



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:47 PM UTC

PDB ID : 3UES / pdb_00003ues
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

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

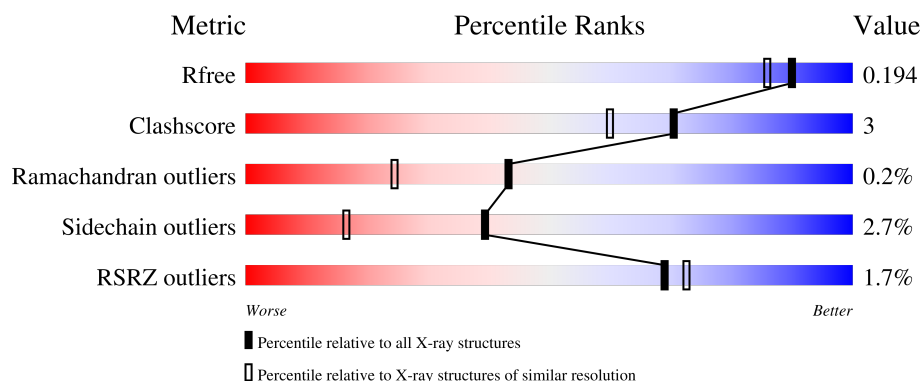
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

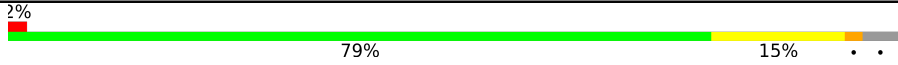
The reported resolution of this entry is 1.60 Å.

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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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	478	
1	B	478	

2 Entry composition [i](#)

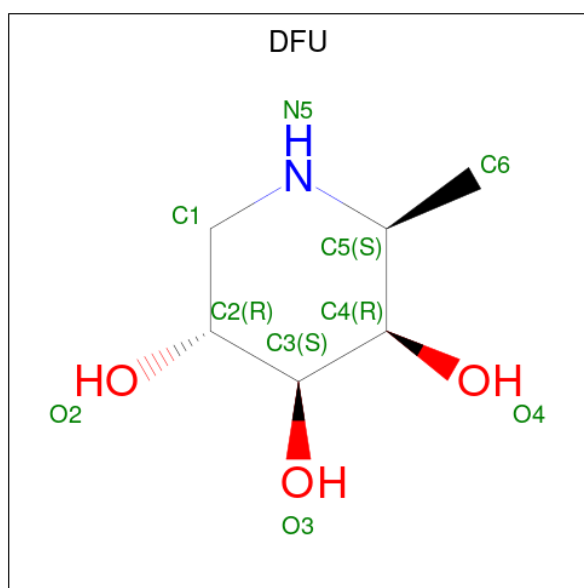
There are 5 unique types of molecules in this entry. The entry contains 8320 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: DFU) (formula: C₆H₁₃NO₃).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: NA) (formula: Na).

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

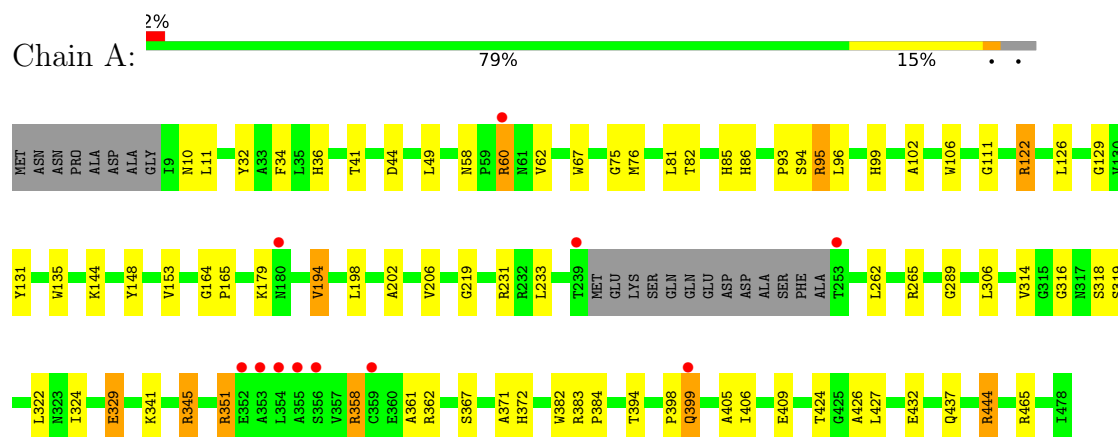
- Molecule 5 is water.

