0.55
1:A:9:THR:HG22	1:A:24:ARG:HH11	1.72	0.55
1:B:129:VAL:HG21	1:B:139:MET:HG2	1.89	0.55
1:B:334:PRO:CD	1:B:372:TYR:HD1	2.18	0.55
1:B:338:PRO:HB3	1:B:346:TRP:CH2	2.42	0.55
1:A:140:ILE:O	1:A:140:ILE:HG13	2.07	0.54
1:A:605:LEU:HB3	1:A:621:PHE:HB2	1.89	0.54
1:B:265:LEU:HB3	1:B:587:ARG:HA	1.89	0.53
1:B:275:LYS:CB	1:B:296:LEU:HD12	2.37	0.53
1:B:40:THR:HG22	1:B:111:ASP:HB2	1.90	0.53
1:B:82:GLU:CB	1:B:99:VAL:HG13	2.37	0.53
1:A:35:ILE:HD12	1:A:35:ILE:O	2.08	0.53
1:B:144:TRP:O	1:B:198:GLY:HA2	2.07	0.53
1:B:269:TRP:CH2	1:B:490:PHE:CD2	2.95	0.53
1:B:289:GLN:N	1:B:290:PRO:HD3	2.23	0.52
1:A:333:HIS:CD2	1:A:368:GLN:HB3	2.45	0.52
1:B:292:LYS:O	1:B:293:ASN:O	2.27	0.52
1:B:275:LYS:HB2	1:B:296:LEU:CD1	2.39	0.52
1:A:605:LEU:CD1	1:A:605:LEU:H	2.19	0.52
1:B:139:MET:HB3	1:B:510:ILE:HB	1.92	0.52
1:B:270:VAL:HG13	1:B:552:ILE:CG2	2.39	0.52
1:A:605:LEU:CD1	1:A:605:LEU:N	2.73	0.52
1:B:326:GLN:O	1:B:328:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASP:CB	1:B:17:THR:HG22	2.40	0.51
1:B:385:ILE:CD1	1:B:445:CYS:HB2	2.40	0.51
1:A:445:CYS:HB3	1:A:452:MET:HB3	1.92	0.51
1:B:326:GLN:CD	1:B:341:ARG:HH12	2.14	0.51
1:B:129:VAL:HG11	1:B:139:MET:HE3	1.93	0.51
1:B:326:GLN:CD	1:B:341:ARG:NH1	2.64	0.51
1:B:250:THR:HB	4:B:813:HOH:O	2.11	0.51
1:A:129:VAL:HG12	1:A:141:PRO:HA	1.91	0.51
1:A:21:SER:HB2	1:A:29:TRP:O	2.11	0.51
1:A:135:GLU:OE2	1:A:479:GLU:OE2	2.29	0.51
1:B:269:TRP:CH2	1:B:490:PHE:CE2	2.97	0.51
1:B:537:ASP:OD1	1:B:578:ARG:NH2	2.41	0.51
1:B:129:VAL:HG22	1:B:139:MET:HG2	1.91	0.51
1:B:257:ARG:NH1	1:B:466:GLU:OE2	2.41	0.51
1:A:171:GLN:HB2	1:A:179:TYR:CE1	2.46	0.51
1:A:128:ASP:CB	1:A:173:ARG:HA	2.40	0.50
1:B:433:TYR:HE2	1:B:492:HIS:HB2	1.76	0.50
1:B:275:LYS:HE2	1:B:277:ASN:ND2	2.26	0.50
1:B:323:GLY:HA2	1:B:336:TYR:OH	2.12	0.50
1:A:461:ARG:O	1:A:464:CYS:HB2	2.12	0.50
1:B:22:PHE:CD1	1:B:225:LEU:HD21	2.46	0.50
1:B:622:HIS:CE1	4:B:829:HOH:O	2.64	0.50
1:B:74:PHE:O	1:B:75:ALA:C	2.49	0.50
1:B:82:GLU:HB2	1:B:99:VAL:HG13	1.93	0.50
1:A:64:GLY:HA2	1:A:89:ARG:HG3	1.94	0.49
1:B:543:LEU:HD12	1:B:582:VAL:HG13	1.93	0.49
1:B:37:PRO:HB3	1:B:115:TRP:HD1	1.77	0.49
1:B:334:PRO:CD	1:B:372:TYR:CD1	2.94	0.49
1:A:37:PRO:HB3	1:A:115:TRP:HD1	1.77	0.49
1:A:32:CYS:HB2	1:A:35:ILE:HG13	1.95	0.49
1:B:298:THR:HG22	1:B:301:GLN:HB2	1.92	0.49
1:A:9:THR:CG2	1:A:24:ARG:HH11	2.25	0.49
1:A:115:TRP:HA	1:A:116:PRO:C	2.32	0.48
1:A:594:LEU:HD11	1:A:609:SER:HB2	1.95	0.48
1:B:139:MET:HB2	1:B:512:VAL:HG22	1.95	0.48
1:A:93:ASP:OD2	1:A:224:ARG:HD2	2.13	0.48
1:A:467:TYR:C	1:A:467:TYR:CD1	2.86	0.48
