



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:18 pm BST

PDB ID : 3UES  
Title : Crystal structure of alpha-1,3/4-fucosidase from Bifidobacterium longum subsp. infantis complexed with deoxyfuconojirimycin  
Authors : Sakurama, H.; Fushinobu, S.; Yoshida, E.; Honda, Y.; Hidaka, M.; Ashida, H.; Kitaoka, M.; Katayama, T.; Yamamoto, K.; Kumagai, H.  
Deposited on : 2011-10-31  
Resolution : 1.60 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

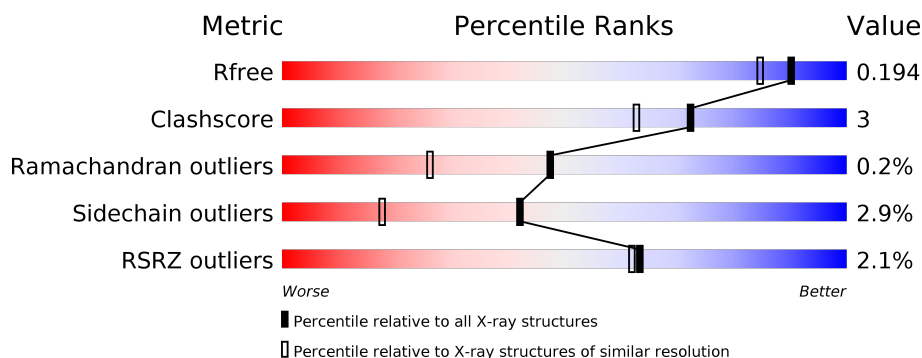
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	478	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• •</div> </div> </div>
1	B	478	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

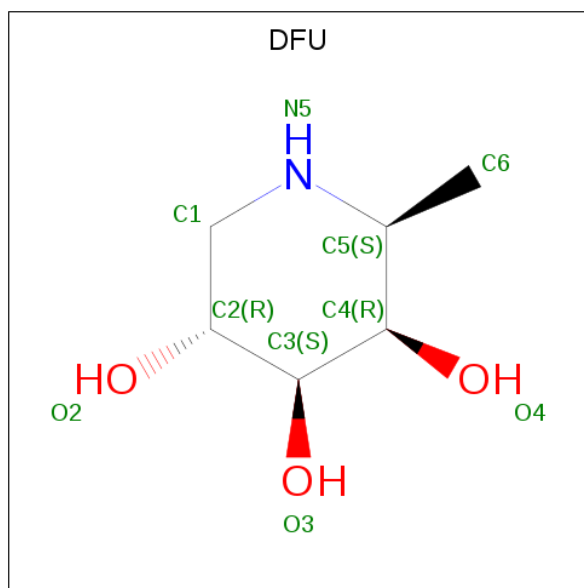
There are 5 unique types of molecules in this entry. The entry contains 8320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-1,3/4-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3583	2241	645	684	13			
1	B	458	Total	C	N	O	S	0	0	0
			3587	2243	646	685	13			

- Molecule 2 is (2S,3R,4S,5R)-2-METHYLPYPERIDINE-3,4,5-TRIOL (three-letter code: DFU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

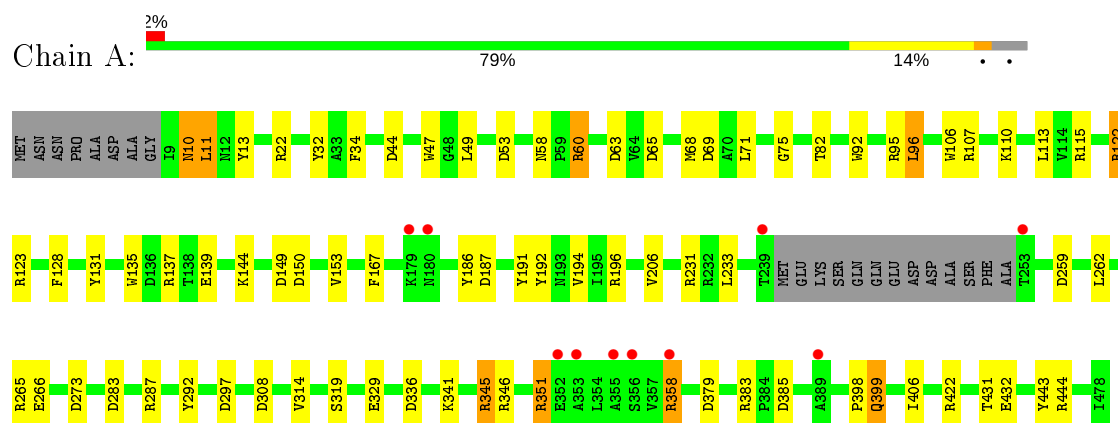
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	542	Total	O	0	0
			542	542		
5	B	578	Total	O	0	0
			578	578		

