



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:15 AM UTC

PDB ID : 2EAC / pdb_00002eac
Title : Crystal structure of 1,2- α -L-fucosidase from *Bifidobacterium bifidum* in complex with deoxyfuconojirimycin
Authors : Nagae, M.; Tsuchiya, A.; Katayama, T.; Yamamoto, K.; Wakatsuki, S.; Kato, R.
Deposited on : 2007-01-31
Resolution : 2.10 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

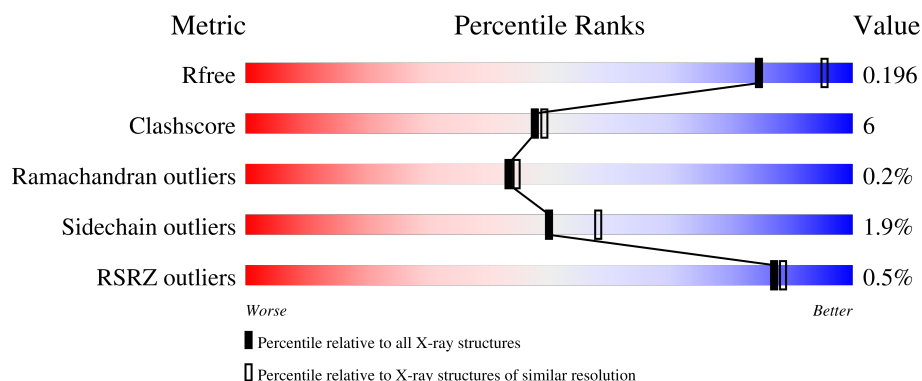
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	899	 88% 9% ..
1	B	899	 87% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15171 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-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	881	Total	C	N	O	S	0	0	0
			6719	4183	1161	1360	15			
1	B	885	Total	C	N	O	S	0	0	0
			6743	4196	1165	1367	15			

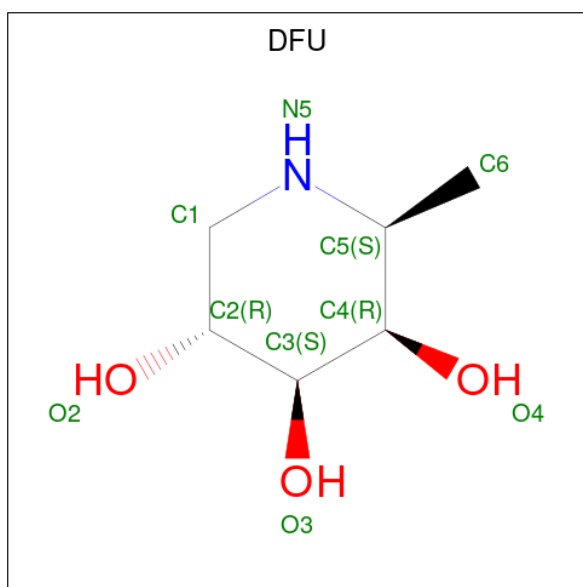
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q6JV24
B	0	MET	-	initiating methionine	UNP Q6JV24

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is (2S,3R,4S,5R)-2-METHYLPYPERIDINE-3,4,5-TRIOL (CCD ID: DFU) (formula: C₆H₁₃NO₃).



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

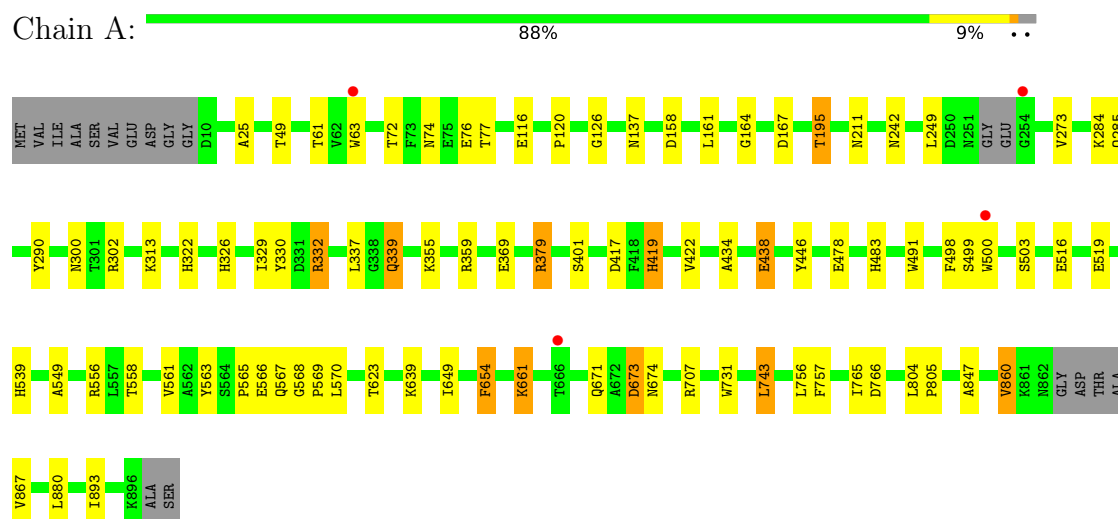
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	896	Total	O	0	0
			896	896		
4	B	789	Total	O	0	0
			789	789		

