



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:07 PM BST

PDB ID : 3KF3  
Title : Structure of fructofuranosidase from Schwanniomyces occidentalis complexed with fructose  
Authors : Sanz-Aparicio, J.; Polo, A.  
Deposited on : 2009-10-27  
Resolution : 1.90 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 : 2.13.1  
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) : 2.13.1

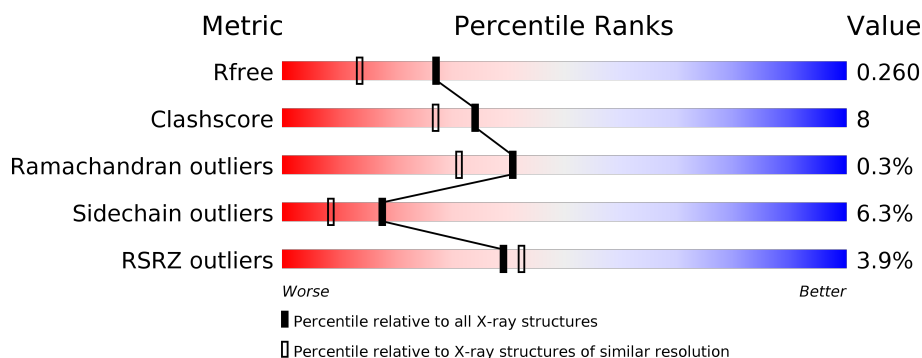
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	509	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	509	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

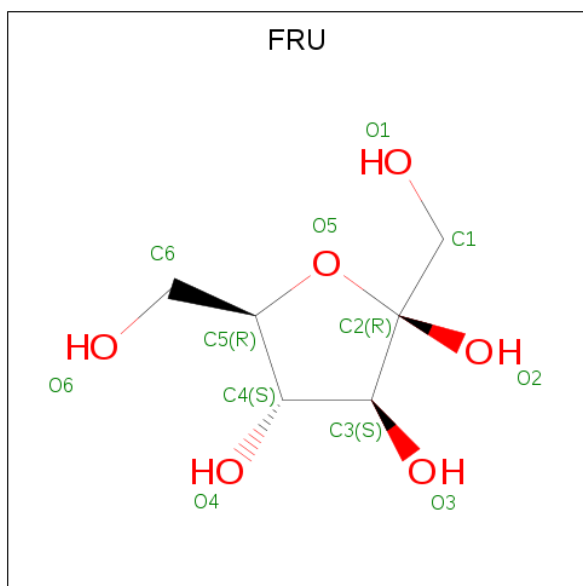
There are 4 unique types of molecules in this entry. The entry contains 9197 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Invertase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4134	2657	677	794	6			
1	B	509	Total	C	N	O	S	0	0	0
			4134	2657	677	794	6			

- Molecule 2 is beta-D-fructofuranose (three-letter code: FRU) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

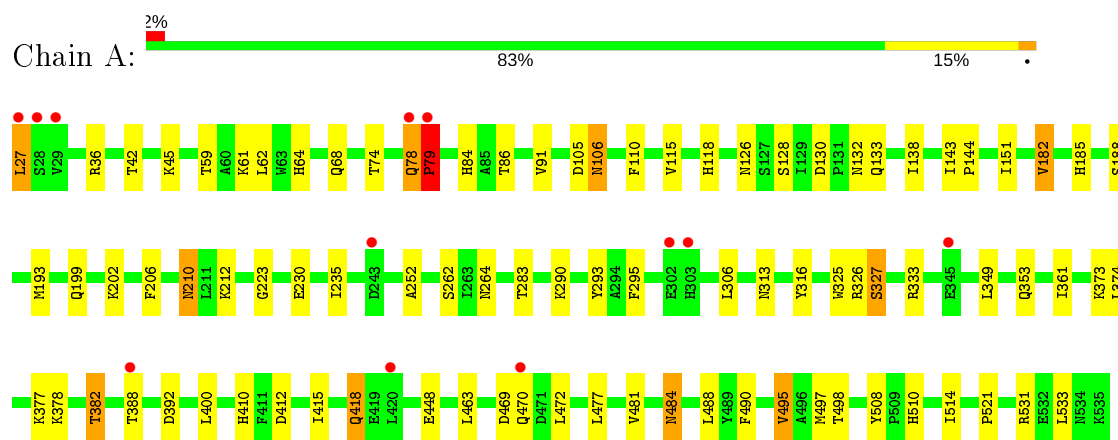
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	424	Total	O	0	0
			424	424		
4	B	383	Total	O	0	0
			383	383		