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

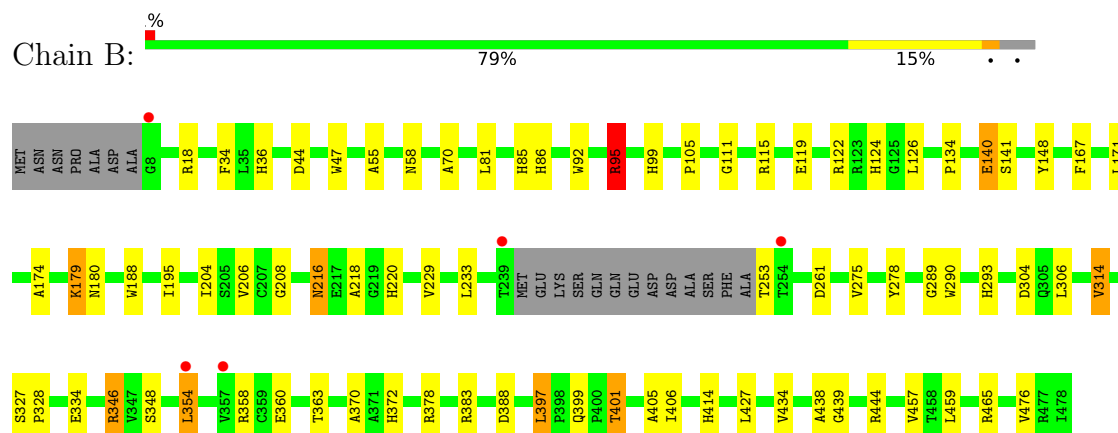
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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, α , β , γ	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) 99.7 (25.91-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: NA, DFU, 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	1.81	49/3670 (1.3%)	1.55	18/4993 (0.4%)
1	B	1.85	45/3674 (1.2%)	1.58	15/4998 (0.3%)
All	All	1.83	94/7344 (1.3%)	1.56	33/9991 (0.3%)