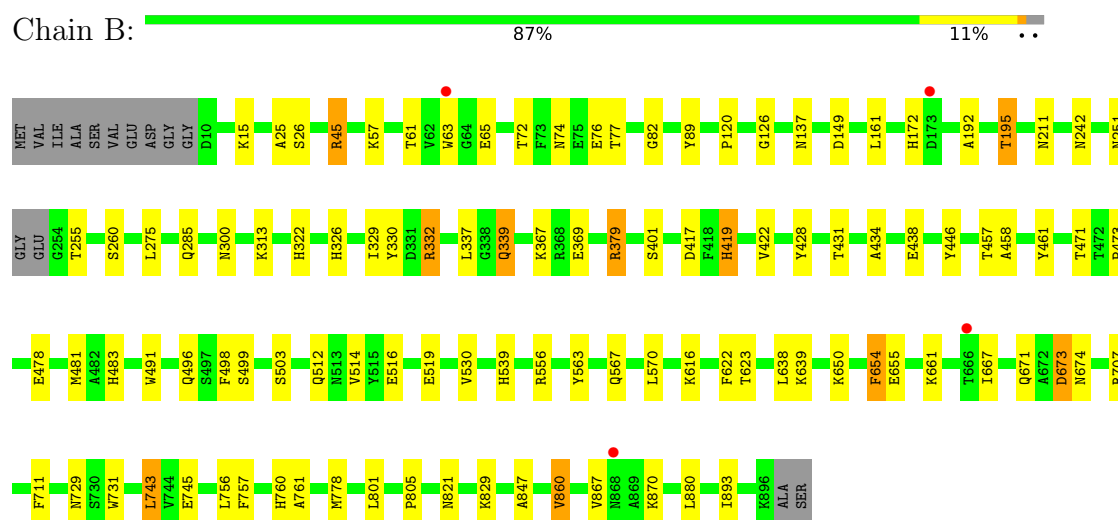
3 Residue-property plots

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-fucosidase



• Molecule 1: Alpha-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.67Å 111.70Å 98.35Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	48.97 – 2.10 48.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.97-2.10) 100.0 (48.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.150 , 0.198 0.151 , 0.196	Depositor DCC
R_{free} test set	5697 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15171	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, DFU

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	0.92	2/6863 (0.0%)	0.95	10/9332 (0.1%)
1	B	0.90	2/6888 (0.0%)	0.95	8/9368 (0.1%)
All	All	0.91	4/13751 (0.0%)	0.95	18/18700 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	801	LEU	N-CA	6.35	1.50	1.46
1	A	674	ASN	N-CA	5.95	1.52	1.46
1	B	674	ASN	N-CA	5.84	1.52	1.46
1	A	649	ILE	CA-CB	5.69	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	ASP	CA-C-N	-11.30	105.42	122.83
1	A	673	ASP	C-N-CA	-11.30	105.42	122.83
1	B	673	ASP	CA-C-N	-9.67	107.94	122.83
1	B	673	ASP	C-N-CA	-9.67	107.94	122.83
1	A	379	ARG	NE-CZ-NH2	-8.99	111.11	119.20
1	A	673	ASP	N-CA-C	-8.54	99.90	110.41
1	B	673	ASP	N-CA-C	-8.06	100.50	110.41
1	B	379	ARG	NE-CZ-NH2	-7.23	112.69	119.20
1	A	673	ASP	O-C-N	-6.34	114.91	122.65
1	A	379	ARG	CD-NE-CZ	6.13	132.98	124.40
1	A	379	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	B	332	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	A	568	GLY	CA-C-N	5.63	125.39	119.76
1	A	568	GLY	C-N-CA	5.63	125.39	119.76
1	A	332	ARG	CB-CG-CD	5.36	123.63	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	ARG	CB-CG-CD	5.34	123.59	111.30
1	B	729	ASN	N-CA-C	5.28	117.44	111.11
1	B	332	ARG	NE-CZ-NH2	-5.27	114.46	119.20

