



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:51 am BST

PDB ID : 5WZR  
Title : Alpha-N-acetylgalactosaminidase NagBb from Bifidobacterium bifidum - Gal-NHAc-DNJ complex  
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Deposited on : 2017-01-18  
Resolution : 2.79 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	:	2.11
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

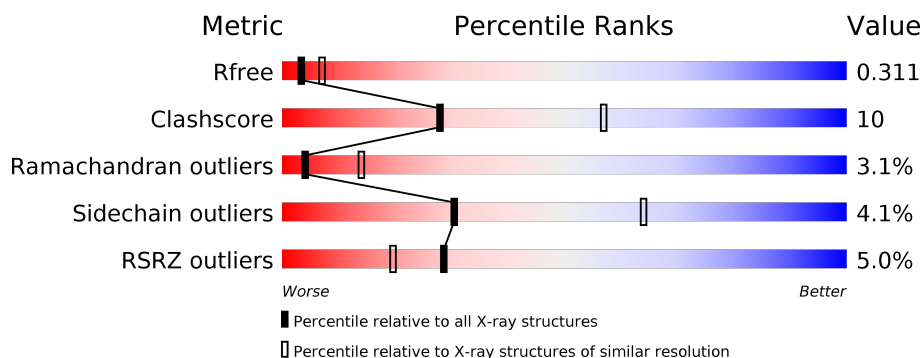
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	640	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10008 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	630	Total	C	N	O	S	0	0	0
			4984	3126	891	929	38			
1	B	630	Total	C	N	O	S	0	0	0
			4988	3129	893	928	38			

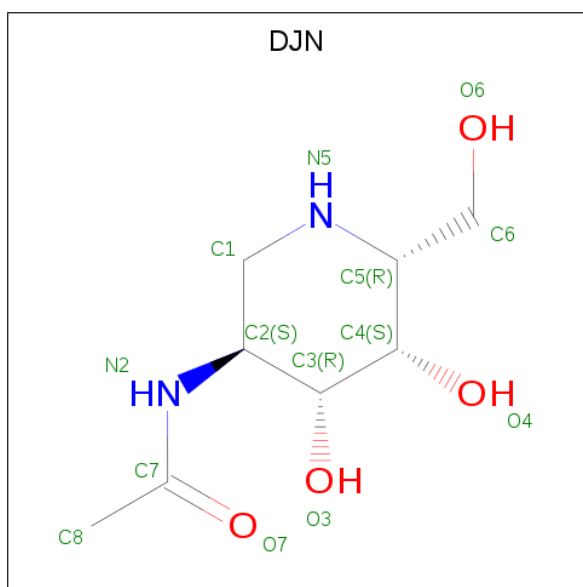
There are 12 discrepancies between the modelled and reference sequences:

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 N-[(3S,4R,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)piperidin-3-yl]acetamide (three-letter code: DJN) (formula: C<sub>8</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	2	4		
3	B	1	Total	C	N	O	0	0
			14	8	2	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