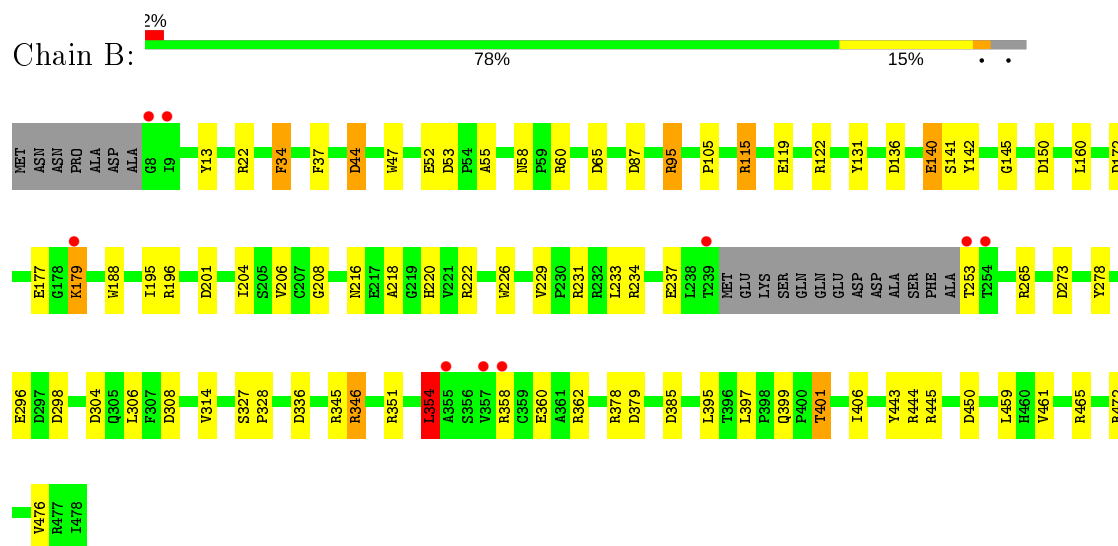
### 3 Residue-property plots [i](#)

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-1,3/4-fucosidase



- Molecule 1: Alpha-1,3/4-fucosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.98Å 120.60Å 142.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.91 – 1.60 25.91 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.91-1.60) 99.4 (25.91-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.160 , 0.191 0.163 , 0.194	Depositor DCC
$R_{free}$ test set	7303 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8320	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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: DFU, NA, EDO

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	1.45	11/3670 (0.3%)	1.50	54/4993 (1.1%)
1	B	1.49	13/3674 (0.4%)	1.55	56/4998 (1.1%)
All	All	1.47	24/7344 (0.3%)	1.53	110/9991 (1.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	TRP	CD2-CE2	7.97	1.50	1.41
1	B	177	GLU	CD-OE1	7.80	1.34	1.25
1	A	135	TRP	CD2-CE2	7.45	1.50	1.41
1	A	106	TRP	CD2-CE2	7.15	1.50	1.41
1	B	378	ARG	CZ-NH1	6.71	1.41	1.33
1	A	432	GLU	CB-CG	-6.70	1.39	1.52
1	B	95	ARG	CZ-NH2	6.43	1.41	1.33
1	A	266	GLU	CD-OE2	6.29	1.32	1.25
1	B	13	TYR	CZ-OH	6.26	1.48	1.37
1	B	226	TRP	CD2-CE2	6.16	1.48	1.41
1	A	186	TYR	CE2-CZ	6.14	1.46	1.38
1	B	142	TYR	CE2-CZ	5.91	1.46	1.38
1	A	139	GLU	CG-CD	5.88	1.60	1.51
1	A	432	GLU	CD-OE2	5.84	1.32	1.25
1	B	296	GLU	CD-OE2	5.79	1.32	1.25
1	A	167	PHE	CE2-CZ	5.52	1.47	1.37
1	B	145	GLY	C-O	5.49	1.32	1.23
1	A	92	TRP	CD2-CE2	5.41	1.47	1.41
1	B	47	TRP	NE1-CE2	5.39	1.44	1.37
1	A	47	TRP	CZ3-CH2	5.35	1.48	1.40
1	B	443	TYR	CE2-CZ	5.33	1.45	1.38
1	B	237	GLU	CG-CD	5.21	1.59	1.51
1	B	142	TYR	CG-CD1	5.11	1.45	1.39
1	A	32	TYR	CA-CB	5.09	1.65	1.53