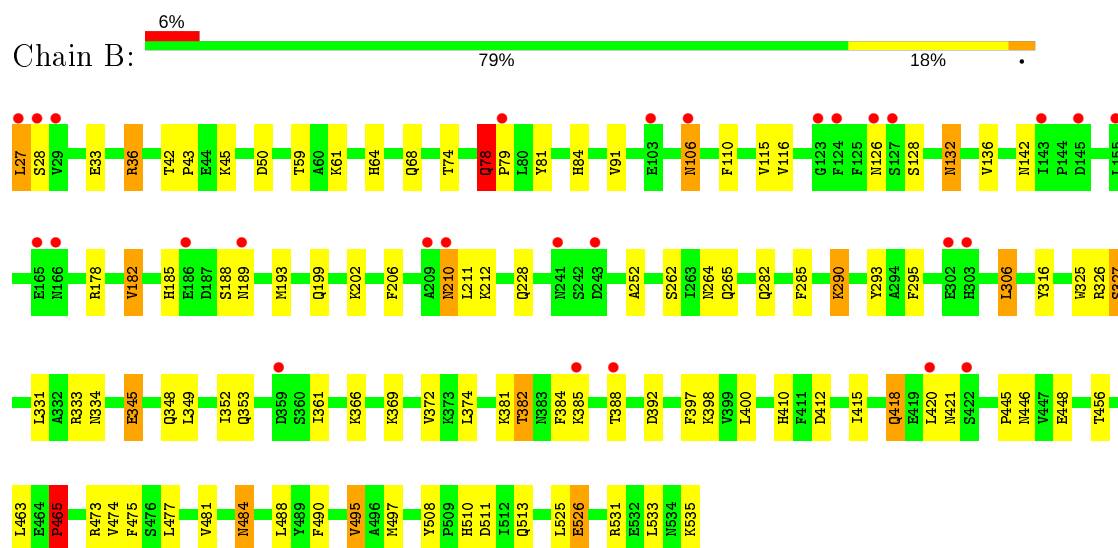
### 3 Residue-property plots

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: Invertase



#### • Molecule 1: Invertase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.87Å 92.27Å 116.28Å 90.00° 104.81° 90.00°	Depositor
Resolution (Å)	49.62 – 1.90 49.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.62-1.90) 99.6 (49.62-1.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.220 , 0.261 0.220 , 0.260	Depositor DCC
$R_{free}$ test set	4866 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9197	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: 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	0.45	1/4255 (0.0%)	0.65	5/5795 (0.1%)
1	B	0.42	0/4255	0.62	3/5795 (0.1%)
All	All	0.44	1/8510 (0.0%)	0.63	8/11590 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLN	C-N	8.50	1.50	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLN	CB-CA-C	9.11	128.62	110.40
1	B	78	GLN	C-N-CD	-7.43	104.26	120.60
1	A	78	GLN	C-N-CD	-6.69	105.88	120.60
1	A	79	PRO	CA-CB-CG	-6.23	92.16	104.00
1	A	78	GLN	C-N-CA	5.72	146.04	122.00
1	A	27	LEU	CA-CB-CG	5.60	128.17	115.30
1	B	27	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	465	PRO	CA-N-CD	-5.06	104.42	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	GLN	Peptide
1	B	78	GLN	Mainchain,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	4134	0	3918	64	0
1	B	4134	0	3919	74	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
3	A	56	0	52	0	0
3	B	42	0	39	1	0
4	A	424	0	0	11	0
4	B	383	0	0	12	0
All	All	9197	0	7952	137	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 8.