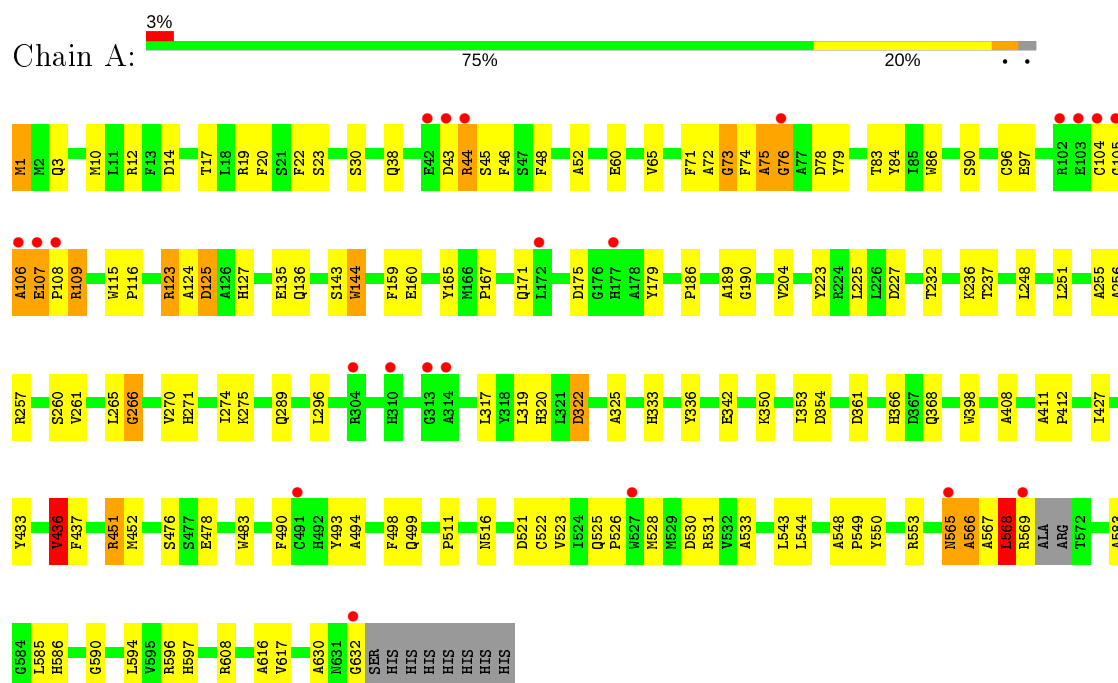
- Molecule 5 is water.

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

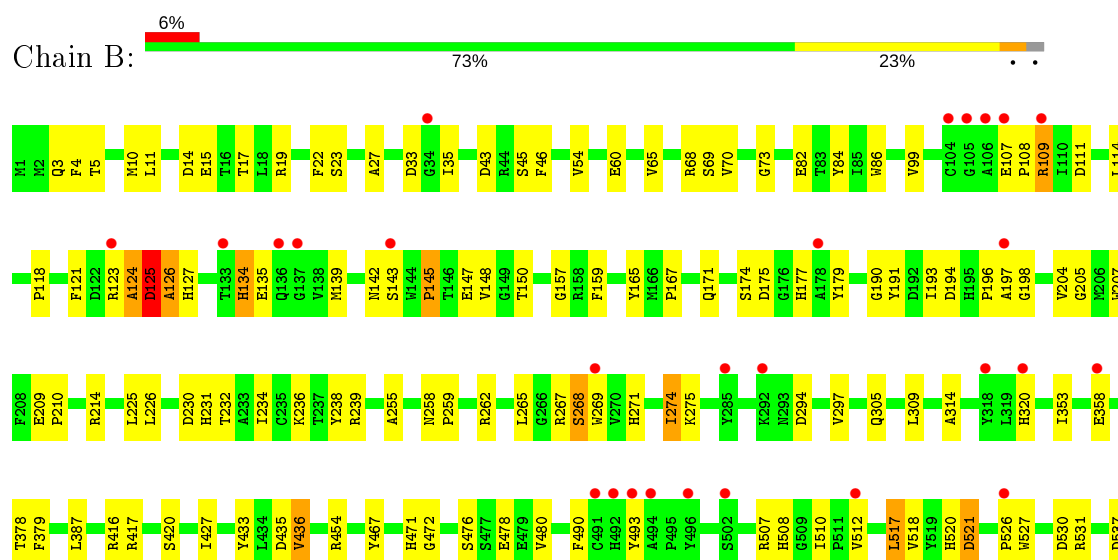
### 3 Residue-property plots

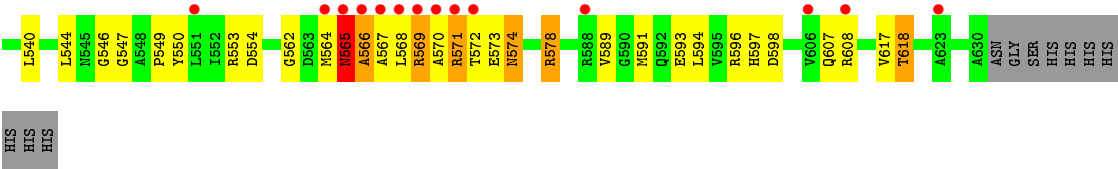
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	64.63Å 128.48Å 176.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.95 – 2.79 33.10 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (103.95-2.79) 98.7 (33.10-2.79)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.229 , 0.313 0.233 , 0.311	Depositor DCC
$R_{free}$ test set	1852 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: ZN, CA, DJN