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	HIS	CE1-NE2	10.26	1.42	1.32
1	B	334	GLU	N-CA	8.17	1.54	1.46
1	A	67	TRP	N-CA	8.11	1.56	1.46
1	A	372	HIS	ND1-CE1	7.92	1.40	1.32
1	B	124	HIS	ND1-CE1	7.74	1.40	1.32
1	B	126	LEU	N-CA	7.66	1.55	1.46
1	B	85	HIS	CE1-NE2	7.64	1.40	1.32
1	A	85	HIS	CE1-NE2	7.37	1.40	1.32
1	B	99	HIS	CE1-NE2	6.75	1.39	1.32
1	A	85	HIS	CG-CD2	6.72	1.43	1.35
1	B	439	GLY	CA-C	6.56	1.55	1.51
1	A	372	HIS	CG-CD2	6.52	1.43	1.35
1	A	394	THR	CA-C	-6.50	1.44	1.52
1	B	47	TRP	NE1-CE2	6.46	1.44	1.37
1	B	378	ARG	CZ-NH1	6.44	1.41	1.32
1	A	81	LEU	N-CA	6.41	1.53	1.46
1	B	293	HIS	ND1-CE1	6.39	1.39	1.32
1	A	36	HIS	ND1-CE1	6.34	1.38	1.32
1	A	437	GLN	CA-C	6.33	1.60	1.52
1	A	32	TYR	CA-CB	6.27	1.65	1.53
1	B	438	ALA	N-CA	6.26	1.53	1.45
1	B	289	GLY	N-CA	6.23	1.51	1.44
1	B	36	HIS	ND1-CE1	6.18	1.38	1.32
1	A	95	ARG	C-O	6.15	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	ARG	CZ-NH2	6.12	1.41	1.33
1	B	372	HIS	ND1-CE1	6.09	1.38	1.32
1	A	106	TRP	CA-CB	6.06	1.63	1.53
1	B	397	LEU	CA-C	5.98	1.60	1.52
1	B	434	VAL	N-CA	5.94	1.53	1.46
1	A	94	SER	C-O	5.91	1.31	1.23
1	A	198	LEU	CA-C	-5.89	1.44	1.52
1	B	174	ALA	N-CA	5.88	1.53	1.46
1	B	383	ARG	CD-NE	-5.84	1.38	1.46
1	A	426	ALA	N-CA	5.83	1.53	1.46
1	A	322	LEU	N-CA	5.81	1.53	1.46
1	A	289	GLY	N-CA	5.78	1.52	1.44
1	B	81	LEU	N-CA	5.76	1.53	1.46
1	A	306	LEU	N-CA	5.75	1.53	1.46
1	A	424	THR	N-CA	5.72	1.52	1.45
1	A	164	GLY	N-CA	5.71	1.52	1.44
1	B	372	HIS	CG-CD2	5.65	1.42	1.35
1	B	405	ALA	C-O	5.64	1.30	1.23
1	B	92	TRP	CA-CB	5.63	1.60	1.54
1	B	188	TRP	CD2-CE2	5.63	1.50	1.41
1	B	86	HIS	ND1-CE1	5.62	1.38	1.32
1	A	444	ARG	N-CA	5.61	1.52	1.46
1	B	363	THR	CA-C	-5.59	1.45	1.52
1	B	314	VAL	CA-C	5.59	1.61	1.52
1	B	290	TRP	CA-C	-5.58	1.45	1.52
1	B	278	TYR	CA-CB	5.55	1.59	1.53
1	A	362	ARG	N-CA	-5.54	1.38	1.45
1	B	414	HIS	ND1-CE1	5.54	1.38	1.32
1	B	378	ARG	CD-NE	-5.53	1.38	1.46
1	A	86	HIS	CG-CD2	5.50	1.42	1.35
1	B	134	PRO	CA-C	5.50	1.59	1.52
1	B	167	PHE	N-CA	5.50	1.53	1.46
1	A	129	GLY	CA-C	-5.49	1.47	1.52
1	A	361	ALA	CA-C	-5.47	1.46	1.52
1	A	44	ASP	CA-CB	5.47	1.61	1.53
1	A	371	ALA	N-CA	-5.47	1.39	1.46
1	B	18	ARG	CA-CB	5.43	1.60	1.53
1	A	164	GLY	C-N	-5.41	1.26	1.33
1	A	93	PRO	CA-CB	5.40	1.60	1.53
1	A	318	SER	N-CA	5.35	1.52	1.46
1	B	348	SER	N-CA	5.34	1.52	1.46
1	A	324	ILE	N-CA	5.34	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	SER	C-O	-5.33	1.17	1.24
