



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 5WZR / pdb_00005wzr
Title : Alpha-N-acetylgalactosaminidase NagBb from Bifidobacterium bifidum - Gal-NHAc-DNJ complex
Authors : Sato, M.; Arakawa, T.; Ashida, H.; Fushinobu, S.
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

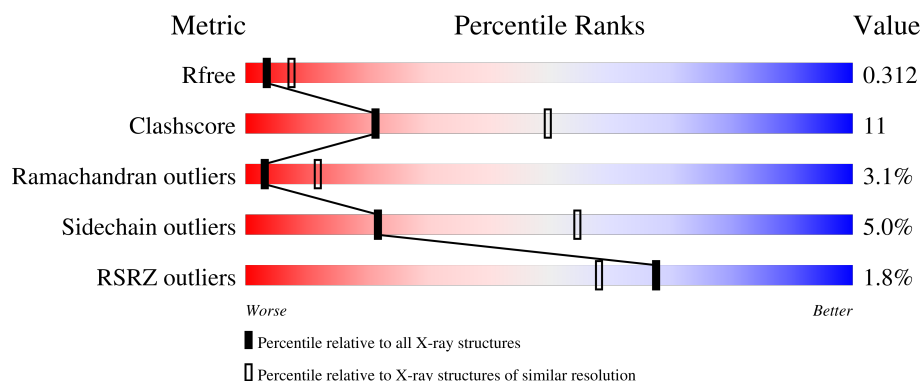
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	% 72% 23% ..
1	B	640	3% 71% 25% ..

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			

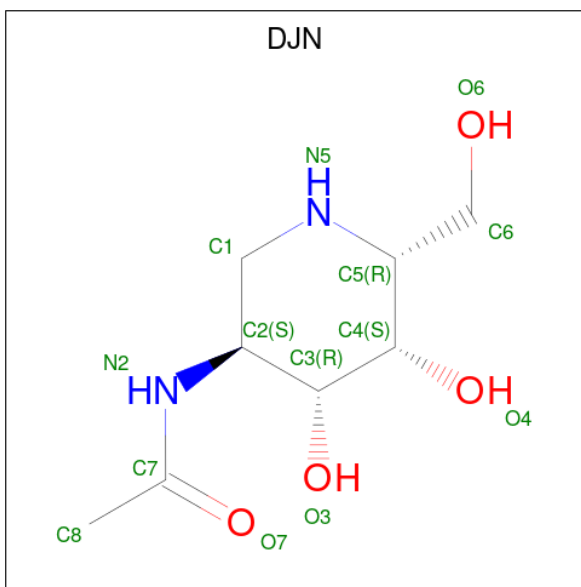
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is N-[(3S,4R,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)piperidin-3-yl]acetamide (CCD ID: DJN) (formula: C₈H₁₆N₂O₄).



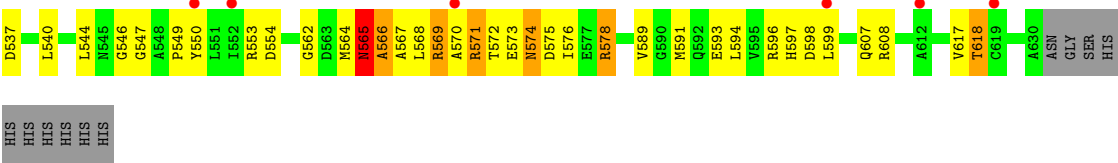
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	2	4		
3	B	1	Total	C	N	O	0	0
			14	8	2	4		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.63Å 128.48Å 176.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.95 – 2.79 103.95 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (103.95-2.79) 98.7 (103.95-2.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.229 , 0.313 0.232 , 0.312	Depositor DCC
R_{free} test set	1852 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10008	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, ZN, 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	0.69	0/5124	0.95	7/6963 (0.1%)
1	B	0.66	0/5129	0.97	6/6971 (0.1%)
All	All	0.67	0/10253	0.96	13/13934 (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	B	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	99	VAL	N-CA-C	7.93	116.09	107.60
1	B	99	VAL	CB-CA-C	-6.05	104.22	111.18
1	B	485	VAL	CA-C-N	-6.04	113.40	119.56
1	B	485	VAL	C-N-CA	-6.04	113.40	119.56
1	A	117	ALA	CA-C-N	5.88	125.89	119.90
1	A	117	ALA	C-N-CA	5.88	125.89	119.90
1	A	603	ASP	CA-C-N	5.42	126.62	119.84
1	A	603	ASP	C-N-CA	5.42	126.62	119.84
1	A	43	ASP	N-CA-C	5.25	119.79	113.17
1	B	523	VAL	N-CA-C	5.17	115.42	107.77
1	A	491	CYS	N-CA-C	5.08	116.39	109.18
1	B	189	ALA	N-CA-C	5.06	115.99	108.60
1	A	47	SER	N-CA-C	-5.01	103.11	110.52