1:B:326:GLN:NE2	1:B:341:ARG:NH1	2.58	0.48
1:A:421:GLU:O	1:A:424:THR:HB	2.13	0.48
1:B:144:TRP:O	1:B:198:GLY:HA3	2.13	0.48
1:B:22:PHE:CE1	1:B:225:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:HIS:HD2	1:A:609:SER:HB3	1.78	0.48
1:A:329:TYR:O	1:A:331:ASN:ND2	2.46	0.48
1:A:320:HIS:NE2	1:A:366:HIS:HB2	2.29	0.48
1:B:532:VAL:HG22	1:B:536:ASP:H	1.78	0.48
1:A:131:LEU:HD21	1:A:231:HIS:HB2	1.96	0.47
1:B:297:VAL:HG12	1:B:298:THR:N	2.28	0.47
1:B:589:VAL:O	1:B:589:VAL:HG12	2.14	0.47
1:B:115:TRP:CG	1:B:116:PRO:HA	2.50	0.47
1:A:140:ILE:HD11	1:A:195:HIS:CG	2.50	0.47
1:B:129:VAL:HG11	1:B:139:MET:CE	2.44	0.47
1:B:589:VAL:HG11	1:B:611:PHE:CG	2.50	0.47
1:A:378:THR:O	1:A:378:THR:CG2	2.62	0.47
1:B:61:THR:O	1:B:89:ARG:NH1	2.48	0.47
1:B:136:GLN:OE1	1:B:513:PRO:HA	2.14	0.47
1:B:292:LYS:C	1:B:293:ASN:O	2.54	0.46
1:B:543:LEU:HD11	1:B:582:VAL:HG22	1.97	0.46
1:A:16:THR:HG23	1:A:17:THR:HG23	1.98	0.46
1:B:143:SER:HA	1:B:198:GLY:O	2.15	0.46
1:B:27:ALA:HB2	1:B:177:HIS:ND1	2.31	0.46
1:B:147:GLU:HB3	1:B:197:ALA:HB2	1.98	0.46
1:B:337:LEU:HD13	1:B:421:GLU:HG2	1.98	0.46
1:A:83:THR:HA	1:A:97:GLU:O	2.15	0.46
1:B:110:ILE:O	1:B:210:PRO:HG3	2.15	0.46
1:B:519:TYR:O	1:B:522:CYS:HB2	2.16	0.45
1:B:99:VAL:HA	1:B:100:PRO:HD2	1.83	0.45
1:A:185:THR:HB	1:A:217:TYR:HE2	1.81	0.45
1:A:476:SER:HA	1:A:490:PHE:O	2.16	0.45
1:B:15:GLU:HB2	1:B:56:HIS:CD2	2.52	0.45
1:B:171:GLN:HB2	1:B:179:TYR:CE2	2.51	0.45
1:B:322:ASP:O	1:B:324:TRP:N	2.49	0.45
1:B:142:ASN:O	1:B:199:GLY:HA2	2.17	0.45
1:B:158:ARG:O	1:B:161:THR:OG1	2.32	0.45
1:B:320:HIS:CD2	1:B:320:HIS:C	2.90	0.45
1:B:476:SER:HB2	1:B:490:PHE:CZ	2.51	0.45
1:B:467:TYR:CE2	1:B:471:HIS:CE1	3.04	0.45
1:A:543:LEU:HB3	1:A:617:VAL:HG11	1.98	0.45
1:B:510:ILE:HA	1:B:511:PRO:HD2	1.80	0.44
1:A:288:ALA:HA	1:A:289:GLN:HA	1.83	0.44
1:B:82:GLU:HG3	1:B:101:LEU:HD11	1.99	0.44
1:A:328:GLY:O	1:A:331:ASN:HB2	2.18	0.44
1:A:333:HIS:HD2	4:A:805:HOH:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:THR:CG2	1:A:477:SER:CB	2.94	0.44
1:A:190:GLY:HA3	1:A:207:TRP:CE2	2.53	0.44
1:B:185:THR:CG2	1:B:217:TYR:CE2	2.98	0.44
1:B:197:ALA:HA	1:B:198:GLY:HA2	1.81	0.44
1:B:232:THR:HG21	1:B:596:ARG:HA	1.99	0.44
1:A:416:ARG:NH2	1:A:463:GLU:OE2	2.51	0.44
1:A:600:VAL:HB	1:A:606:VAL:HG12	1.98	0.44
1:B:406:LEU:O	1:B:407:CYS:C	2.55	0.44
1:B:20:PHE:HE1	1:B:22:PHE:CE2	2.36	0.43
1:B:433:TYR:CE2	1:B:492:HIS:HB2	2.53	0.43
1:A:133:THR:HG23	1:A:164:GLY:HA2	2.00	0.43
1:B:121:PHE:O	1:B:142:ASN:ND2	2.49	0.43
1:A:234:ILE:O	1:A:237:THR:OG1	2.35	0.43
1:A:449:GLU:HG2	1:B:68:ARG:NH1	2.34	0.43
1:A:354:ASP:O	1:A:358:GLU:HB2	2.18	0.43