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	6719	0	6400	66	0
1	B	6743	0	6420	82	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	13	0	0
3	B	10	0	13	0	0
4	A	896	0	0	8	0
4	B	789	0	0	13	0
All	All	15171	0	12846	148	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 6.

All (148) 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:137:ASN:HD22	1:B:211:ASN:HD22	1.06	0.94
1:A:63:TRP:HZ3	1:A:72:THR:HG1	0.94	0.91
1:A:313:LYS:HD2	4:A:2556:HOH:O	1.70	0.91
1:B:63:TRP:HZ3	1:B:72:THR:OG1	1.53	0.91
1:A:137:ASN:HD22	1:A:211:ASN:HD22	1.22	0.86
1:B:63:TRP:HZ3	1:B:72:THR:HG1	0.86	0.84
1:A:242:ASN:HD21	1:A:300:ASN:HD22	1.26	0.83
1:B:556:ARG:HH12	1:B:639:LYS:HB2	1.45	0.82
1:A:63:TRP:HZ3	1:A:72:THR:OG1	1.65	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:ND2	1:B:211:ASN:HD22	1.80	0.79
1:B:379:ARG:CD	1:B:434:ALA:HB1	2.13	0.79
1:B:337:LEU:H	1:B:339:GLN:HE22	1.30	0.77
1:A:417:ASP:OD1	1:A:419:HIS:HD2	1.69	0.76
1:A:337:LEU:H	1:A:339:GLN:HE22	1.34	0.76
1:A:556:ARG:NH1	1:A:639:LYS:O	2.19	0.73
1:A:161:LEU:O	1:A:326:HIS:HE1	1.72	0.73
1:A:483:HIS:HD2	1:A:503:SER:H	1.33	0.73
1:A:330:TYR:O	1:A:379:ARG:NH2	2.22	0.72
1:A:339:GLN:HE21	1:A:339:GLN:H	1.36	0.72
1:B:483:HIS:HD2	1:B:503:SER:H	1.37	0.71
1:B:137:ASN:HD22	1:B:211:ASN:ND2	1.85	0.71
1:B:458:ALA:HA	1:B:481:MET:CE	2.21	0.71
1:B:539:HIS:HD2	4:B:2176:HOH:O	1.74	0.70
1:B:242:ASN:HD21	1:B:300:ASN:HD22	1.39	0.70
1:A:379:ARG:HD2	1:A:434:ALA:HB1	1.73	0.69
1:B:74:ASN:HD21	1:B:401:SER:H	1.41	0.69
1:A:379:ARG:CD	1:A:434:ALA:HB1	2.22	0.68
1:B:313:LYS:HD2	4:B:2476:HOH:O	1.95	0.65
1:A:567:GLN:NE2	1:A:671:GLN:H	1.94	0.65
1:B:379:ARG:HD2	1:B:434:ALA:HB1	1.78	0.65
1:B:458:ALA:HA	1:B:481:MET:HE2	1.79	0.64
1:B:379:ARG:HD3	1:B:434:ALA:HB1	1.78	0.64
1:B:860:VAL:HG22	1:B:867:VAL:HB	1.80	0.64
1:A:539:HIS:HD2	4:A:2293:HOH:O	1.80	0.63
1:B:707:ARG:NH2	4:B:1899:HOH:O	2.32	0.63
1:B:567:GLN:NE2	1:B:671:GLN:H	1.98	0.62
1:B:161:LEU:O	1:B:326:HIS:HE1	1.83	0.62
1:A:195:THR:CG2	4:A:1703:HOH:O	2.49	0.61
1:B:556:ARG:NH1	1:B:639:LYS:HB2	2.13	0.60
1:A:285:GLN:HE22	1:A:446:TYR:HA	1.66	0.60
1:B:731:TRP:CD1	1:B:743:LEU:HD13	2.36	0.60
1:B:417:ASP:OD1	1:B:419:HIS:HD2	1.84	0.60
1:A:137:ASN:ND2	1:A:211:ASN:HD22	1.96	0.60
1:B:25:ALA:HB3	1:B:63:TRP:CD1	2.36	0.60
1:B:26:SER:HA	1:B:45:ARG:HD2	1.84	0.60
1:A:249:LEU:HD23	1:A:273:VAL:HG12	1.83	0.59
