



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3U14  
Title : Structure of D50A-fructofuranosidase from Schwanniomyces occidentalis complexed with inulin  
Authors : Sainz-Polo, M.A.; Sanz-Aparicio, J.  
Deposited on : 2011-09-29  
Resolution : 2.24 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

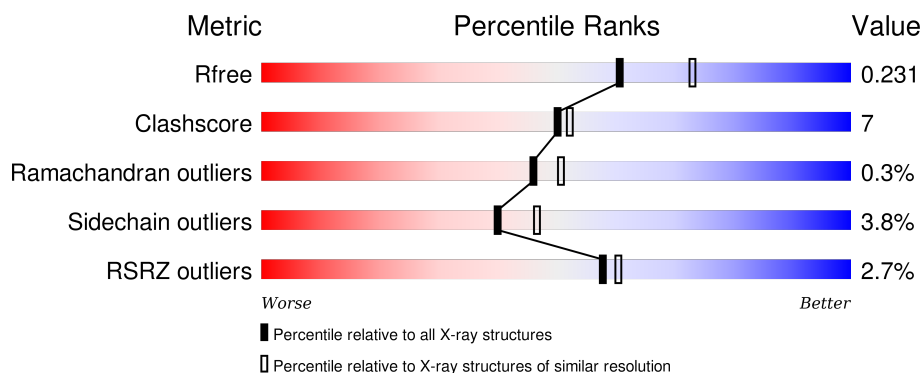
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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))
$R_{free}$	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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. 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	535	
1	B	535	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	A	1005	X	-	-	-
2	FRU	B	1002	-	-	-	X
2	FRU	B	1005	X	-	-	-
3	NAG	A	1072	-	-	-	X
3	NAG	A	1219	-	-	-	X
3	NAG	B	1126	-	-	-	X
3	NAG	B	1219	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9123 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 Fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4131	2656	677	792	6			
1	B	509	Total	C	N	O	S	0	0	0
			4131	2656	677	792	6			

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	6	Total	C	O	0	0
			66	36	30		
2	B	6	Total	C	O	0	0
			66	36	30		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

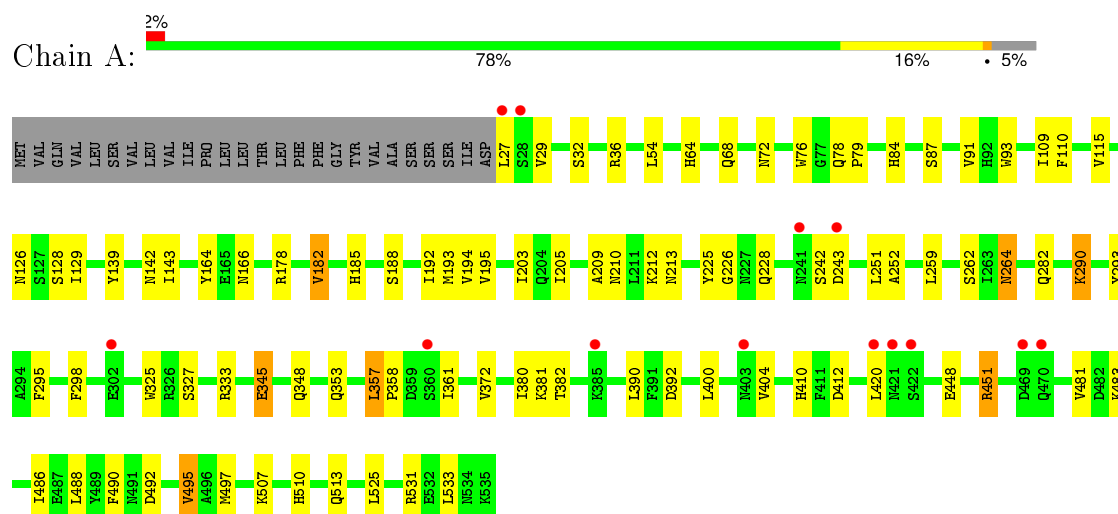
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	298	Total	O	0	0
			298	298		
4	B	319	Total	O	0	0
			319	319		