1	B	171	LEU	N-CA	5.33	1.53	1.46
1	B	457	VAL	CA-C	-5.33	1.46	1.52
1	B	261	ASP	N-CA	-5.31	1.39	1.46
1	A	111	GLY	N-CA	5.30	1.51	1.44
1	A	409	GLU	N-CA	5.29	1.52	1.46
1	A	165	PRO	C-O	5.29	1.29	1.23
1	B	122	ARG	CA-C	5.28	1.59	1.52
1	A	126	LEU	N-CA	5.27	1.52	1.46
1	A	135	TRP	CD2-CE2	5.26	1.50	1.41
1	A	427	LEU	CA-C	5.22	1.58	1.52
1	A	465	ARG	C-O	5.21	1.30	1.23
1	A	405	ALA	C-O	5.18	1.30	1.23
1	A	316	GLY	CA-C	5.18	1.59	1.51
1	B	275	VAL	N-CA	5.14	1.51	1.46
1	A	76	MET	N-CA	5.13	1.52	1.45
1	A	384	PRO	CA-CB	5.13	1.60	1.53
1	B	388	ASP	C-O	5.12	1.30	1.24
1	A	62	VAL	N-CA	5.12	1.52	1.46
1	B	188	TRP	NE1-CE2	-5.11	1.31	1.37
1	A	405	ALA	CA-C	-5.10	1.46	1.52
1	A	382	TRP	C-O	5.10	1.29	1.23
1	B	179	LYS	C-O	5.09	1.30	1.24
1	A	329	GLU	C-O	5.09	1.30	1.24
1	B	216	ASN	CA-CB	5.09	1.62	1.53
1	B	465	ARG	CA-CB	5.06	1.59	1.52
1	A	106	TRP	CD2-CE2	5.05	1.50	1.41
1	B	111	GLY	N-CA	5.01	1.51	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ASN	CA-C-N	-8.82	112.85	122.55
1	B	180	ASN	C-N-CA	-8.82	112.85	122.55
1	B	122	ARG	NE-CZ-NH1	7.40	128.90	121.50
1	A	122	ARG	NE-CZ-NH1	6.92	128.42	121.50
1	B	122	ARG	NE-CZ-NH2	-6.75	113.12	119.20
1	B	179	LYS	CD-CE-NZ	-6.27	91.83	111.90
1	A	122	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	A	432	GLU	CG-CD-OE2	6.22	132.71	118.40
1	B	122	ARG	CD-NE-CZ	6.13	132.98	124.40
1	A	122	ARG	CD-NE-CZ	6.09	132.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	TYR	N-CA-C	-5.88	104.95	111.36
1	A	319	SER	N-CA-CB	-5.78	101.84	110.17
1	A	427	LEU	CA-C-N	-5.78	113.72	119.56
1	A	427	LEU	C-N-CA	-5.78	113.72	119.56
1	B	92	TRP	O-C-N	5.73	126.02	121.55
1	B	95	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	B	427	LEU	CA-C-N	-5.58	113.92	119.56
1	B	427	LEU	C-N-CA	-5.58	113.92	119.56
1	A	179	LYS	N-CA-C	5.44	117.91	111.33
1	A	102	ALA	N-CA-C	-5.32	106.04	112.54
1	B	346	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	A	41	THR	O-C-N	5.27	127.70	122.12
1	A	383	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	148	TYR	CA-C-O	-5.20	114.91	120.42
1	B	70	ALA	N-CA-C	-5.19	105.70	111.36
1	A	194	VAL	N-CA-C	-5.18	105.66	110.53
1	B	434	VAL	N-CA-C	-5.17	101.14	108.58
1	A	265	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	219	GLY	N-CA-C	-5.09	108.25	115.43
1	A	231	ARG	CG-CD-NE	-5.05	100.90	112.00
1	B	370	ALA	N-CA-C	5.01	117.39	111.33
1	A	202	ALA	CA-C-N	-5.00	115.92	122.37
1	A	202	ALA	C-N-CA	-5.00	115.92	122.37