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	105	0
1	B	4988	0	4685	108	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	212	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 11.

All (212) 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:124:ALA:C	1:B:126:ALA:H	2.03	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:125:ASP:C	1:B:127:HIS:H	2.09	0.60
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:139:MET:HE3	1:A:512:VAL:HG11	1.86	0.58
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:537:ASP:CG	1:B:578:ARG:HH22	2.12	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:171:GLN:HB2	1:B:179:TYR:CE2	2.41	0.56
1:B:521:ASP:OD1	1:B:521:ASP:N	2.34	0.56
1:B:239:ARG:NH1	1:B:518:VAL:O	2.38	0.56
1:A:104:CYS:C	1:A:106:ALA:H	2.13	0.55
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:HH11	1:A:451:ARG:HG2	1.71	0.55
1:B:225:LEU:HD12	1:B:225:LEU:N	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:5:THR:HG22	1:B:10:MET:HG2	1.89	0.54
1:B:267:ARG:O	1:B:549:PRO:HD2	2.07	0.54
1:B:121:PHE:O	1:B:142:ASN:ND2	2.41	0.54
1:A:125:ASP:C	1:A:127:HIS:H	2.15	0.54
1:A:14:ASP:CG	1:A:17:THR:HG22	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:96:CYS:C	1:A:115:TRP:HH2	2.18	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:123:ARG:O	1:B:124:ALA:HB2	2.08	0.52
1:B:531:ARG:CZ	1:B:572:THR:HB	2.40	0.52
1:B:19:ARG:NH2	1:B:33:ASP:O	2.43	0.52
1:B:143:SER:O	1:B:198:GLY:O	2.28	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:236:LYS:O	1:A:237:THR:C	2.55	0.50
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:B:225:LEU:N	1:B:225:LEU:CD1	2.76	0.49
1:B:84:TYR:CE2	1:B:86:TRP:CD1	3.01	0.49
1:B:416:ARG:O	1:B:420:SER:HB3	2.12	0.49
1:A:104:CYS:C	1:A:106:ALA:N	2.70	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:46:PHE:HZ	1:A:75:ALA:HB2	1.78	0.48
1:A:125:ASP:O	1:A:127:HIS:N	2.42	0.48
1:B:435:ASP:O	1:B:436:VAL:HB	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:GLU:HB3	1:B:99:VAL:HB	1.95	0.48
1:B:165:TYR:CE2	1:B:480:VAL:CG2	2.96	0.48
1:A:107:GLU:HA	1:A:108:PRO:HA	1.74	0.47
1:A:171:GLN:HB2	1:A:179:TYR:CE1	2.49	0.47
1:A:260:SER:O	1:A:261:VAL:C	2.56	0.47
1:A:543:LEU:O	1:A:544:LEU:C	2.57	0.47
1:B:305:GLN:O	1:B:309:LEU:HD13	2.14	0.47
1:A:526:PRO:HB2	1:A:550:TYR:CE2	2.50	0.47
1:A:566:ALA:C	1:A:568:LEU:N	2.73	0.47
1:B:262:ARG:HA	1:B:591:MET:CE	2.45	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:147:GLU:HG3	1:B:196:PRO:HA	1.97	0.47
1:B:353:ILE:HD13	1:B:427:ILE:HG23	1.96	0.47
1:B:10:MET:SD	1:B:10:MET:C	2.98	0.46
1:A:608:ARG:HA	1:A:617:VAL:O	2.16	0.46
1:B:134:HIS:C	1:B:134:HIS:CD2	2.94	0.46
1:B:378:THR:O	1:B:379:PHE:C	2.59	0.46
1:B:320:HIS:CD2	1:B:320:HIS:C	2.94	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:251:LEU:HD12	1:A:521:ASP:C	2.41	0.45