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	0.51	0/5124	0.75	3/6963 (0.0%)
1	B	0.49	0/5129	0.75	0/6971
All	All	0.50	0/10253	0.75	3/13934 (0.0%)

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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	322	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	568	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	451	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	174	SER	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	4984	0	4675	92	0
1	B	4988	0	4685	100	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	16	1	0
3	B	14	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
All	All	10008	0	9392	191	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 10.

All (191) 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:124:ALA:O	1:B:126:ALA:N	1.98	0.94
1:A:74:PHE:O	1:A:76:GLY:N	2.05	0.89
1:B:573:GLU:O	1:B:574:ASN:OD1	1.91	0.86
1:B:107:GLU:HB3	1:B:108:PRO:HA	1.60	0.83
1:A:533:ALA:N	1:A:568:LEU:O	2.19	0.76
1:B:236:LYS:NZ	1:B:593:GLU:OE2	2.23	0.71
1:A:266:GLY:O	1:A:583:ALA:HB1	1.94	0.68
1:B:22:PHE:HD1	1:B:225:LEU:HD21	1.62	0.64
1:B:159:PHE:CD1	1:B:167:PRO:HA	2.33	0.64
1:A:516:ASN:HD21	1:A:525:GLN:HE22	1.46	0.64
1:A:265:LEU:HD22	1:A:590:GLY:HA3	1.80	0.63
1:A:3:GLN:NE2	1:A:10:MET:SD	2.71	0.63
1:B:262:ARG:O	1:B:265:LEU:HB2	1.99	0.62
1:B:124:ALA:C	1:B:126:ALA:H	2.03	0.61
1:B:125:ASP:O	1:B:127:HIS:N	2.31	0.61
1:B:565:ASN:OD1	1:B:567:ALA:HB3	2.01	0.61
1:A:271:HIS:CE1	1:A:322:ASP:OD2	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:12:ARG:NH1	2.73	0.60
1:A:476:SER:HA	1:A:490:PHE:O	2.02	0.60
1:B:517:LEU:HD13	1:B:594:LEU:HD22	1.83	0.60
1:A:531:ARG:O	1:A:568:LEU:HD12	2.02	0.60
1:B:22:PHE:CD1	1:B:225:LEU:HD21	2.37	0.59
1:A:516:ASN:ND2	1:A:525:GLN:HE22	2.02	0.58
1:A:265:LEU:CD2	1:A:590:GLY:HA3	2.34	0.57
1:B:147:GLU:HB2	1:B:197:ALA:HB2	1.87	0.57
1:B:564:MET:O	1:B:566:ALA:N	2.37	0.57
1:A:46:PHE:CZ	1:A:75:ALA:HB2	2.39	0.57
1:B:4:PHE:HD2	1:B:11:LEU:HD23	1.70	0.56
1:A:96:CYS:HB3	1:A:115:TRP:CH2	2.41	0.56
1:B:125:ASP:C	1:B:127:HIS:H	2.09	0.56
1:B:171:GLN:HB2	1:B:179:TYR:CE2	2.41	0.56
1:B:521:ASP:N	1:B:521:ASP:OD1	2.34	0.56
1:B:239:ARG:NH1	1:B:518:VAL:O	2.38	0.56
1:A:159:PHE:CD1	1:A:167:PRO:HA	2.42	0.55