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ARG	NE-CZ-NH1	17.20	128.90	120.30
1	A	122	ARG	NE-CZ-NH1	16.25	128.42	120.30
1	B	122	ARG	NE-CZ-NH2	-14.36	113.12	120.30
1	A	122	ARG	NE-CZ-NH2	-13.47	113.56	120.30
1	B	346	ARG	NE-CZ-NH1	13.02	126.81	120.30
1	A	385	ASP	CB-CG-OD1	12.07	129.16	118.30
1	B	196	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	B	378	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	351	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	B	385	ASP	CB-CG-OD1	10.39	127.65	118.30
1	A	346	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	B	231	ARG	NE-CZ-NH2	-10.33	115.13	120.30
1	A	385	ASP	CB-CG-OD2	-10.29	109.04	118.30
1	A	150	ASP	CB-CG-OD1	9.79	127.11	118.30
1	B	351	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	A	231	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	B	53	ASP	CB-CG-OD1	9.04	126.43	118.30
1	A	287	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	A	53	ASP	CB-CG-OD2	-8.97	110.22	118.30
1	B	95	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	A	192	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	B	179	LYS	CD-CE-NZ	-8.64	91.83	111.70
1	B	345	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	B	201	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	196	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	222	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	265	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	A	65	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	22	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	201	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	B	354	LEU	CB-CG-CD2	-7.65	98.00	111.00
1	A	192	TYR	CB-CG-CD1	7.60	125.56	121.00
1	A	128	PHE	CB-CG-CD2	-7.57	115.50	120.80
1	B	60	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	B	37	PHE	CB-CG-CD2	-7.46	115.58	120.80
1	B	44	ASP	CB-CG-OD1	7.44	124.99	118.30
1	B	385	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	A	383	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	A	115	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	432	GLU	CG-CD-OE2	7.21	132.71	118.30
1	A	308	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	379	ASP	CB-CG-OD1	7.19	124.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	B	150	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	443	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	B	362	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	122	ARG	CD-NE-CZ	6.70	132.98	123.60
1	B	379	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	122	ARG	CD-NE-CZ	6.67	132.93	123.60
1	A	53	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	273	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	273	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	69	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	308	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	379	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	346	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	69	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	65	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	472	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	11	LEU	CB-CG-CD1	6.20	121.53	111.00
1	A	149	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	136	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	123	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	115	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	298	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	346	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	191	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	445	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	87	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	A	107	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	142	TYR	CB-CG-CD2	5.78	124.47	121.00
1	A	319	SER	N-CA-CB	-5.77	101.84	110.50
1	A	196	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	22	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	345	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	278	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	113	LEU	CB-CG-CD2	-5.66	101.39	111.00
1	B	465	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	137	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	13	TYR	CZ-CE2-CD2	-5.56	114.80	119.80
1	B	196	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	431	THR	CA-CB-CG2	-5.52	104.67	112.40
1	B	95	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	297	ASP	CB-CG-OD1	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	443	TYR	CZ-CE2-CD2	-5.45	114.89	119.80
1	A	44	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	259	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	110	LYS	CD-CE-NZ	-5.38	99.32	111.70
1	B	265	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	283	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	292	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	B	308	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	187	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	71	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	B	53	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	96	LEU	CA-CB-CG	-5.24	103.24	115.30
1	A	63	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	68	MET	CA-CB-CG	5.20	122.14	113.30
1	A	231	ARG	CG-CD-NE	-5.19	100.90	111.80
1	B	160	LEU	CB-CG-CD2	5.19	119.82	111.00
1	B	131	TYR	CG-CD2-CE2	-5.17	117.17	121.30
1	B	234	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	395	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	B	445	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	52	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	B	450	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	115	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	422	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	461	VAL	CA-CB-CG1	-5.00	103.39	110.90

There are no chirality outliers.