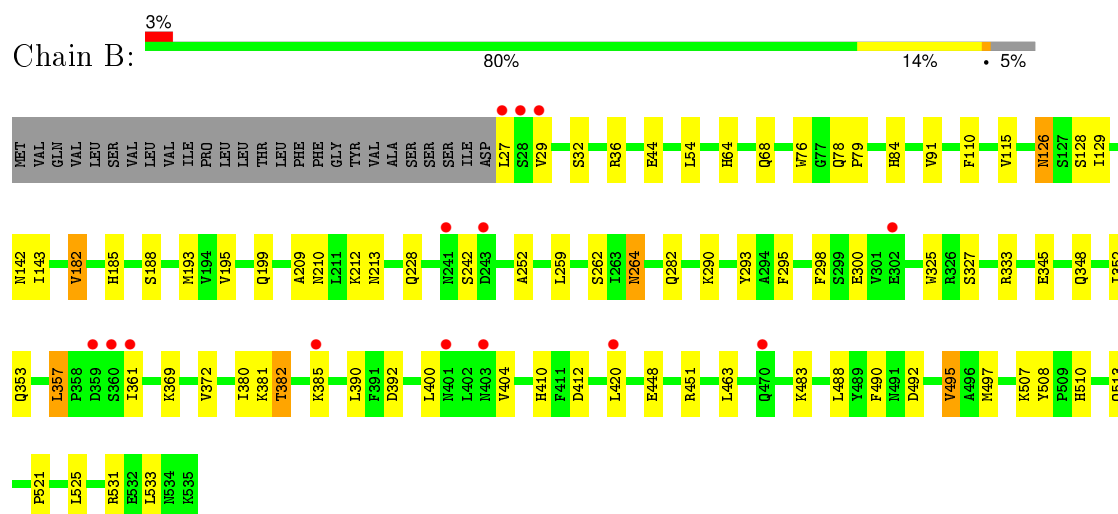
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Fructofuranosidase



#### • Molecule 1: Fructofuranosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.98Å 107.67Å 96.46Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.24 35.91 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.24) 98.2 (35.91-2.24)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.194 , 0.231 0.194 , 0.231	Depositor DCC
$R_{free}$ test set	3263 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.4	EDS
Estimated twinning fraction	0.040 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 64600 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG, FRU

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	0.55	0/4252	0.67	4/5791 (0.1%)
1	B	0.54	0/4252	0.65	1/5791 (0.0%)
All	All	0.55	0/8504	0.66	5/11582 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	A	1	0
2	B	1	0
All	All	2	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	TYR	C-N-CA	-6.82	107.98	122.30
1	A	225	TYR	O-C-N	-5.62	113.64	123.20
1	A	226	GLY	N-CA-C	-5.41	99.57	113.10
1	A	225	TYR	CA-C-N	5.26	126.73	116.20
1	B	126	ASN	CB-CA-C	-5.01	100.38	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1005	FRU	C2

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Mol	Chain	Res	Type	Atom
2	B	1005	FRU	C2

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	ALA	Peptide
1	B	209	ALA	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	4131	0	3919	60	0
1	B	4131	0	3918	54	0
2	A	66	0	59	2	0
2	B	66	0	59	1	0
3	A	56	0	52	3	0
3	B	56	0	51	0	0
4	A	298	0	0	7	0
4	B	319	0	0	6	0
All	All	9123	0	8058	116	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 7.