1:A:333:HIS:ND1	1:A:368:GLN:HB3	2.22	0.55
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.71	0.55
1:B:225:LEU:N	1:B:225:LEU:HD12	2.21	0.55
1:A:116:PRO:HG2	1:A:223:TYR:OH	2.07	0.55
1:B:22:PHE:CE1	1:B:225:LEU:HD11	2.41	0.55
1:B:267:ARG:O	1:B:549:PRO:HD2	2.07	0.54
1:B:5:THR:HG22	1:B:10:MET:HG2	1.89	0.54
1:B:121:PHE:O	1:B:142:ASN:ND2	2.41	0.54
1:A:20:PHE:HE2	1:A:22:PHE:HE2	1.54	0.53
1:B:4:PHE:CD2	1:B:11:LEU:HD23	2.43	0.53
1:A:14:ASP:HB3	1:A:17:THR:HG23	1.89	0.53
1:A:333:HIS:CE1	1:A:368:GLN:HB3	2.43	0.53
1:A:568:LEU:O	1:A:569:ARG:CB	2.56	0.53
1:A:1:MET:CE	1:A:14:ASP:OD2	2.56	0.53
1:A:271:HIS:HE1	1:A:322:ASP:OD2	1.90	0.53
1:B:271:HIS:CD2	1:B:320:HIS:CD2	2.97	0.53
1:A:608:ARG:HD2	1:A:616:ALA:HB1	1.90	0.53
1:B:123:ARG:O	1:B:124:ALA:HB2	2.08	0.53
1:A:14:ASP:HB3	1:A:17:THR:CG2	2.38	0.53
1:B:531:ARG:NH1	1:B:572:THR:HB	2.24	0.53
1:A:353:ILE:CD1	1:A:427:ILE:HG23	2.39	0.53
1:B:159:PHE:CD2	1:B:190:GLY:HA2	2.44	0.52
1:A:135:GLU:HA	1:A:165:TYR:CE2	2.45	0.52
1:A:568:LEU:O	1:A:569:ARG:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ASP:CG	1:B:578:ARG:HH22	2.12	0.52
1:B:60:GLU:HA	1:B:65:VAL:HG12	1.92	0.52
1:A:353:ILE:HD13	1:A:427:ILE:HG23	1.92	0.52
1:B:531:ARG:CZ	1:B:572:THR:HB	2.40	0.52
1:B:143:SER:O	1:B:198:GLY:O	2.28	0.52
1:B:19:ARG:NH2	1:B:33:ASP:O	2.43	0.52
1:A:516:ASN:HD21	1:A:525:GLN:NE2	2.08	0.51
1:A:123:ARG:O	1:A:124:ALA:HB3	2.09	0.51
1:A:159:PHE:CD2	1:A:190:GLY:HA2	2.46	0.51
1:B:476:SER:HA	1:B:490:PHE:O	2.10	0.51
1:B:544:LEU:HD21	1:B:607:GLN:OE1	2.10	0.51
1:A:317:LEU:N	1:A:361:ASP:OD1	2.40	0.51
1:B:148:VAL:HG22	1:B:508:HIS:HD2	1.76	0.51
1:B:608:ARG:HA	1:B:617:VAL:O	2.10	0.51
1:A:104:CYS:C	1:A:106:ALA:H	2.13	0.51
1:B:226:LEU:HD12	1:B:234:ILE:HG12	1.92	0.50
1:B:107:GLU:HB3	1:B:108:PRO:CA	2.38	0.50
1:B:232:THR:O	1:B:236:LYS:HG2	2.12	0.49
1:B:353:ILE:CD1	1:B:427:ILE:HG23	2.41	0.49
1:A:14:ASP:CG	1:A:17:THR:HG22	2.32	0.49
1:B:225:LEU:N	1:B:225:LEU:CD1	2.76	0.49
1:B:416:ARG:O	1:B:420:SER:HB3	2.12	0.49
1:B:84:TYR:CE2	1:B:86:TRP:CD1	3.01	0.49
1:B:531:ARG:HD2	1:B:570:ALA:HB3	1.94	0.49
1:B:568:LEU:O	1:B:569:ARG:HG3	2.13	0.49
1:A:333:HIS:CG	1:A:368:GLN:HB3	2.47	0.49
1:A:125:ASP:O	1:A:127:HIS:N	2.42	0.48
1:A:46:PHE:HZ	1:A:75:ALA:HB2	1.78	0.48
1:B:435:ASP:O	1:B:436:VAL:HB	2.12	0.48
1:B:565:ASN:O	1:B:566:ALA:HB3	2.13	0.48