All (137) 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:488:LEU:HD12	1:B:497:MET:HE2	1.29	1.08
1:B:497:MET:SD	4:B:601:HOH:O	2.12	1.08
1:A:497:MET:SD	4:A:694:HOH:O	2.12	1.07
1:B:488:LEU:HD12	1:B:497:MET:CE	1.85	1.06
1:A:488:LEU:HD12	1:A:497:MET:HE2	1.40	1.04
1:A:488:LEU:HD12	1:A:497:MET:CE	1.86	1.03
1:A:79:PRO:HG3	1:A:105:ASP:HA	1.48	0.93
1:A:418:GLN:HE21	1:A:418:GLN:H	1.13	0.91
1:B:59:THR:HG23	1:B:132:ASN:HD21	1.39	0.87
1:A:415:ILE:HD13	1:A:481:VAL:HG21	1.55	0.86
1:B:78:GLN:HE22	1:B:142:ASN:HD22	1.19	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:THR:HG23	1:B:132:ASN:ND2	1.92	0.84
1:B:418:GLN:H	1:B:418:GLN:HE21	1.28	0.82
1:A:313:ASN:ND2	4:A:939:HOH:O	2.06	0.81
1:B:42:THR:HG23	1:B:325:TRP:CD1	2.16	0.80
1:A:42:THR:HG23	1:A:325:TRP:CD1	2.19	0.77
1:B:415:ILE:HD13	1:B:481:VAL:HG21	1.65	0.77
1:A:193:MET:CE	1:A:206:PHE:CD2	2.69	0.76
1:B:42:THR:CG2	1:B:325:TRP:CD1	2.70	0.75
1:B:64:HIS:HD2	1:B:84:HIS:NE2	1.84	0.75
1:A:382:THR:CG2	4:A:613:HOH:O	2.36	0.73
1:A:42:THR:CG2	1:A:325:TRP:CD1	2.72	0.72
1:A:382:THR:HG22	4:A:613:HOH:O	1.89	0.71
1:A:68:GLN:HE22	1:A:110:PHE:HA	1.56	0.69
1:B:78:GLN:NE2	1:B:142:ASN:HD22	1.89	0.69
1:B:382:THR:HG22	4:B:541:HOH:O	1.92	0.68
1:A:418:GLN:N	1:A:418:GLN:HE21	1.90	0.67
1:B:290:LYS:HE2	1:B:456:THR:OG1	1.95	0.67
1:A:392:ASP:OD1	1:A:531:ARG:HD3	1.95	0.66
1:B:290:LYS:HD2	4:B:730:HOH:O	1.96	0.65
1:A:79:PRO:CG	1:A:105:ASP:HA	2.25	0.65
1:A:79:PRO:HD3	1:A:105:ASP:O	1.97	0.65
1:B:418:GLN:HE21	1:B:418:GLN:N	1.94	0.62
1:B:210:ASN:HB3	1:B:212:LYS:H	1.65	0.61
1:A:185:HIS:HD2	1:A:188:SER:OG	1.84	0.61
1:B:68:GLN:HE22	1:B:110:PHE:HA	1.65	0.61
1:B:264:ASN:HD21	1:B:295:PHE:H	1.49	0.61
1:B:193:MET:CE	1:B:206:PHE:CD2	2.84	0.60
1:B:398:LYS:HG2	1:B:474:VAL:HG22	1.85	0.59
1:A:210:ASN:HB3	1:A:212:LYS:H	1.67	0.59
1:B:282:GLN:HE22	1:B:348:GLN:HE21	1.49	0.59
1:A:418:GLN:HE22	1:A:508:TYR:H	1.52	0.58
1:A:64:HIS:HD2	1:A:84:HIS:NE2	2.02	0.58
1:A:235:ILE:HD12	4:A:885:HOH:O	2.03	0.58
1:A:193:MET:HE2	1:A:206:PHE:CD2	2.38	0.58
1:B:418:GLN:HE22	1:B:508:TYR:H	1.50	0.58
1:A:484:ASN:C	1:A:484:ASN:HD22	2.08	0.56
1:B:535:LYS:C	4:B:638:HOH:O	2.44	0.56
1:A:264:ASN:HD21	1:A:295:PHE:H	1.53	0.56
1:B:252:ALA:HB1	1:B:293:TYR:CE1	2.41	0.55
1:B:508:TYR:O	1:B:510:HIS:HD2	1.88	0.55
1:A:290:LYS:HG2	1:A:316:TYR:OH	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:HD1	1:A:495:VAL:HG22	1.71	0.55
1:A:333:ARG:HH11	1:A:353:GLN:NE2	2.05	0.54
1:A:488:LEU:HD12	1:A:497:MET:HE1	1.84	0.54
1:A:59:THR:HG23	1:A:132:ASN:HD22	1.70	0.54
1:A:252:ALA:HB1	1:A:293:TYR:CE1	2.43	0.54
1:B:126:ASN:ND2	4:B:816:HOH:O	2.41	0.53
1:B:178:ARG:HH22	1:B:228:GLN:NE2	2.06	0.53
1:B:465:PRO:HG3	1:B:473:ARG:HB3	1.89	0.53
1:B:262:SER:HB2	1:B:293:TYR:CD1	2.45	0.52
1:B:333:ARG:HH11	1:B:353:GLN:NE2	2.07	0.52
1:A:42:THR:HG21	1:A:325:TRP:CD1	2.44	0.52
1:A:410:HIS:HD2	1:A:412:ASP:OD1	1.92	0.52
1:B:306:LEU:HD21	3:B:4001:NAG:H82	1.91	0.52
1:A:74:THR:HG21	4:A:696:HOH:O	2.09	0.52
1:B:535:LYS:O	4:B:638:HOH:O	2.19	0.51
1:B:42:THR:HG21	1:B:325:TRP:CD1	2.46	0.51
1:A:62:LEU:HG	1:A:86:THR:HB	1.91	0.51
1:A:290:LYS:HG3	1:A:313:ASN:HD22	1.76	0.51
1:A:326:ARG:O	1:A:327:SER:HB2	2.11	0.50