1:A:302:ARG:NH1	4:A:2241:HOH:O	2.30	0.59
1:B:285:GLN:HE22	1:B:446:TYR:HA	1.66	0.59
1:A:339:GLN:H	1:A:339:GLN:NE2	2.01	0.59
1:B:367:LYS:NZ	1:B:745:GLU:OE1	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:TRP:CZ3	1:B:72:THR:OG1	2.41	0.58
1:A:25:ALA:HB3	1:A:63:TRP:CD1	2.40	0.57
1:A:74:ASN:HD21	1:A:401:SER:H	1.51	0.57
1:A:120:PRO:HB2	1:A:498:PHE:CD1	2.40	0.57
1:B:337:LEU:H	1:B:339:GLN:NE2	1.99	0.56
1:A:499:SER:HB3	1:A:570:LEU:HD21	1.88	0.56
1:B:499:SER:HB3	1:B:570:LEU:HD21	1.88	0.56
1:A:332:ARG:HD3	4:A:2323:HOH:O	2.06	0.55
1:A:707:ARG:NH1	4:A:2379:HOH:O	2.38	0.55
1:A:483:HIS:CD2	1:A:503:SER:H	2.20	0.55
1:B:483:HIS:CD2	1:B:503:SER:H	2.22	0.55
1:A:355:LYS:NZ	1:A:359:ARG:NE	2.55	0.54
1:A:671:GLN:O	1:A:673:ASP:O	2.26	0.54
1:B:251:ASN:HB2	4:B:2227:HOH:O	2.07	0.54
1:B:671:GLN:O	1:B:673:ASP:O	2.26	0.54
1:A:161:LEU:O	1:A:326:HIS:CE1	2.59	0.53
1:A:867:VAL:HA	4:A:2119:HOH:O	2.08	0.53
1:A:355:LYS:HZ3	1:A:359:ARG:HE	1.57	0.53
1:B:870:LYS:HE3	4:B:1827:HOH:O	2.08	0.53
1:B:650:LYS:HE2	1:B:655:GLU:O	2.09	0.52
1:B:330:TYR:O	1:B:379:ARG:NH2	2.41	0.52
1:B:458:ALA:HA	1:B:481:MET:HE3	1.92	0.52
1:A:25:ALA:HB1	1:A:49:THR:OG1	2.10	0.52
1:A:731:TRP:CD1	1:A:743:LEU:HD13	2.44	0.51
1:B:322:HIS:HD2	4:B:1829:HOH:O	1.92	0.51
1:B:847:ALA:HB1	1:B:880:LEU:HD13	1.91	0.51
1:B:339:GLN:HE21	1:B:339:GLN:H	1.58	0.51
1:A:76:GLU:HG3	1:A:77:THR:HG23	1.93	0.51
1:A:116:GLU:OE1	1:A:661:LYS:HE3	2.12	0.50
1:B:76:GLU:HG3	1:B:77:THR:HG23	1.94	0.50
1:A:847:ALA:HB1	1:A:880:LEU:HD13	1.94	0.50
1:A:860:VAL:HB	1:A:893:ILE:HG12	1.92	0.49
1:A:355:LYS:NZ	1:A:359:ARG:HE	2.09	0.49
1:B:498:PHE:HE2	1:B:563:TYR:HB2	1.78	0.49
1:A:337:LEU:H	1:A:339:GLN:NE2	2.08	0.49
1:A:417:ASP:OD1	1:A:419:HIS:CD2	2.58	0.49
1:A:478:GLU:OE1	1:A:539:HIS:HE1	1.96	0.49
1:B:329:ILE:O	1:B:332:ARG:HG3	2.13	0.49
1:B:556:ARG:NH1	1:B:639:LYS:O	2.46	0.49
1:B:516:GLU:HA	1:B:519:GLU:HB2	1.95	0.48
1:B:120:PRO:HB2	1:B:498:PHE:CE1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLY:HA2	1:A:491:TRP:CZ2	2.50	0.47
1:B:326:HIS:HD2	4:B:1808:HOH:O	1.96	0.47
1:A:329:ILE:O	1:A:332:ARG:HG3	2.14	0.47
1:B:57:LYS:HD2	4:B:2085:HOH:O	2.14	0.47
1:B:499:SER:O	1:B:563:TYR:CE2	2.68	0.47
1:B:829:LYS:HD3	1:B:829:LYS:HA	1.74	0.47
1:A:516:GLU:HA	1:A:519:GLU:HB2	1.96	0.47
1:A:74:ASN:ND2	1:A:401:SER:H	2.12	0.46
1:A:355:LYS:HG2	1:A:359:ARG:HE	1.81	0.46
1:B:778:MET:CE	1:B:805:PRO:HG3	2.46	0.46