All (116) 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:451:ARG:NH1	4:A:740:HOH:O	1.82	1.11
1:A:492:ASP:HB2	4:A:792:HOH:O	1.65	0.94
1:B:210:ASN:HD22	1:B:213:ASN:HD22	1.06	0.93
1:B:210:ASN:ND2	1:B:213:ASN:HD22	1.69	0.90
1:A:210:ASN:HD22	1:A:213:ASN:HD22	1.22	0.88
1:A:357:LEU:HD23	1:A:361:ILE:HD13	1.55	0.87
1:B:488:LEU:HD12	1:B:497:MET:HE2	1.58	0.85
1:B:78:GLN:HE22	1:B:142:ASN:HD22	1.22	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:LEU:HD12	1:B:497:MET:CE	2.07	0.84
1:A:210:ASN:ND2	1:A:213:ASN:HD22	1.76	0.84
1:B:357:LEU:HD23	1:B:361:ILE:HD13	1.60	0.82
1:A:78:GLN:HE22	1:A:142:ASN:HD22	1.24	0.82
1:A:488:LEU:HD12	1:A:497:MET:CE	2.10	0.81
1:A:259:LEU:O	1:A:290:LYS:HE3	1.82	0.79
1:A:64:HIS:HD2	1:A:84:HIS:NE2	1.80	0.78
1:B:64:HIS:HD2	1:B:84:HIS:NE2	1.82	0.77
1:B:68:GLN:HE22	1:B:110:PHE:HA	1.49	0.77
1:B:126:ASN:HB2	1:B:129:ILE:HG12	1.67	0.74
1:A:488:LEU:HD12	1:A:497:MET:HE2	1.69	0.74
3:A:1072:NAG:H3	3:A:1072:NAG:O7	1.87	0.74
1:A:490:PHE:HD1	1:A:495:VAL:HG22	1.55	0.70
1:B:210:ASN:HB3	1:B:212:LYS:H	1.57	0.70
1:B:300:GLU:OE2	4:B:847:HOH:O	2.11	0.69
1:A:410:HIS:HD2	1:A:412:ASP:OD1	1.75	0.69
1:B:492:ASP:HB2	4:B:612:HOH:O	1.93	0.69
1:B:490:PHE:HD1	1:B:495:VAL:HG22	1.56	0.68
1:B:78:GLN:NE2	1:B:142:ASN:HD22	1.92	0.67
1:B:282:GLN:HE22	1:B:348:GLN:HE21	1.42	0.67
1:B:410:HIS:HD2	1:B:412:ASP:OD1	1.78	0.66
1:B:210:ASN:ND2	1:B:213:ASN:ND2	2.42	0.66
1:A:210:ASN:HB3	1:A:212:LYS:H	1.62	0.64
1:B:282:GLN:HE22	1:B:348:GLN:NE2	1.96	0.62
1:A:126:ASN:HB2	1:A:129:ILE:HG12	1.81	0.62
1:A:252:ALA:HB1	1:A:293:TYR:CE1	2.35	0.61
1:A:68:GLN:HE22	1:A:110:PHE:HA	1.66	0.60
1:B:126:ASN:HB3	1:B:128:SER:H	1.66	0.60
1:B:259:LEU:O	1:B:290:LYS:HE3	2.03	0.58
1:B:262:SER:HB2	1:B:293:TYR:CD1	2.38	0.58
1:A:64:HIS:CD2	1:A:84:HIS:NE2	2.68	0.57
1:A:345:GLU:HB2	1:B:199:GLN:HE21	1.70	0.57
1:A:282:GLN:HE22	1:A:348:GLN:NE2	2.03	0.56
1:A:264:ASN:ND2	1:A:295:PHE:H	2.04	0.56
1:B:64:HIS:CD2	1:B:84:HIS:NE2	2.70	0.56
1:A:228:GLN:NE2	4:A:671:HOH:O	2.23	0.56
1:A:262:SER:HB2	1:A:293:TYR:CD1	2.41	0.56
1:A:282:GLN:HE22	1:A:348:GLN:HE21	1.54	0.55
1:A:488:LEU:HD12	1:A:497:MET:HE3	1.86	0.55
1:A:451:ARG:CZ	4:A:740:HOH:O	2.41	0.54
1:B:185:HIS:HD2	1:B:188:SER:OG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ALA:HB1	1:B:293:TYR:CE1	2.42	0.54
1:B:410:HIS:CD2	1:B:412:ASP:OD1	2.61	0.53
1:B:392:ASP:OD1	1:B:531:ARG:HD3	2.10	0.52
1:A:392:ASP:OD1	1:A:531:ARG:HD3	2.09	0.52
1:B:78:GLN:HE22	1:B:142:ASN:ND2	2.01	0.51
1:A:210:ASN:ND2	1:A:213:ASN:ND2	2.52	0.51
1:A:264:ASN:HD21	1:A:295:PHE:H	1.56	0.51
1:B:91:VAL:HG11	1:B:361:ILE:HD11	1.93	0.51
1:B:420:LEU:HB2	1:B:507:LYS:HE3	1.92	0.51
1:B:264:ASN:HD21	1:B:295:PHE:H	1.60	0.50
1:A:91:VAL:HG11	1:A:361:ILE:HD11	1.93	0.50