1:B:520:HIS:HE1	1:B:589:VAL:O	1.97	0.48
1:B:68:ARG:NH1	1:B:82:GLU:OE2	2.46	0.48
1:A:136:GLN:HB2	1:A:494:ALA:O	2.13	0.48
1:A:411:ALA:HB3	1:A:412:PRO:HD3	1.96	0.48
1:B:165:TYR:CE2	1:B:480:VAL:CG2	2.96	0.48
1:B:82:GLU:HB3	1:B:99:VAL:HB	1.95	0.48
1:A:107:GLU:HA	1:A:108:PRO:HA	1.74	0.47
1:A:125:ASP:C	1:A:127:HIS:H	2.15	0.47
1:A:171:GLN:HB2	1:A:179:TYR:CE1	2.49	0.47
1:A:96:CYS:C	1:A:115:TRP:HH2	2.18	0.47
1:B:305:GLN:O	1:B:309:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PRO:HB2	1:A:550:TYR:CE2	2.50	0.47
1:B:262:ARG:HA	1:B:591:MET:CE	2.45	0.47
1:B:147:GLU:HG3	1:B:196:PRO:HA	1.97	0.47
1:A:270:VAL:O	1:A:319:LEU:HD12	2.15	0.47
1:A:548:ALA:HB2	1:A:586:HIS:CD2	2.49	0.47
1:B:353:ILE:HD13	1:B:427:ILE:HG23	1.96	0.47
1:A:608:ARG:HA	1:A:617:VAL:O	2.16	0.46
1:A:83:THR:HA	1:A:97:GLU:O	2.16	0.46
1:B:167:PRO:HD2	1:B:238:TYR:OH	2.16	0.46
1:A:43:ASP:O	1:A:44:ARG:HB3	2.15	0.46
1:A:296:LEU:HD21	1:A:342:GLU:O	2.16	0.45
1:A:123:ARG:HG2	1:A:125:ASP:HB2	1.98	0.45
1:B:191:TYR:HA	1:B:205:GLY:O	2.16	0.45
1:A:255:ALA:O	1:A:257:ARG:N	2.49	0.45
1:A:123:ARG:O	1:A:124:ALA:CB	2.65	0.45
1:A:236:LYS:O	1:A:237:THR:C	2.55	0.45
1:B:231:HIS:CE1	1:B:597:HIS:HD2	2.34	0.45
1:A:585:LEU:HD12	1:A:585:LEU:O	2.16	0.45
1:B:433:TYR:OH	1:B:478:GLU:HA	2.17	0.45
1:A:104:CYS:C	1:A:106:ALA:N	2.70	0.45
1:B:145:PRO:HA	1:B:198:GLY:HA3	1.98	0.44
1:B:114:LEU:HD23	1:B:207:TRP:HB3	1.99	0.44
1:B:157:GLY:O	1:B:190:GLY:HA3	2.17	0.44
1:B:269:TRP:HB3	1:B:550:TYR:CD1	2.52	0.44
1:B:467:TYR:CE2	1:B:471:HIS:CE1	3.06	0.44
1:A:72:ALA:O	1:A:73:GLY:O	2.35	0.44
1:B:255:ALA:O	1:B:259:PRO:HA	2.17	0.44
1:A:597:HIS:HA	1:A:608:ARG:O	2.18	0.44
1:A:616:ALA:HB2	1:A:632:GLY:HA2	2.00	0.44
1:A:398:TRP:CE2	3:A:702:DJN:H12	2.53	0.44
1:A:143:SER:O	1:A:144:TRP:O	2.35	0.44
1:A:436:VAL:O	1:A:437:PHE:C	2.56	0.43
1:A:186:PRO:HA	1:A:189:ALA:HB3	1.99	0.43
1:B:118:PRO:HB3	1:B:204:VAL:O	2.18	0.43
1:B:607:GLN:O	1:B:618:THR:HA	2.18	0.43
1:A:433:TYR:HA	1:A:476:SER:OG	2.19	0.43
1:A:232:THR:HG21	1:A:596:ARG:HA	2.01	0.43
1:A:248:LEU:HD12	1:A:522:CYS:SG	2.59	0.43
1:A:499:GLN:HB3	1:A:528:MET:SD	2.59	0.43
1:B:14:ASP:HB3	1:B:17:THR:HG23	1.99	0.43
1:B:274:ILE:HG22	1:B:275:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:O	1:B:314:ALA:CB	2.67	0.43
1:B:553:ARG:NH2	1:B:562:GLY:O	2.52	0.43