There are no planarity outliers.

## 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	3583	0	3436	22	0
1	B	3587	0	3439	26	0
2	A	10	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	13	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	542	0	0	5	0
5	B	578	0	0	4	0
All	All	8320	0	6913	48	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 3.

All (48) 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:351:ARG:HH11	1:A:351:ARG:CG	1.73	1.00
1:A:58:ASN:HB3	5:A:852:HOH:O	1.64	0.97
1:A:351:ARG:HG2	1:A:351:ARG:NH1	1.58	0.96
1:A:351:ARG:HH11	1:A:351:ARG:HG2	0.80	0.92
1:B:399:GLN:O	1:B:401:THR:HG22	1.89	0.71
1:B:216:ASN:HD22	1:B:218:ALA:H	1.37	0.70
1:A:398:PRO:HB2	1:A:399:GLN:HE21	1.56	0.69
1:B:216:ASN:HD21	1:B:220:HIS:H	1.44	0.65
1:B:58:ASN:HB3	5:B:832:HOH:O	1.97	0.63
1:A:314:VAL:HG12	1:A:444:ARG:HH11	1.63	0.62
1:B:95:ARG:HD2	5:B:603:HOH:O	2.01	0.60
1:A:314:VAL:HG12	1:A:444:ARG:NH1	2.17	0.60
1:A:95:ARG:HD2	5:A:808:HOH:O	2.03	0.58
1:B:354:LEU:HD22	1:B:476:VAL:HG11	1.85	0.57
1:B:95:ARG:CD	5:B:603:HOH:O	2.52	0.56
1:B:358:ARG:CZ	1:B:358:ARG:HB2	2.35	0.56
1:A:95:ARG:CD	5:A:808:HOH:O	2.52	0.56
1:A:341:LYS:HE2	1:A:345:ARG:HH12	1.72	0.55
1:A:406:ILE:HD12	1:A:406:ILE:C	2.28	0.53
1:B:399:GLN:O	1:B:401:THR:CG2	2.55	0.53
1:B:216:ASN:ND2	1:B:218:ALA:H	2.05	0.53
1:A:351:ARG:NH1	1:A:351:ARG:CG	2.43	0.52
1:A:60:ARG:CD	1:A:329:GLU:HG2	2.40	0.51
1:B:229:VAL:HB	1:B:233:LEU:HD12	1.92	0.50
1:B:314:VAL:HG12	1:B:444:ARG:HH11	1.76	0.50
1:B:304:ASP:OD1	1:B:346:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG13	1:A:194:VAL:HG21	1.93	0.50
1:A:233:LEU:HD11	1:A:262:LEU:HD22	1.92	0.50
1:A:60:ARG:HD3	1:A:329:GLU:HG2	1.93	0.49
1:B:406:ILE:C	1:B:406:ILE:HD12	2.35	0.47
1:B:314:VAL:HG12	1:B:444:ARG:NH1	2.29	0.47
1:A:358:ARG:O	1:A:398:PRO:HD3	2.15	0.46
1:B:115:ARG:NH2	5:B:482:HOH:O	2.47	0.45
1:B:140:GLU:HG2	1:B:141:SER:N	2.31	0.45
1:B:459:LEU:N	1:B:459:LEU:HD12	2.32	0.45
1:A:82:THR:HA	1:A:131:TYR:HB3	1.97	0.45
1:B:115:ARG:HD2	1:B:119:GLU:OE2	2.15	0.45
1:B:204:ILE:HG22	1:B:208:GLY:HA3	1.99	0.44
1:B:327:SER:HB2	1:B:328:PRO:HD2	2.01	0.43
1:A:122:ARG:NH1	5:A:786:HOH:O	2.37	0.42
1:A:75:GLY:HA3	5:A:765:HOH:O	2.20	0.42
1:A:314:VAL:CG1	1:A:444:ARG:NH1	2.83	0.42
1:B:216:ASN:ND2	1:B:220:HIS:H	2.15	0.41
1:B:306:LEU:HA	1:B:306:LEU:HD23	1.90	0.41
1:B:55:ALA:HA	1:B:105:PRO:HD3	2.02	0.41
1:B:358:ARG:CZ	1:B:358:ARG:CB	2.98	0.41
1:A:10:ASN:HD22	1:A:10:ASN:C	2.23	0.41
1:B:195:ILE:HG21	1:B:204:ILE:HG12	2.03	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	453/478 (95%)	443 (98%)	9 (2%)	1 (0%)	47	26
1	B	454/478 (95%)	441 (97%)	12 (3%)	1 (0%)	47	26
All	All	907/956 (95%)	884 (98%)	21 (2%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	VAL
1	B	206	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	377/393 (96%)	365 (97%)	12 (3%)	39	15
1	B	377/393 (96%)	367 (97%)	10 (3%)	44	20
All	All	754/786 (96%)	732 (97%)	22 (3%)	42	18