1:B:68:GLN:NE2	1:B:110:PHE:HA	2.24	0.49
1:A:410:HIS:CD2	1:A:412:ASP:OD1	2.60	0.49
1:B:210:ASN:HD22	1:B:213:ASN:ND2	1.90	0.49
1:A:193:MET:HE2	1:A:195:VAL:CG1	2.42	0.49
1:A:78:GLN:NE2	1:A:142:ASN:HD22	2.02	0.49
1:B:382:THR:HG22	4:B:786:HOH:O	2.14	0.48
1:A:372:VAL:HG22	1:A:525:LEU:HB2	1.96	0.48
1:A:72:ASN:OD1	3:A:1072:NAG:H2	2.14	0.47
1:B:54:LEU:HB3	1:B:298:PHE:CD2	2.49	0.47
1:A:126:ASN:ND2	4:A:562:HOH:O	2.48	0.47
2:A:1000:FRU:H12	2:A:1001:FRU:H11	1.68	0.47
1:A:32:SER:HA	1:A:36:ARG:HB2	1.97	0.47
1:A:185:HIS:HE1	4:A:748:HOH:O	1.98	0.46
1:A:358:PRO:HD2	1:A:361:ILE:HD12	1.98	0.46
1:A:126:ASN:HB3	1:A:128:SER:H	1.80	0.46
1:B:488:LEU:HD12	1:B:497:MET:HE3	1.93	0.46
1:B:264:ASN:ND2	1:B:295:PHE:H	2.14	0.46
1:A:193:MET:CE	1:A:195:VAL:HG11	2.46	0.46
1:B:115:VAL:HG11	1:B:182:VAL:HG22	1.97	0.46
1:B:463:LEU:HD21	1:B:495:VAL:HG13	1.98	0.45
1:B:76:TRP:HE1	2:B:1000:FRU:HO6	1.64	0.45
1:B:78:GLN:HA	1:B:79:PRO:C	2.37	0.45
1:A:333:ARG:HH11	1:A:353:GLN:NE2	2.15	0.45
1:A:420:LEU:HB2	1:A:507:LYS:HE3	1.99	0.45
1:B:44:GLU:HG2	4:B:837:HOH:O	2.18	0.44
1:A:115:VAL:HG11	1:A:182:VAL:HG22	2.00	0.44
1:A:78:GLN:HA	1:A:79:PRO:C	2.38	0.44
1:A:510:HIS:HB3	4:A:729:HOH:O	2.18	0.44
1:B:228:GLN:NE2	4:B:672:HOH:O	2.27	0.43
1:B:369:LYS:HD2	1:B:380:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:HD11	1:A:488:LEU:HD21	2.01	0.43
3:A:1072:NAG:O7	3:A:1072:NAG:C3	2.61	0.43
1:A:54:LEU:HB3	1:A:298:PHE:CD2	2.54	0.43
1:A:182:VAL:HA	1:A:192:ILE:O	2.19	0.43
1:B:372:VAL:HG22	1:B:525:LEU:HB2	2.01	0.43
1:A:194:VAL:HG12	1:A:205:ILE:HG12	1.99	0.43
1:A:390:LEU:HG	1:A:533:LEU:HB2	2.01	0.42
1:B:381:LYS:HG2	1:B:513:GLN:HG2	2.00	0.42
1:B:382:THR:CG2	4:B:786:HOH:O	2.67	0.42
1:A:76:TRP:HE1	2:A:1000:FRU:HO6	1.67	0.42
1:A:87:SER:HB2	1:A:93:TRP:CE3	2.55	0.42
1:B:32:SER:HA	1:B:36:ARG:HB2	2.02	0.42
1:B:390:LEU:HG	1:B:533:LEU:HB2	2.02	0.42
1:A:178:ARG:HH22	1:A:228:GLN:NE2	2.17	0.42
1:B:372:VAL:HG21	1:B:380:ILE:HD11	2.02	0.42
1:B:508:TYR:O	1:B:510:HIS:HD2	2.03	0.41
1:A:381:LYS:HG2	1:A:513:GLN:HG2	2.01	0.41
1:B:193:MET:HE3	1:B:195:VAL:CG1	2.50	0.41
1:A:185:HIS:HD2	1:A:188:SER:OG	2.03	0.41
1:A:164:TYR:CE2	1:A:166:ASN:HB2	2.55	0.41
1:A:372:VAL:HG21	1:A:380:ILE:HD11	2.01	0.41
1:A:36:ARG:O	1:A:483:LYS:HD3	2.21	0.41
1:B:333:ARG:HH11	1:B:353:GLN:NE2	2.19	0.40
1:B:36:ARG:O	1:B:483:LYS:HD3	2.21	0.40
1:A:203:ILE:HD11	1:A:251:LEU:HD13	2.03	0.40
1:A:109:ILE:HG23	1:A:139:TYR:CD1	2.56	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	507/535 (95%)	477 (94%)	29 (6%)	1 (0%)	52	60
1	B	507/535 (95%)	475 (94%)	30 (6%)	2 (0%)	39	42
All	All	1014/1070 (95%)	952 (94%)	59 (6%)	3 (0%)	46	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	B	327	SER
1	B	521	PRO