1:A:120:PRO:HB2	1:A:498:PHE:CE1	2.49	0.46
1:B:457:THR:O	1:B:481:MET:HE3	2.15	0.46
1:B:149:ASP:O	1:B:172:HIS:HE1	1.99	0.46
1:B:74:ASN:ND2	1:B:401:SER:H	2.11	0.46
1:A:438:GLU:HG3	4:A:1984:HOH:O	2.16	0.46
1:B:326:HIS:CD2	4:B:1808:HOH:O	2.68	0.46
1:A:164:GLY:O	1:A:322:HIS:HE1	1.98	0.45
1:A:498:PHE:HE2	1:A:563:TYR:HB2	1.81	0.45
1:B:471:THR:O	1:B:473:PRO:HD3	2.16	0.45
1:B:195:THR:CG2	4:B:1985:HOH:O	2.65	0.45
1:A:498:PHE:CE2	1:A:563:TYR:HB2	2.52	0.45
1:B:499:SER:O	1:B:563:TYR:CD2	2.70	0.45
1:A:549:ALA:HB2	1:A:558:THR:HG23	1.99	0.45
1:A:860:VAL:HG22	1:A:867:VAL:HB	1.98	0.45
1:B:126:GLY:HA2	1:B:491:TRP:CZ2	2.52	0.45
1:B:461:TYR:HB2	1:B:481:MET:HE1	1.99	0.45
1:A:565:PRO:HA	1:A:566:GLU:HA	1.79	0.45
1:A:63:TRP:CZ3	1:A:72:THR:OG1	2.52	0.45
1:B:15:LYS:HB2	4:B:2169:HOH:O	2.16	0.44
1:A:339:GLN:HB2	1:A:369:GLU:HA	1.99	0.44
1:B:496:GLN:NE2	4:B:2271:HOH:O	2.51	0.43
1:A:567:GLN:HE21	1:A:671:GLN:H	1.61	0.43
1:B:192:ALA:HB3	1:B:275:LEU:HB2	2.01	0.42
1:B:707:ARG:O	1:B:711:PHE:HB2	2.19	0.42
1:B:760:HIS:N	1:B:761:ALA:HA	2.34	0.42
1:B:654:PHE:C	1:B:654:PHE:CD1	2.98	0.42
1:B:457:THR:C	1:B:481:MET:HE3	2.45	0.42
1:B:512:GLN:O	1:B:516:GLU:HG3	2.19	0.42
1:A:284:LYS:O	1:A:290:TYR:HA	2.19	0.41
1:B:339:GLN:HB2	1:B:369:GLU:HA	2.01	0.41
1:B:82:GLY:HA2	1:B:89:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LYS:HG3	1:B:667:ILE:HG12	2.02	0.41
1:B:860:VAL:HB	1:B:893:ILE:HG12	2.03	0.41
1:B:63:TRP:HB3	1:B:65:GLU:HG2	2.03	0.41
1:B:428:TYR:HA	1:B:431:THR:OG1	2.21	0.41
1:B:285:GLN:NE2	4:B:1726:HOH:O	2.52	0.41
1:B:478:GLU:OE1	1:B:539:HIS:HE1	2.03	0.41
1:B:498:PHE:CE2	1:B:563:TYR:HB2	2.56	0.41
1:A:569:PRO:HG2	1:A:654:PHE:HZ	1.86	0.41
1:B:339:GLN:NE2	1:B:339:GLN:H	2.18	0.41
1:B:556:ARG:NH1	1:B:638:LEU:O	2.54	0.41
1:A:158:ASP:OD1	1:A:167:ASP:OD2	2.39	0.41
1:A:765:ILE:O	1:A:766:ASP:C	2.64	0.41
1:B:514:VAL:HG12	1:B:530:VAL:HG12	2.03	0.40
1:A:355:LYS:HZ1	1:A:359:ARG:NE	2.19	0.40
1:A:804:LEU:HD12	1:A:805:PRO:HD2	2.03	0.40
1:B:616:LYS:HE3	1:B:622:PHE:CE1	2.56	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	875/899 (97%)	846 (97%)	27 (3%)	2 (0%)	43	44
1	B	881/899 (98%)	856 (97%)	23 (3%)	2 (0%)	43	44
All	All	1756/1798 (98%)	1702 (97%)	50 (3%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	VAL
1	A	500	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	422	VAL
1	B	821	ASN