1:A:59:THR:HG21	1:A:130:ASP:OD2	2.11	0.50
1:B:185:HIS:HD2	1:B:188:SER:OG	1.94	0.50
1:B:91:VAL:HG11	1:B:361:ILE:HD11	1.92	0.50
1:A:374:LEU:HD11	1:A:514:ILE:HG22	1.94	0.49
1:B:326:ARG:O	1:B:327:SER:HB2	2.13	0.49
1:A:118:HIS:HE1	4:A:23:HOH:O	1.95	0.49
1:A:378:LYS:HE3	4:A:726:HOH:O	2.12	0.48
1:B:410:HIS:HD2	1:B:412:ASP:OD1	1.96	0.48
1:B:488:LEU:CD1	1:B:497:MET:CE	2.76	0.48
1:B:484:ASN:C	1:B:484:ASN:HD22	2.16	0.48
1:A:262:SER:HB2	1:A:293:TYR:CD1	2.49	0.47
1:B:445:PRO:O	1:B:446:ASN:HB2	2.14	0.47
1:A:333:ARG:NH2	1:A:498:THR:OG1	2.43	0.47
1:B:116:VAL:HG11	1:B:132:ASN:HA	1.97	0.46
1:B:79:PRO:HB2	1:B:81:TYR:CE1	2.51	0.46
1:B:228:GLN:NE2	4:B:818:HOH:O	2.45	0.45
1:B:490:PHE:HD1	1:B:495:VAL:HG22	1.81	0.45
1:A:199:GLN:HE21	1:B:345:GLU:HB2	1.81	0.45
1:A:508:TYR:O	1:A:510:HIS:HD2	1.99	0.45
1:B:193:MET:HE3	1:B:206:PHE:CD2	2.52	0.45
1:B:74:THR:OG1	1:B:326:ARG:HG3	2.16	0.45
1:A:469:ASP:O	1:A:470:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLN:NE2	4:A:585:HOH:O	2.49	0.45
1:A:74:THR:HG23	4:A:868:HOH:O	2.17	0.45
1:B:397:PHE:CZ	1:B:475:PHE:HB2	2.51	0.45
1:B:418:GLN:NE2	1:B:418:GLN:H	2.05	0.44
1:A:115:VAL:HG11	1:A:182:VAL:HG22	1.99	0.44
1:B:36:ARG:NH1	1:B:42:THR:HG22	2.32	0.44
1:A:484:ASN:C	1:A:484:ASN:ND2	2.70	0.44
1:B:331:LEU:HD22	4:B:837:HOH:O	2.17	0.44
1:B:64:HIS:CD2	1:B:84:HIS:NE2	2.75	0.44
1:B:372:VAL:CG2	1:B:525:LEU:HB2	2.48	0.44
1:A:415:ILE:CD1	1:A:481:VAL:HG21	2.39	0.43
1:A:126:ASN:HB3	1:A:128:SER:H	1.83	0.43
1:A:230:GLU:OE2	2:A:600:FRU:H12	2.19	0.43
1:A:143:ILE:HG23	1:A:144:PRO:HD2	2.01	0.43
1:A:373:LYS:HB3	1:A:521:PRO:HB3	2.00	0.43
1:B:36:ARG:HH11	1:B:42:THR:CG2	2.32	0.42
1:B:136:VAL:HG11	1:B:211:LEU:HD13	2.01	0.42
1:B:290:LYS:HG2	1:B:316:TYR:OH	2.19	0.42
1:B:79:PRO:HB2	1:B:81:TYR:CZ	2.54	0.42
1:B:74:THR:HG21	4:B:610:HOH:O	2.19	0.42
1:A:264:ASN:ND2	1:A:295:PHE:H	2.16	0.42
1:B:306:LEU:HD12	1:B:334:ASN:HA	2.02	0.42
1:A:118:HIS:CE1	4:A:23:HOH:O	2.72	0.42
1:B:392:ASP:OD1	1:B:531:ARG:HD3	2.20	0.42
1:B:384:PHE:HB2	4:B:698:HOH:O	2.20	0.42
1:A:410:HIS:CD2	1:A:412:ASP:OD1	2.73	0.41
1:A:91:VAL:HG11	1:A:361:ILE:HD11	2.01	0.41
1:B:381:LYS:HG2	1:B:513:GLN:HG2	2.03	0.41
1:B:42:THR:HG22	1:B:43:PRO:O	2.21	0.41
1:B:265:GLN:HA	1:B:285:PHE:HA	2.03	0.41
1:A:106:ASN:HA	1:A:106:ASN:HD22	1.66	0.41
1:A:223:GLY:HA2	1:A:283:THR:OG1	2.21	0.41
1:B:199:GLN:HG2	1:B:228:GLN:HG2	2.01	0.41
1:B:398:LYS:NZ	1:B:526:GLU:OE1	2.47	0.41
1:A:290:LYS:HG3	1:A:313:ASN:ND2	2.35	0.41
1:A:463:LEU:HD21	1:A:495:VAL:HG13	2.03	0.41
1:B:420:LEU:HB3	1:B:421:ASN:H	1.57	0.41
1:A:138:ILE:HG13	1:A:151:ILE:HG22	2.03	0.40
1:B:126:ASN:HB3	1:B:128:SER:H	1.86	0.40
1:B:410:HIS:HE1	4:B:587:HOH:O	2.04	0.40
1:B:106:ASN:HA	1:B:106:ASN:HD22	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:VAL:HG11	1:B:182:VAL:HG22	2.03	0.40
1:B:465:PRO:HD3	1:B:475:PHE:CZ	2.57	0.40
1:B:484:ASN:N	4:B:724:HOH:O	2.54	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	507/509 (100%)	484 (96%)	21 (4%)	2 (0%)	34	24
1	B	507/509 (100%)	482 (95%)	24 (5%)	1 (0%)	47	38
All	All	1014/1018 (100%)	966 (95%)	45 (4%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	PRO
1	A	327	SER
1	B	327	SER