### 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	460/484 (95%)	442 (96%)	18 (4%)	39	45
1	B	460/484 (95%)	443 (96%)	17 (4%)	41	48
All	All	920/968 (95%)	885 (96%)	35 (4%)	40	47

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	29	VAL
1	A	143	ILE
1	A	182	VAL
1	A	242	SER
1	A	243	ASP
1	A	264	ASN
1	A	290	LYS
1	A	325	TRP
1	A	345	GLU
1	A	357	LEU
1	A	382	THR
1	A	400	LEU

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Mol	Chain	Res	Type
1	A	404	VAL
1	A	448	GLU
1	A	451	ARG
1	A	481	VAL
1	A	495	VAL
1	B	27	LEU
1	B	29	VAL
1	B	143	ILE
1	B	182	VAL
1	B	242	SER
1	B	264	ASN
1	B	325	TRP
1	B	345	GLU
1	B	352	ILE
1	B	357	LEU
1	B	382	THR
1	B	385	LYS
1	B	400	LEU
1	B	404	VAL
1	B	448	GLU
1	B	451	ARG
1	B	495	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	64	HIS
1	A	68	GLN
1	A	78	GLN
1	A	126	ASN
1	A	185	HIS
1	A	199	GLN
1	A	210	ASN
1	A	264	ASN
1	A	296	GLN
1	A	348	GLN
1	A	353	GLN
1	A	362	ASN
1	A	410	HIS
1	A	513	GLN
1	B	52	ASN

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Mol	Chain	Res	Type
1	B	64	HIS
1	B	68	GLN
1	B	78	GLN
1	B	118	HIS
1	B	133	GLN
1	B	185	HIS
1	B	199	GLN
1	B	213	ASN
1	B	227	ASN
1	B	264	ASN
1	B	296	GLN
1	B	348	GLN
1	B	353	GLN
1	B	362	ASN
1	B	401	ASN
1	B	410	HIS
1	B	421	ASN
1	B	513	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

12 carbohydrates are modelled in this entry.

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	FRU	A	1000	2	11,11,12	0.37	0	15,15,18	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FRU	A	1001	2	11,11,12	0.28	0	15,15,18	0.78	0
2	FRU	A	1002	2	11,11,12	0.44	0	15,15,18	1.26	1 (6%)
2	FRU	A	1003	2	11,11,12	0.28	0	15,15,18	0.77	0
2	FRU	A	1004	2	11,11,12	0.40	0	15,15,18	0.68	0
2	FRU	A	1005	2	11,11,12	2.78	2 (18%)	15,15,18	5.43	5 (33%)
2	FRU	B	1000	2	11,11,12	0.30	0	15,15,18	0.79	0
2	FRU	B	1001	2	11,11,12	0.33	0	15,15,18	0.96	1 (6%)
2	FRU	B	1002	2	11,11,12	0.41	0	15,15,18	1.32	1 (6%)
2	FRU	B	1003	2	11,11,12	0.36	0	15,15,18	0.69	0
2	FRU	B	1004	2	11,11,12	0.30	0	15,15,18	0.78	0
2	FRU	B	1005	2	11,11,12	2.63	2 (18%)	15,15,18	5.58	5 (33%)