1:A:436:VAL:O	1:A:437:PHE:C	2.56	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:B:231:HIS:CE1	1:B:597:HIS:HD2	2.34	0.45
1:A:498:PHE:CD1	1:A:498:PHE:C	2.94	0.45
1:A:585:LEU:O	1:A:585:LEU:HD12	2.16	0.45
1:B:433:TYR:OH	1:B:478:GLU:HA	2.17	0.45
1:B:393:PRO:O	1:B:404:THR:OG1	2.34	0.45
1:B:114:LEU:HD23	1:B:207:TRP:HB3	1.99	0.44
1:B:145:PRO:HA	1:B:198:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:HIS:C	1:A:320:HIS:CD2	2.95	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:613:ASP:OD1	1:A:615:THR:OG1	2.34	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:B:125:ASP:C	1:B:127:HIS:N	2.76	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:306:MET:O	1:B:307:ARG:C	2.61	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:41:ARG:O	1:A:42:GLU:C	2.62	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:574:ASN:O	1:B:575:ASP:C	2.61	0.43
1:B:274:ILE:HG22	1:B:275:LYS:N	2.33	0.43
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:B:27:ALA:HB2	1:B:177:HIS:ND1	2.34	0.42
1:B:35:ILE:HG21	1:B:118:PRO:HD2	2.00	0.42
1:B:143:SER:O	1:B:144:TRP:C	2.62	0.42
1:A:325:ALA:HB3	1:A:336:TYR:CE1	2.54	0.42
1:A:201:TYR:CD1	1:A:201:TYR:C	2.97	0.42
1:A:238:TYR:O	1:A:239:ARG:C	2.62	0.42
1:A:528:MET:HE1	1:A:562:GLY:HA3	2.02	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:A:105:GLY:O	1:A:106:ALA:C	2.62	0.42
1:B:366:HIS:CD2	1:B:366:HIS:C	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:135:GLU:C	1:A:165:TYR:CD2	2.99	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:594:LEU:HD12	1:A:594:LEU:C	2.46	0.41
1:A:60:GLU:HA	1:A:65:VAL:HG12	2.03	0.41
1:A:48:PHE:HB3	1:A:71:PHE:CE2	2.56	0.41
1:A:328:GLY:O	1:A:329:TYR:C	2.62	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:B:575:ASP:O	1:B:576:ILE:C	2.64	0.41
1:A:37:PRO:C	1:A:38:GLN:HG2	2.45	0.41
1:A:325:ALA:HB3	1:A:336:TYR:CD1	2.56	0.41
1:A:350:LYS:NZ	1:A:354:ASP:OD2	2.52	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:B:268:SER:HA	1:B:549:PRO:HG2	2.03	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: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
1:A:476:SER:HB3	1:A:490:PHE:CZ	2.57	0.40
1:B:251:LEU:HD12	1:B:521:ASP:C	2.46	0.40
1:A:22:PHE:CE1	1:A:225:LEU:HD11	2.56	0.40
1:A:626:TYR:CD1	1:A:626:TYR:C	2.99	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: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
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

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	626/640 (98%)	542 (87%)	61 (10%)	23 (4%)	2	9
1	B	628/640 (98%)	537 (86%)	75 (12%)	16 (2%)	4	16
All	All	1254/1280 (98%)	1079 (86%)	136 (11%)	39 (3%)	3	12

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
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