### 5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	461/461 (100%)	438 (95%)	23 (5%)	24 15
1	B	461/461 (100%)	426 (92%)	35 (8%)	13 5
All	All	922/922 (100%)	864 (94%)	58 (6%)	18 8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ARG
1	A	45	LYS
1	A	61	LYS
1	A	79	PRO
1	A	106	ASN
1	A	133	GLN
1	A	182	VAL
1	A	202	LYS
1	A	210	ASN
1	A	306	LEU
1	A	349	LEU
1	A	377	LYS
1	A	382	THR
1	A	388	THR
1	A	400	LEU
1	A	418	GLN
1	A	448	GLU
1	A	472	LEU
1	A	477	LEU
1	A	484	ASN
1	A	495	VAL
1	A	533	LEU
1	B	27	LEU
1	B	28	SER
1	B	33	GLU
1	B	36	ARG
1	B	45	LYS
1	B	50	ASP
1	B	61	LYS
1	B	106	ASN
1	B	132	ASN

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Mol	Chain	Res	Type
1	B	182	VAL
1	B	189	ASN
1	B	202	LYS
1	B	210	ASN
1	B	290	LYS
1	B	306	LEU
1	B	345	GLU
1	B	349	LEU
1	B	352	ILE
1	B	366	LYS
1	B	369	LYS
1	B	374	LEU
1	B	382	THR
1	B	385	LYS
1	B	388	THR
1	B	400	LEU
1	B	418	GLN
1	B	448	GLU
1	B	463	LEU
1	B	465	PRO
1	B	477	LEU
1	B	484	ASN
1	B	495	VAL
1	B	511	ASP
1	B	526	GLU
1	B	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) 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	106	ASN
1	A	118	HIS
1	A	132	ASN
1	A	133	GLN
1	A	185	HIS
1	A	199	GLN
1	A	210	ASN
1	A	213	ASN