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	FRU	A	1000	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1001	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1002	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1003	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1004	2	-	0/4/20/24	0/1/1/1
2	FRU	A	1005	2	1/1/4/4	0/4/20/24	0/1/1/1
2	FRU	B	1000	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1001	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1002	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1003	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1004	2	-	0/4/20/24	0/1/1/1
2	FRU	B	1005	2	1/1/4/4	0/4/20/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	FRU	C1-C2	-7.62	1.24	1.51
2	B	1005	FRU	C1-C2	-7.29	1.26	1.51
2	A	1005	FRU	O1-C1	-4.79	1.21	1.42
2	B	1005	FRU	O1-C1	-4.48	1.23	1.42

All (14) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	FRU	C6-C5-C4	-2.96	108.07	115.08
2	A	1002	FRU	C6-C5-C4	-2.44	109.32	115.08
2	B	1001	FRU	C6-C5-C4	-2.28	109.69	115.08
2	A	1000	FRU	O5-C2-C1	2.12	113.76	109.17
2	B	1005	FRU	C3-C4-C5	2.52	107.79	102.61
2	A	1005	FRU	C1-C2-C3	2.75	121.59	115.08
2	A	1005	FRU	C3-C4-C5	2.80	108.36	102.61
2	B	1005	FRU	C1-C2-C3	3.21	122.68	115.08
2	B	1005	FRU	O5-C2-C3	4.69	114.59	105.15
2	A	1005	FRU	O5-C2-C3	5.11	115.45	105.15
2	B	1005	FRU	O5-C2-C1	6.25	122.71	109.17
2	A	1005	FRU	O5-C2-C1	6.32	122.86	109.17
2	A	1005	FRU	O1-C1-C2	18.81	173.48	111.33
2	B	1005	FRU	O1-C1-C2	19.54	175.90	111.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1005	FRU	C2
2	A	1005	FRU	C2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	FRU	2	0
2	A	1001	FRU	1	0
2	B	1000	FRU	1	0

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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	NAG	A	1072	1	14,14,15	0.54	0	15,19,21	0.59	0
3	NAG	A	1219	1	14,14,15	0.55	0	15,19,21	1.64	1 (6%)
3	NAG	A	1334	1	14,14,15	1.77	1 (7%)	15,19,21	2.75	6 (40%)
3	NAG	A	1394	1	14,14,15	0.81	1 (7%)	15,19,21	3.03	3 (20%)
3	NAG	B	1126	1	14,14,15	1.75	5 (35%)	15,19,21	1.71	2 (13%)
3	NAG	B	1219	1	14,14,15	1.71	2 (14%)	15,19,21	1.88	4 (26%)
3	NAG	B	1334	1	14,14,15	1.82	1 (7%)	15,19,21	2.29	5 (33%)
3	NAG	B	1394	1	14,14,15	0.80	1 (7%)	15,19,21	1.80	5 (33%)

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	NAG	A	1072	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1219	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1334	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1394	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1126	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1219	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1334	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1394	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1334	NAG	O5-C1	-6.56	1.32	1.43
3	A	1334	NAG	O5-C1	-6.13	1.33	1.43
3	B	1219	NAG	O5-C1	-5.12	1.35	1.43
3	B	1126	NAG	O5-C1	-2.91	1.38	1.43
3	B	1126	NAG	C2-N2	-2.48	1.41	1.46
3	B	1126	NAG	O7-C7	-2.37	1.17	1.23
3	B	1126	NAG	O4-C4	-2.17	1.37	1.43
3	B	1126	NAG	C1-C2	2.24	1.55	1.52
3	B	1394	NAG	C1-C2	2.42	1.55	1.52
3	A	1394	NAG	C1-C2	2.69	1.56	1.52
3	B	1219	NAG	C1-C2	3.45	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1334	NAG	C1-O5-C5	-7.17	103.15	112.25
3	B	1334	NAG	C1-O5-C5	-5.94	104.71	112.25
3	A	1334	NAG	C2-N2-C7	-4.83	116.83	123.04
3	B	1334	NAG	C2-N2-C7	-3.35	118.74	123.04
3	B	1394	NAG	C3-C4-C5	-3.31	104.42	110.20
3	A	1394	NAG	C3-C2-N2	-3.25	102.78	110.56
3	B	1334	NAG	C4-C3-C2	-3.13	106.36	111.23
3	B	1219	NAG	C1-O5-C5	-2.99	108.45	112.25
3	B	1394	NAG	C3-C2-N2	-2.54	104.48	110.56
3	B	1219	NAG	C3-C4-C5	-2.36	106.09	110.20
3	A	1334	NAG	C4-C3-C2	-2.31	107.64	111.23
3	A	1334	NAG	O4-C4-C3	-2.11	105.58	110.34
3	B	1394	NAG	O5-C5-C6	2.04	111.77	107.35
3	B	1334	NAG	O3-C3-C2	2.30	113.67	109.11
3	B	1394	NAG	C1-O5-C5	2.34	115.22	112.25
3	A	1334	NAG	C3-C4-C5	2.35	114.30	110.20
3	B	1334	NAG	C3-C2-N2	2.38	116.26	110.56
3	A	1394	NAG	O5-C5-C6	2.53	112.83	107.35
3	B	1219	NAG	O3-C3-C2	2.57	114.20	109.11
3	B	1394	NAG	C2-N2-C7	2.83	126.67	123.04
3	A	1334	NAG	O5-C5-C6	3.39	114.69	107.35
3	B	1126	NAG	O3-C3-C2	3.87	116.78	109.11
3	B	1219	NAG	O5-C5-C6	4.09	116.20	107.35
3	B	1126	NAG	O5-C5-C6	4.49	117.06	107.35
3	A	1219	NAG	C1-O5-C5	5.41	119.11	112.25
3	A	1394	NAG	C1-O5-C5	10.64	125.75	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1072	NAG	3	0