1:B:310:HIS:HB2	1:B:359:GLN:CD	2.39	0.43
1:B:543:LEU:CD1	1:B:582:VAL:HG22	2.49	0.43
1:B:433:TYR:HA	1:B:476:SER:HB3	2.01	0.43
1:B:226:LEU:HD11	1:B:237:THR:HG21	2.01	0.43
1:A:20:PHE:HE2	1:A:22:PHE:CE2	2.37	0.42
1:A:298:THR:OG1	1:A:301:GLN:HG3	2.19	0.42
1:B:236:LYS:NZ	1:B:593:GLU:OE1	2.46	0.42
1:B:536:ASP:OD1	1:B:621:PHE:HD1	2.02	0.42
1:A:129:VAL:HG12	1:A:141:PRO:CA	2.49	0.42
1:A:59:ILE:HD12	1:A:68:ARG:HB2	2.00	0.42
1:A:549:PRO:HG3	1:A:582:VAL:HB	2.02	0.42
1:A:22:PHE:CD1	1:A:225:LEU:HD11	2.54	0.42
1:A:528:MET:HG2	1:A:553:ARG:NH2	2.34	0.42
1:B:139:MET:HB2	1:B:512:VAL:CG2	2.49	0.42
1:B:320:HIS:NE2	1:B:366:HIS:HB2	2.35	0.42
1:B:381:PRO:HA	1:B:392:MET:HE3	2.01	0.42
1:B:623:ALA:HB3	1:B:625:THR:HG22	2.02	0.42
1:A:594:LEU:HD12	1:A:610:VAL:O	2.20	0.42
1:B:421:GLU:O	1:B:424:THR:HB	2.19	0.42
1:B:527:TRP:CD1	1:B:547:GLY:HA3	2.54	0.42
1:A:135:GLU:HB3	1:A:495:PRO:O	2.19	0.42
1:B:468:LEU:HB3	1:B:473:ILE:HB	2.01	0.42
1:A:382:ARG:HH21	1:B:68:ARG:HD2	1.85	0.42
1:A:159:PHE:CE1	1:A:167:PRO:HA	2.54	0.42
1:B:297:VAL:HG21	1:B:302:ARG:NH2	2.35	0.42
1:B:22:PHE:CD1	1:B:225:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:O	1:B:554:ASP:HB2	2.20	0.41
1:B:476:SER:HA	1:B:490:PHE:O	2.19	0.41
1:B:112:ARG:HG2	1:B:112:ARG:NH1	2.33	0.41
1:B:19:ARG:NH1	1:B:32:CYS:O	2.53	0.41
1:A:368:GLN:HE22	1:A:436:VAL:HG13	1.86	0.41
1:B:159:PHE:CD1	1:B:167:PRO:HA	2.55	0.41
1:B:266:GLY:O	1:B:583:ALA:HB1	2.20	0.41
1:B:140:ILE:HA	1:B:141:PRO:HD2	1.93	0.41
1:A:322:ASP:HA	1:A:366:HIS:HB3	2.02	0.41
1:B:144:TRP:HA	1:B:145:PRO:HD2	1.73	0.41
1:A:290:PRO:C	1:A:292:LYS:H	2.24	0.41
1:B:589:VAL:CG1	1:B:611:PHE:CG	3.03	0.41
1:A:271:HIS:CE1	1:A:322:ASP:OD2	2.74	0.41
1:B:276:THR:O	1:B:294:ASP:HA	2.21	0.41
1:B:41:ARG:CD	1:B:110:ILE:HG22	2.51	0.41
1:A:480:VAL:HG22	1:A:515:TYR:OH	2.21	0.40
1:B:408:ALA:O	1:B:412:PRO:HD3	2.21	0.40
1:A:122:ASP:HA	1:A:123:ARG:HA	1.85	0.40
1:A:236:LYS:HA	1:A:236:LYS:HD3	1.96	0.40
1:A:333:HIS:CE1	1:A:368:GLN:HB3	2.56	0.40
1:A:144:TRP:O	1:A:198:GLY:HA2	2.21	0.40
1:A:438:THR:OG1	1:A:477:SER:CB	2.67	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	593/640 (93%)	545 (92%)	43 (7%)	5 (1%)	19	28
1	B	592/640 (92%)	534 (90%)	48 (8%)	10 (2%)	9	12
All	All	1185/1280 (93%)	1079 (91%)	91 (8%)	15 (1%)	12	17



All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ALA
1	B	293	ASN
1	B	436	VAL
1	A	137	GLY
1	A	436	VAL
1	B	294	ASP
1	B	323	GLY
1	B	292	LYS
1	B	75	ALA
1	B	145	PRO
1	B	326	GLN
1	B	511	PRO
1	A	345	GLY
1	A	606	VAL