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Mol	Chain	Res	Type
1	A	227	ASN
1	A	228	GLN
1	A	264	ASN
1	A	296	GLN
1	A	348	GLN
1	A	353	GLN
1	A	401	ASN
1	A	410	HIS
1	A	418	GLN
1	A	435	GLN
1	A	484	ASN
1	A	510	HIS
1	A	513	GLN
1	B	52	ASN
1	B	64	HIS
1	B	68	GLN
1	B	78	GLN
1	B	106	ASN
1	B	118	HIS
1	B	132	ASN
1	B	133	GLN
1	B	185	HIS
1	B	199	GLN
1	B	210	ASN
1	B	213	ASN
1	B	227	ASN
1	B	228	GLN
1	B	264	ASN
1	B	296	GLN
1	B	348	GLN
1	B	353	GLN
1	B	410	HIS
1	B	418	GLN
1	B	435	GLN
1	B	484	ASN
1	B	510	HIS
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	3001	1	14,14,15	0.57	0	17,19,21	1.11	1 (5%)
3	NAG	B	3001	1	14,14,15	0.59	0	17,19,21	1.50	1 (5%)
3	NAG	A	5001	1	14,14,15	0.57	0	17,19,21	1.07	1 (5%)
3	NAG	B	4001	1	14,14,15	0.56	0	17,19,21	0.88	0
2	FRU	B	600	-	11,12,12	1.16	2 (18%)	10,18,18	1.49	1 (10%)
3	NAG	A	1001	1	14,14,15	0.57	0	17,19,21	1.28	2 (11%)
3	NAG	B	5001	1	14,14,15	0.47	0	17,19,21	1.39	1 (5%)
2	FRU	A	600	-	11,12,12	1.17	2 (18%)	10,18,18	1.50	1 (10%)
3	NAG	A	4001	1	14,14,15	0.55	0	17,19,21	1.17	2 (11%)