1:A:260:SER:O	1:A:261:VAL:C	2.56	0.43
1:A:543:LEU:O	1:A:544:LEU:C	2.57	0.43
1:B:27:ALA:HB2	1:B:177:HIS:ND1	2.34	0.42
1:A:566:ALA:C	1:A:568:LEU:N	2.73	0.42
1:B:35:ILE:HG21	1:B:118:PRO:HD2	2.00	0.42
1:A:325:ALA:HB3	1:A:336:TYR:CE1	2.54	0.42
1:A:160:GLU:OE1	1:A:483:TRP:HB3	2.19	0.42
1:A:274:ILE:HG22	1:A:275:LYS:N	2.35	0.42
1:A:90:SER:HB3	1:B:417:ARG:HA	2.02	0.42
1:B:10:MET:C	1:B:10:MET:SD	2.98	0.42
1:B:231:HIS:HE1	1:B:597:HIS:HD2	1.67	0.42
1:B:230:ASP:OD2	1:B:596:ARG:NH2	2.48	0.42
1:B:135:GLU:HA	1:B:165:TYR:CE1	2.54	0.41
1:B:197:ALA:HA	1:B:198:GLY:HA2	1.82	0.41
1:B:145:PRO:O	1:B:197:ALA:HB1	2.20	0.41
1:B:258:ASN:ND2	1:B:472:GLY:HA2	2.35	0.41
1:A:84:TYR:CD2	1:A:86:TRP:CD1	3.08	0.41
1:B:134:HIS:C	1:B:134:HIS:CD2	2.94	0.41
1:B:378:THR:O	1:B:379:PHE:C	2.59	0.41
1:A:322:ASP:HA	1:A:366:HIS:HB3	2.02	0.41
1:A:433:TYR:OH	1:A:478:GLU:HA	2.21	0.41
1:A:498:PHE:HE2	1:A:511:PRO:HB3	1.85	0.41
1:A:60:GLU:HA	1:A:65:VAL:HG12	2.03	0.41
1:B:320:HIS:C	1:B:320:HIS:CD2	2.94	0.41
1:A:48:PHE:HB3	1:A:71:PHE:CE2	2.56	0.41
1:A:52:ALA:HB3	1:A:73:GLY:HA3	2.02	0.41
1:B:109:ARG:NH2	1:B:111:ASP:OD1	2.53	0.41
1:B:435:ASP:OD2	3:B:702:DJN:N5	2.54	0.41
1:A:325:ALA:HB3	1:A:336:TYR:CD1	2.56	0.41
1:A:408:ALA:HB3	1:A:452:MET:SD	2.61	0.41
1:B:209:GLU:HB2	1:B:210:PRO:HD2	2.01	0.41
1:A:251:LEU:HD12	1:A:521:ASP:C	2.41	0.41
1:A:350:LYS:NZ	1:A:354:ASP:OD2	2.52	0.41
1:B:416:ARG:O	1:B:420:SER:CB	2.69	0.41
1:B:527:TRP:CD1	1:B:547:GLY:HA3	2.55	0.41
1:B:268:SER:HA	1:B:549:PRO:HG2	2.03	0.41
1:A:550:TYR:CG	1:A:553:ARG:HD3	2.55	0.41
1:B:269:TRP:CE2	1:B:526:PRO:HG3	2.57	0.40
1:B:570:ALA:O	1:B:571:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:HB3	1:A:490:PHE:CZ	2.57	0.40
1:A:22:PHE:CE1	1:A:225:LEU:HD11	2.56	0.40
1:A:498:PHE:CD1	1:A:498:PHE:C	2.94	0.40
1:B:123:ARG:O	1:B:124:ALA:CB	2.69	0.40
1:B:139:MET:HB3	1:B:510:ILE:HB	2.04	0.40
1:A:565:ASN:O	1:A:566:ALA:HB2	2.22	0.40
1:B:193:ILE:CG1	1:B:194:ASP:N	2.84	0.40
1:B:209:GLU:OE2	1:B:454:ARG:NE	2.52	0.40
1:B:46:PHE:N	1:B:46:PHE:CD1	2.90	0.40
1:B:54:VAL:HA	1:B:70:VAL:O	2.21	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	626/640 (98%)	542 (87%)	61 (10%)	23 (4%)	3	11
1	B	628/640 (98%)	537 (86%)	75 (12%)	16 (2%)	5	19
All	All	1254/1280 (98%)	1079 (86%)	136 (11%)	39 (3%)	4	14