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
2	B	10	0	13	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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:NH1	1:A:351:ARG:HG2	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:406:ILE:C	1:A:406:ILE:HD12	2.28	0.58
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:HB2	1:B:358:ARG:CZ	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: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:B:406:ILE:HD12	1:B:406:ILE:C	2.35	0.52
1:A:351:ARG:CG	1:A:351:ARG:NH1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HD3	1:A:329:GLU:HG2	1.93	0.49
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:A:10:ASN:C	1:A:10:ASN:HD22	2.23	0.45
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:HD23	1:B:306:LEU:HA	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:B:195:ILE:HG21	1:B:204:ILE:HG12	2.03	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	453/478 (95%)	443 (98%)	9 (2%)	1 (0%)	43	24
1	B	454/478 (95%)	441 (97%)	12 (3%)	1 (0%)	43	24
All	All	907/956 (95%)	884 (98%)	21 (2%)	2 (0%)	43	24

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%)	367 (97%)	10 (3%)	39	16
1	B	377/393 (96%)	367 (97%)	10 (3%)	39	16
All	All	754/786 (96%)	734 (97%)	20 (3%)	39	16

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	345	ARG
1	A	351	ARG
1	A	358	ARG
1	A	399	GLN
1	B	34	PHE
1	B	44	ASP
1	B	95	ARG
1	B	140	GLU
1	B	179	LYS
1	B	253	THR
1	B	354	LEU
1	B	360	GLU
1	B	397	LEU
1	B	401	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	180	ASN
1	A	338	GLN
1	A	399	GLN
1	B	61	ASN
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 oligosaccharides 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	A	501	-	10,10,10	1.91	3 (30%)	12,14,14	1.31	2 (16%)
3	EDO	B	502	-	3,3,3	0.72	0	2,2,2	0.47	0
3	EDO	A	502	-	3,3,3	0.59	0	2,2,2	0.22	0
2	DFU	B	501	-	10,10,10	3.04	6 (60%)	12,14,14	1.72	2 (16%)

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	A	501	-	-	-	0/1/1/1
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
2	DFU	B	501	-	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	DFU	C1-N5	5.79	1.55	1.47
2	B	501	DFU	C5-N5	4.48	1.51	1.45
2	A	501	DFU	C1-N5	4.25	1.53	1.47
2	B	501	DFU	C6-C5	3.85	1.60	1.52
2	A	501	DFU	C4-C5	2.98	1.59	1.53
2	B	501	DFU	C2-C3	2.93	1.57	1.52
2	B	501	DFU	C1-C2	-2.19	1.50	1.52
2	A	501	DFU	C6-C5	2.09	1.56	1.52
2	B	501	DFU	O2-C2	2.02	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	DFU	C3-C4-C5	-4.30	104.14	110.40
2	B	501	DFU	C6-C5-N5	-2.84	102.71	109.47
2	A	501	DFU	C1-N5-C5	2.66	116.23	109.48
2	A	501	DFU	O3-C3-C4	-2.17	105.27	110.38

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 [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, 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	457/478 (95%)	-0.25	11 (2%) 59 63	13, 19, 36, 62	0
1	B	458/478 (95%)	-0.39	5 (1%) 78 82	12, 18, 33, 57	0
All	All	915/956 (95%)	-0.32	16 (1%) 69 72	12, 19, 34, 62	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	5.3
1	A	239	THR	5.0
1	B	239	THR	4.3
1	A	354	LEU	2.8
1	B	254	THR	2.8
1	B	8	GLY	2.6
1	A	180	ASN	2.5
1	B	354	LEU	2.5
1	A	353	ALA	2.4
1	A	356	SER	2.3
1	A	60	ARG	2.3
1	A	352	GLU	2.2
1	A	359	CYS	2.2
1	A	253	THR	2.1
1	A	399	GLN	2.1
1	B	357	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	EDO	A	502	4/4	0.97	0.06	17,17,18,18	0
2	DFU	A	501	10/10	0.98	0.04	15,16,17,18	0
4	NA	B	503	1/1	0.98	0.05	20,20,20,20	0
3	EDO	B	502	4/4	0.99	0.03	16,17,17,18	0
4	NA	A	503	1/1	0.99	0.04	21,21,21,21	0
2	DFU	B	501	10/10	0.99	0.04	12,13,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.