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	3001	1	-	2/6/23/26	0/1/1/1
3	NAG	B	3001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	5001	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	4001	1	-	2/6/23/26	0/1/1/1
2	FRU	B	600	-	-	3/5/24/24	0/1/1/1
3	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
3	NAG	B	5001	1	-	0/6/23/26	0/1/1/1
2	FRU	A	600	-	-	3/5/24/24	0/1/1/1
3	NAG	A	4001	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FRU	O2-C2	2.78	1.45	1.40
2	B	600	FRU	O2-C2	2.73	1.45	1.40
2	B	600	FRU	O5-C2	-2.09	1.40	1.43
2	A	600	FRU	O5-C2	-2.07	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3001	NAG	C1-O5-C5	4.93	118.88	112.19
3	B	5001	NAG	C1-O5-C5	4.39	118.15	112.19
3	A	3001	NAG	C1-O5-C5	3.98	117.58	112.19
2	A	600	FRU	O2-C2-O5	-3.67	102.41	109.50
2	B	600	FRU	O2-C2-O5	-3.66	102.43	109.50
3	A	4001	NAG	C1-O5-C5	3.23	116.56	112.19
3	A	5001	NAG	C1-O5-C5	3.10	116.39	112.19
3	A	1001	NAG	C4-C3-C2	2.64	114.89	111.02
3	A	1001	NAG	C1-O5-C5	2.58	115.69	112.19
3	A	4001	NAG	O5-C1-C2	-2.52	107.31	111.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	FRU	O1-C1-C2-O2
2	B	600	FRU	O1-C1-C2-O5
2	A	600	FRU	O1-C1-C2-O2
2	A	600	FRU	O1-C1-C2-O5
3	A	5001	NAG	O5-C5-C6-O6
3	A	1001	NAG	O5-C5-C6-O6
3	B	3001	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	3001	NAG	O5-C5-C6-O6
3	A	3001	NAG	C4-C5-C6-O6
3	A	3001	NAG	O5-C5-C6-O6
3	B	4001	NAG	C4-C5-C6-O6
3	A	5001	NAG	C4-C5-C6-O6
3	A	1001	NAG	C4-C5-C6-O6
3	B	4001	NAG	O5-C5-C6-O6
2	B	600	FRU	O1-C1-C2-C3
2	A	600	FRU	O1-C1-C2-C3
3	A	4001	NAG	C4-C5-C6-O6
3	A	4001	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4001	NAG	1	0
2	A	600	FRU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	509/509 (100%)	0.09	12 (2%) 59 62	7, 16, 26, 34	0
1	B	509/509 (100%)	0.28	28 (5%) 25 28	7, 17, 28, 36	0
All	All	1018/1018 (100%)	0.18	40 (3%) 39 42	7, 16, 27, 36	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	LEU	7.9
1	B	27	LEU	6.3
1	A	28	SER	4.8
1	B	302	GLU	3.8
1	B	143	ILE	3.6
1	A	470	GLN	3.3
1	B	385	LYS	3.2
1	B	422	SER	3.2
1	B	165	GLU	3.2
1	B	127	SER	3.2
1	A	420	LEU	3.1
1	A	302	GLU	2.9
1	B	420	LEU	2.8
1	A	79	PRO	2.8
1	B	126	ASN	2.8
1	B	166	ASN	2.7
1	A	78	GLN	2.7
1	B	106	ASN	2.7
1	B	103	GLU	2.6
1	B	124	PHE	2.6
1	B	303	HIS	2.5
1	B	79	PRO	2.5
1	B	155	LEU	2.4
1	A	303	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	210	ASN	2.4
1	B	189	ASN	2.4
1	A	29	VAL	2.3
1	B	28	SER	2.3
1	A	243	ASP	2.3
1	B	186	GLU	2.3
1	A	388	THR	2.3
1	B	123	GLY	2.2
1	A	345	GLU	2.2
1	B	241	ASN	2.2
1	B	145	ASP	2.1
1	B	388	THR	2.1
1	B	209	ALA	2.1
1	B	243	ASP	2.1
1	B	29	VAL	2.0
1	B	359	ASP	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 monosaccharides 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
3	NAG	B	5001	14/15	0.69	0.30	30,35,37,37	0
3	NAG	A	1001	14/15	0.70	0.29	31,35,37,37	0
3	NAG	A	5001	14/15	0.75	0.23	30,34,35,36	0
2	FRU	B	600	12/12	0.75	0.26	12,20,25,27	0
2	FRU	A	600	12/12	0.76	0.27	12,20,25,27	0
3	NAG	B	4001	14/15	0.82	0.15	22,25,26,26	0
3	NAG	A	4001	14/15	0.82	0.16	23,26,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	3001	14/15	0.86	0.14	29,32,34,35	0
3	NAG	A	3001	14/15	0.86	0.13	25,28,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.