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLY
1	A	75	ALA
1	A	78	ASP
1	A	106	ALA
1	A	125	ASP
1	A	566	ALA
1	A	630	ALA
1	B	43	ASP

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Mol	Chain	Res	Type
1	B	45	SER
1	B	124	ALA
1	B	125	ASP
1	B	126	ALA
1	B	175	ASP
1	B	507	ARG
1	B	565	ASN
1	B	569	ARG
1	A	79	TYR
1	A	256	ALA
1	A	567	ALA
1	B	436	VAL
1	A	76	GLY
1	A	109	ARG
1	A	289	GLN
1	B	134	HIS
1	B	546	GLY
1	A	44	ARG
1	A	107	GLU
1	A	123	ARG
1	A	144	TRP
1	A	175	ASP
1	A	565	ASN
1	B	274	ILE
1	A	549	PRO
1	B	566	ALA
1	A	105	GLY
1	A	266	GLY
1	B	73	GLY
1	B	145	PRO
1	A	436	VAL

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	511/520 (98%)	495 (97%)	16 (3%)	40 74
1	B	511/520 (98%)	485 (95%)	26 (5%)	24 55
All	All	1022/1040 (98%)	980 (96%)	42 (4%)	30 64

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	ARG
1	A	23	SER
1	A	30	SER
1	A	38	GLN
1	A	45	SER
1	A	109	ARG
1	A	204	VAL
1	A	227	ASP
1	A	320	HIS
1	A	436	VAL
1	A	493	TYR
1	A	523	VAL
1	A	530	ASP
1	A	568	LEU
1	A	594	LEU
1	B	3	GLN
1	B	15	GLU
1	B	23	SER
1	B	69	SER
1	B	109	ARG
1	B	125	ASP
1	B	150	THR
1	B	214	ARG
1	B	268	SER
1	B	294	ASP
1	B	297	VAL
1	B	358	GLU
1	B	387	LEU
1	B	493	TYR
1	B	512	VAL
1	B	517	LEU

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Mol	Chain	Res	Type
1	B	521	ASP
1	B	530	ASP
1	B	540	LEU
1	B	554	ASP
1	B	565	ASN
1	B	571	ARG
1	B	574	ASN
1	B	578	ARG
1	B	598	ASP
1	B	618	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	188	ASN
1	A	508	HIS
1	A	516	ASN
1	B	231	HIS
1	B	258	ASN
1	B	333	HIS
1	B	368	GLN
1	B	574	ASN
1	B	592	GLN
1	B	597	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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
3	DJN	B	702	-	14,14,14	1.62	1 (7%)	16,19,19	1.83	3 (18%)
3	DJN	A	702	-	14,14,14	1.56	2 (14%)	16,19,19	1.53	5 (31%)