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Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	511/520 (98%)	490 (96%)	21 (4%)	27	62
1	B	511/520 (98%)	481 (94%)	30 (6%)	18	48
All	All	1022/1040 (98%)	971 (95%)	51 (5%)	22	54

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	LEU
1	A	19	ARG
1	A	23	SER
1	A	30	SER
1	A	38	GLN
1	A	45	SER
1	A	67	VAL
1	A	109	ARG

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Mol	Chain	Res	Type
1	A	204	VAL
1	A	227	ASP
1	A	320	HIS
1	A	352	LEU
1	A	359	GLN
1	A	436	VAL
1	A	486	PRO
1	A	493	TYR
1	A	501	ARG
1	A	523	VAL
1	A	568	LEU
1	A	594	LEU
1	B	3	GLN
1	B	9	THR
1	B	15	GLU
1	B	23	SER
1	B	28	THR
1	B	60	GLU
1	B	69	SER
1	B	109	ARG
1	B	125	ASP
1	B	133	THR
1	B	150	THR
1	B	214	ARG
1	B	268	SER
1	B	294	ASP
1	B	297	VAL
1	B	377	ARG
1	B	387	LEU
1	B	493	TYR
1	B	512	VAL
1	B	517	LEU
1	B	521	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	599	LEU
1	B	618	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	289	GLN
1	A	333	HIS
1	A	508	HIS
1	A	516	ASN
1	A	631	ASN
1	B	38	GLN
1	B	171	GLN
1	B	258	ASN
1	B	310	HIS
1	B	333	HIS
1	B	368	GLN
1	B	440	ASN
1	B	574	ASN
1	B	597	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	702	-	14,14,14	1.56	2 (14%)	15,19,19	1.59	5 (33%)
3	DJN	B	702	-	14,14,14	1.62	1 (7%)	15,19,19	1.87	3 (20%)

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	A	702	-	-	0/6/23/23	0/1/1/1
3	DJN	B	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	2.00	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	-4.36	103.34	112.47
3	B	702	DJN	C3-C4-C5	-3.71	105.58	111.02
3	B	702	DJN	O6-C6-C5	-3.38	102.90	111.10
3	A	702	DJN	C3-C4-C5	-2.95	106.70	111.02
3	A	702	DJN	O7-C7-C8	-2.71	117.23	122.05
3	A	702	DJN	O7-C7-N2	2.51	126.42	121.98
3	A	702	DJN	O6-C6-C5	-2.21	105.73	111.10
3	A	702	DJN	C1-N5-C5	2.06	114.23	109.71

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	A	702	DJN	1	0
3	B	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	630/640 (98%)	0.05	6 (0%) 79 72	40, 73, 113, 164	0
1	B	630/640 (98%)	0.34	17 (2%) 56 46	47, 84, 122, 175	0
All	All	1260/1280 (98%)	0.19	23 (1%) 67 58	40, 79, 118, 175	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	TRP	4.2
1	A	567	ALA	3.1
1	B	552	ILE	3.0
1	B	1	MET	2.8
1	B	114	LEU	2.8
1	B	306	MET	2.8
1	A	630	ALA	2.7
1	B	314	ALA	2.7
1	A	544	LEU	2.6
1	B	124	ALA	2.6
1	A	632	GLY	2.5
1	B	178	ALA	2.4
1	B	570	ALA	2.4
1	A	306	MET	2.4
1	B	599	LEU	2.3
1	A	612	ALA	2.2
1	B	612	ALA	2.2
1	B	508	HIS	2.2
1	B	324	TRP	2.2
1	B	550	TYR	2.2
1	B	270	VAL	2.1
1	B	619	CYS	2.1
1	B	272	VAL	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 oligosaccharides 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, 95th 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	0.91	0.08	56,65,68,71	0
3	DJN	A	702	14/14	0.95	0.10	43,47,58,59	0
4	CA	B	703	1/1	0.98	0.04	49,49,49,49	0
4	CA	A	703	1/1	0.99	0.05	37,37,37,37	0
2	ZN	A	701	1/1	1.00	0.04	50,50,50,50	0
2	ZN	B	701	1/1	1.00	0.01	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.