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	LEU
1	A	34	PHE
1	A	49	LEU
1	A	60	ARG
1	A	96	LEU
1	A	144	LYS
1	A	336	ASP
1	A	345	ARG
1	A	351	ARG
1	A	358	ARG
1	A	399	GLN
1	B	34	PHE
1	B	44	ASP
1	B	140	GLU
1	B	179	LYS
1	B	253	THR
1	B	336	ASP
1	B	354	LEU
1	B	360	GLU
1	B	397	LEU

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Mol	Chain	Res	Type
1	B	401	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	399	GLN
1	B	216	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
2	DFU	B	501	-	10,10,10	3.01	5 (50%)	12,14,14	1.85	2 (16%)
2	DFU	A	501	-	10,10,10	1.87	3 (30%)	12,14,14	1.31	2 (16%)
3	EDO	B	502	-	3,3,3	0.78	0	2,2,2	0.43	0
3	EDO	A	502	-	3,3,3	0.60	0	2,2,2	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DFU	B	501	-	-	-	0/1/1/1
2	DFU	A	501	-	-	-	0/1/1/1
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	DFU	C1-N5	5.60	1.55	1.47
2	B	501	DFU	C5-N5	4.55	1.51	1.45
2	A	501	DFU	C1-N5	4.11	1.53	1.47
2	B	501	DFU	C6-C5	3.79	1.60	1.52
2	B	501	DFU	C2-C3	3.02	1.57	1.52
2	A	501	DFU	C4-C5	2.88	1.59	1.53
2	B	501	DFU	C1-C2	-2.19	1.50	1.52
2	A	501	DFU	C6-C5	2.06	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	DFU	C3-C4-C5	-4.24	104.14	110.34
2	B	501	DFU	C6-C5-N5	-3.78	102.71	109.91
2	A	501	DFU	C1-N5-C5	2.61	116.23	109.57
2	A	501	DFU	O3-C3-C4	-2.20	105.27	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	457/478 (95%)	-0.21	10 (2%) 62 60	13, 19, 36, 62	0
1	B	458/478 (95%)	-0.27	9 (1%) 65 64	12, 18, 33, 57	0
All	All	915/956 (95%)	-0.24	19 (2%) 63 62	12, 19, 34, 62	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	5.4
1	B	8	GLY	4.4
1	A	239	THR	4.4
1	A	180	ASN	4.1
1	A	179	LYS	3.6
1	A	389	ALA	3.3
1	A	358	ARG	3.3
1	B	239	THR	3.2
1	B	254	THR	3.1
1	B	358	ARG	2.8
1	A	253	THR	2.6
1	B	253	THR	2.6
1	A	356	SER	2.6
1	A	352	GLU	2.5
1	B	179	LYS	2.4
1	B	9	ILE	2.4
1	A	353	ALA	2.3
1	B	355	ALA	2.1
1	B	357	VAL	2.1

### 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	DFU	A	501	10/10	0.96	0.07	15,16,17,18	0
2	DFU	B	501	10/10	0.98	0.08	12,13,14,14	0
3	EDO	A	502	4/4	0.98	0.08	17,17,18,18	0
4	NA	B	503	1/1	0.98	0.05	20,20,20,20	0
4	NA	A	503	1/1	0.99	0.04	21,21,21,21	0
3	EDO	B	502	4/4	0.99	0.07	16,17,17,18	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.