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
3	DJN	B	702	-	-	0/6/23/23	0/1/1/1
3	DJN	A	702	-	-	0/6/23/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	DJN	C1-C2	-5.16	1.47	1.52
3	A	702	DJN	C1-C2	-4.64	1.47	1.52
3	A	702	DJN	O4-C4	2.10	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	DJN	C2-C1-N5	-4.54	103.34	112.33
3	B	702	DJN	C3-C4-C5	-3.71	105.58	111.02
3	B	702	DJN	O6-C6-C5	-3.38	102.90	111.09
3	A	702	DJN	C3-C4-C5	-2.95	106.70	111.02
3	A	702	DJN	O7-C7-C8	-2.60	117.23	122.06
3	A	702	DJN	O7-C7-N2	2.43	126.42	121.95
3	A	702	DJN	O6-C6-C5	-2.21	105.73	111.09
3	A	702	DJN	C1-N5-C5	2.14	114.23	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	DJN	1	0
3	A	702	DJN	1	0

## 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	630/640 (98%)	0.05	22 (3%)	44 34	40, 73, 113, 164	0
1	B	630/640 (98%)	0.32	41 (6%)	18 11	47, 84, 122, 175	0
All	All	1260/1280 (98%)	0.18	63 (5%)	28 19	40, 79, 118, 175	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	ALA	8.9
1	B	571	ARG	8.7
1	A	104	CYS	7.0
1	B	105	GLY	6.6
1	B	104	CYS	6.3
1	B	570	ALA	6.1
1	A	106	ALA	5.2
1	B	566	ALA	4.8
1	B	572	THR	4.7
1	B	567	ALA	4.6
1	A	43	ASP	4.2
1	A	107	GLU	4.2
1	B	107	GLU	4.0
1	B	565	ASN	4.0
1	A	569	ARG	3.9
1	A	108	PRO	3.7
1	B	569	ARG	3.7
1	B	494	ALA	3.6
1	A	105	GLY	3.2
1	B	197	ALA	3.1
1	B	512	VAL	3.1
1	A	42	GLU	3.0
1	A	102	ARG	2.8
1	B	606	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	109	ARG	2.8
1	B	526	PRO	2.8
1	B	178	ALA	2.8
1	A	103	GLU	2.8
1	B	493	TYR	2.7
1	A	44	ARG	2.6
1	B	358	GLU	2.6
1	B	568	LEU	2.5
1	A	632	GLY	2.5
1	B	491	CYS	2.5
1	B	137	GLY	2.5
1	B	292	LYS	2.5
1	B	502	SER	2.5
1	B	136	GLN	2.5
1	B	492	HIS	2.5
1	A	565	ASN	2.5
1	B	564	MET	2.4
1	B	320	HIS	2.4
1	A	313	GLY	2.3
1	B	588	ARG	2.3
1	B	608	ARG	2.3
1	A	172	LEU	2.3
1	B	551	LEU	2.3
1	B	623	ALA	2.3
1	A	527	TRP	2.3
1	B	133	THR	2.3
1	B	123	ARG	2.2
1	B	318	TYR	2.2
1	A	310	HIS	2.2
1	A	314	ALA	2.2
1	A	304	ARG	2.1
1	A	76	GLY	2.1
1	A	177	HIS	2.1
1	B	34	GLY	2.1
1	A	491	CYS	2.1
1	B	269	TRP	2.0
1	B	285	TYR	2.0
1	B	496	TYR	2.0
1	B	143	SER	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
3	DJN	B	702	14/14	0.93	0.21	56,65,68,71	0
4	CA	B	703	1/1	0.94	0.17	49,49,49,49	0
3	DJN	A	702	14/14	0.97	0.18	43,47,58,59	0
4	CA	A	703	1/1	0.97	0.18	37,37,37,37	0
2	ZN	B	701	1/1	0.99	0.08	56,56,56,56	0
2	ZN	A	701	1/1	1.00	0.10	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.