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	701/712 (98%)	688 (98%)	13 (2%)	50	58
1	B	703/712 (99%)	689 (98%)	14 (2%)	48	56
All	All	1404/1424 (99%)	1377 (98%)	27 (2%)	50	58

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	THR
1	A	195	THR
1	A	339	GLN
1	A	419	HIS
1	A	438	GLU
1	A	561	VAL
1	A	623	THR
1	A	654	PHE
1	A	661	LYS
1	A	743	LEU
1	A	756	LEU
1	A	757	PHE
1	A	860	VAL
1	B	45	ARG
1	B	61	THR
1	B	195	THR
1	B	255	THR
1	B	260	SER
1	B	339	GLN
1	B	419	HIS
1	B	438	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	623	THR
1	B	654	PHE
1	B	743	LEU
1	B	756	LEU
1	B	757	PHE
1	B	860	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	74	ASN
1	A	100	ASN
1	A	137	ASN
1	A	242	ASN
1	A	244	GLN
1	A	251	ASN
1	A	285	GLN
1	A	322	HIS
1	A	326	HIS
1	A	339	GLN
1	A	342	HIS
1	A	391	GLN
1	A	397	GLN
1	A	407	ASN
1	A	419	HIS
1	A	468	ASN
1	A	483	HIS
1	A	486	ASN
1	A	539	HIS
1	A	543	ASN
1	A	567	GLN
1	A	587	ASN
1	A	675	GLN
1	A	695	ASN
1	A	764	GLN
1	A	771	ASN
1	A	821	ASN
1	A	830	ASN
1	A	868	ASN
1	B	74	ASN
1	B	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	137	ASN
1	B	172	HIS
1	B	185	ASN
1	B	213	ASN
1	B	242	ASN
1	B	244	GLN
1	B	251	ASN
1	B	285	GLN
1	B	322	HIS
1	B	326	HIS
1	B	339	GLN
1	B	342	HIS
1	B	391	GLN
1	B	397	GLN
1	B	419	HIS
1	B	483	HIS
1	B	539	HIS
1	B	543	ASN
1	B	567	GLN
1	B	587	ASN
1	B	675	GLN
1	B	764	GLN
1	B	821	ASN
1	B	830	ASN
1	B	857	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

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	DFU	A	1690	-	10,10,10	0.63	0	12,14,14	1.17	1 (8%)
3	DFU	B	1691	-	10,10,10	0.94	1 (10%)	12,14,14	1.14	1 (8%)

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	DFU	A	1690	-	-	-	0/1/1/1
3	DFU	B	1691	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1691	DFU	C1-C2	2.02	1.54	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1690	DFU	C1-N5-C5	3.60	118.62	109.48
3	B	1691	DFU	C1-N5-C5	3.18	117.56	109.48

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	881/899 (97%)	-0.73	4 (0%) 87 88	6, 13, 27, 41	0
1	B	885/899 (98%)	-0.57	4 (0%) 87 88	7, 16, 32, 47	0
All	All	1766/1798 (98%)	-0.65	8 (0%) 87 88	6, 14, 30, 47	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	666	THR	3.2
1	B	868	ASN	3.0
1	A	500	TRP	2.6
1	B	666	THR	2.6
1	A	63	TRP	2.5
1	B	63	TRP	2.3
1	B	173	ASP	2.1
1	A	254	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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	DFU	A	1690	10/10	0.96	0.06	11,16,19,20	0
3	DFU	B	1691	10/10	0.96	0.06	12,16,18,22	0
2	CA	A	899	1/1	0.97	0.13	22,22,22,22	0
2	CA	A	900	1/1	0.99	0.04	20,20,20,20	0
2	CA	B	900	1/1	0.99	0.10	20,20,20,20	0
2	CA	B	899	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.