## 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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	509/535 (95%)	-0.25	13 (2%) 59 62	6, 14, 31, 46	0
1	B	509/535 (95%)	-0.26	14 (2%) 56 59	6, 14, 31, 46	0
All	All	1018/1070 (95%)	-0.25	27 (2%) 58 60	6, 14, 31, 46	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	LEU	7.1
1	B	27	LEU	6.1
1	A	422	SER	5.7
1	A	421	ASN	4.3
1	A	470	GLN	4.0
1	B	243	ASP	3.9
1	A	302	GLU	3.6
1	B	470	GLN	3.4
1	B	360	SER	3.3
1	B	359	ASP	3.2
1	A	385	LYS	3.2
1	B	29	VAL	3.0
1	B	401	ASN	3.0
1	A	243	ASP	2.9
1	B	385	LYS	2.8
1	B	28	SER	2.8
1	B	241	ASN	2.4
1	B	361	ILE	2.3
1	A	241	ASN	2.3
1	A	469	ASP	2.3
1	B	420	LEU	2.3
1	B	302	GLU	2.3
1	A	403	ASN	2.2
1	A	28	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	403	ASN	2.1
1	A	420	LEU	2.1
1	A	360	SER	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FRU	B	1002	11/12	0.89	0.15	3.31	29,32,36,36	0
2	FRU	B	1003	11/12	0.93	0.12	1.82	28,31,33,33	0
2	FRU	A	1002	11/12	0.90	0.13	0.99	22,29,34,37	0
2	FRU	B	1001	11/12	0.94	0.11	0.82	21,28,30,33	0
2	FRU	A	1001	11/12	0.91	0.12	0.68	16,20,22,25	0
2	FRU	A	1003	11/12	0.94	0.11	0.16	23,26,28,28	0
2	FRU	B	1000	11/12	0.96	0.13	-0.01	15,19,20,20	0
2	FRU	A	1000	11/12	0.95	0.11	-0.32	10,12,13,15	0
2	FRU	A	1005	11/12	0.65	0.37	-	45,56,58,58	0
2	FRU	B	1005	11/12	0.60	0.43	-	49,58,61,62	0
2	FRU	B	1004	11/12	0.89	0.18	-	36,45,46,47	0
2	FRU	A	1004	11/12	0.91	0.17	-	30,41,44,46	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	1126	14/15	0.78	0.30	7.85	20,20,20,20	0
3	NAG	A	1072	14/15	0.71	0.31	4.45	34,38,44,44	0
3	NAG	A	1219	14/15	0.92	0.15	2.43	23,26,32,32	0
3	NAG	B	1219	14/15	0.91	0.15	2.14	19,21,25,25	0
3	NAG	B	1394	14/15	0.88	0.17	-	32,36,37,38	0
3	NAG	A	1394	14/15	0.83	0.25	-	33,39,43,45	0
3	NAG	B	1334	14/15	0.92	0.19	-	26,29,31,31	0
3	NAG	A	1334	14/15	0.90	0.21	-	28,32,35,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.