1	B	601	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	496/520 (95%)	454 (92%)	42 (8%)	10	15
1	B	493/520 (95%)	442 (90%)	51 (10%)	7	9
All	All	989/1040 (95%)	896 (91%)	93 (9%)	8	12

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	22	PHE
1	A	28	THR
1	A	53	THR
1	A	63	THR
1	A	69	SER
1	A	90	SER
1	A	101	LEU

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	122	ASP
1	A	123	ARG
1	A	140	ILE
1	A	175	ASP
1	A	187	TRP
1	A	209	GLU
1	A	212	LEU
1	A	230	ASP
1	A	237	THR
1	A	260	SER
1	A	262	ARG
1	A	264	LEU
1	A	265	LEU
1	A	292	LYS
1	A	342	GLU
1	A	365	THR
1	A	386	ARG
1	A	410	LEU
1	A	417	ARG
1	A	429	LEU
1	A	445	CYS
1	A	446	SER
1	A	468	LEU
1	A	476	SER
1	A	479	GLU
1	A	493	TYR
1	A	517	LEU
1	A	540	LEU
1	A	543	LEU
1	A	574	ASN
1	A	587	ARG
1	A	589	VAL
1	A	628	VAL
1	B	3	GLN
1	B	17	THR
1	B	21	SER
1	B	30	SER
1	B	41	ARG
1	B	45	SER
1	B	53	THR
1	B	79	TYR

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	99	VAL
1	B	109	ARG
1	B	110	ILE
1	B	112	ARG
1	B	119	LEU
1	B	122	ASP
1	B	127	HIS
1	B	129	VAL
1	B	134	HIS
1	B	136	GLN
1	B	151	ASP
1	B	214	ARG
1	B	224	ARG
1	B	268	SER
1	B	277	ASN
1	B	282	SER
1	B	292	LYS
1	B	294	ASP
1	B	295	SER
1	B	320	HIS
1	B	347	LYS
1	B	387	LEU
1	B	403	GLN
1	B	407	CYS
1	B	410	LEU
1	B	417	ARG
1	B	428	VAL
1	B	429	LEU
1	B	436	VAL
1	B	466	GLU
1	B	469	LEU
1	B	487	SER
1	B	493	TYR
1	B	500	MET
1	B	512	VAL
1	B	514	LEU
1	B	517	LEU
1	B	530	ASP
1	B	591	MET
1	B	599	LEU
1	B	606	VAL

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Mol	Chain	Res	Type
1	B	627	GLU

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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, 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	603/640 (94%)	0.00	8 (1%) 77 75	31, 59, 88, 122	0
1	B	602/640 (94%)	0.09	15 (2%) 57 53	39, 70, 97, 135	0
All	All	1205/1280 (94%)	0.05	23 (1%) 66 64	31, 63, 93, 135	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	3.9
1	A	533	ALA	3.8
1	A	177	HIS	3.7
1	B	621	PHE	3.0
1	B	75	ALA	2.9
1	B	358	GLU	2.7
1	B	396	ALA	2.7
1	B	299	PHE	2.6
1	B	76	GLY	2.6
1	B	630	ALA	2.6
1	B	287	PRO	2.5
1	B	281	ASP	2.5
1	A	534	GLY	2.4
1	A	78	ASP	2.3
1	B	12	ARG	2.3
1	B	532	VAL	2.3
1	A	79	TYR	2.3
1	B	535	GLY	2.2
1	B	282	SER	2.2
1	B	623	ALA	2.2
1	A	504	ASP	2.1
1	A	493	TYR	2.0
1	B	534	GLY	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 carbohydrates 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	ZN	B	701	1/1	0.85	0.21	57,57,57,57	0
2	ZN	A	701	1/1	0.93	0.12	51,51,51,51	0
3	CA	B	702	1/1	0.95	0.19	55,55,55,55	0
3	CA	A	702	1/1	0.99	0.17	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.