



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2016 – 05:43 PM EDT

PDB ID : 5FMC  
Title : Structure of D80A-fructofuranosidase from Xanthophyllomyces dendrorhous complexed with fructose and BIS-TRIS propane buffer  
Authors : Ramirez-Escudero, M.; Sanz-Aparicio, J.  
Deposited on : 2015-11-02  
Resolution : 1.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
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) : rb-20027107

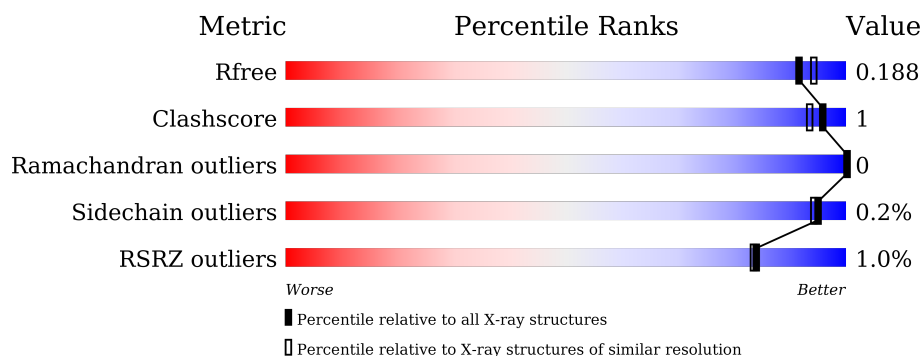
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	663	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
1	B	663	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>

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
3	B3P	A	1001	-	-	-	X
4	NAG	A	1236	-	-	-	X
4	NAG	A	1539	-	-	-	X
4	NAG	A	1606	-	-	-	X
4	NAG	A	1644	-	-	-	X
4	NAG	B	1236	-	-	-	X
4	NAG	B	1471	-	-	-	X
4	NAG	B	1539	-	-	-	X
4	NAG	B	1644	-	-	-	X
5	NAG	A	1058	-	-	-	X
5	MAN	A	1063	X	-	-	-
5	MAN	A	1064	X	-	-	-
6	MAN	B	1115	X	-	-	-
8	MAN	B	1062	X	-	-	-
8	MAN	B	1063	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11999 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.

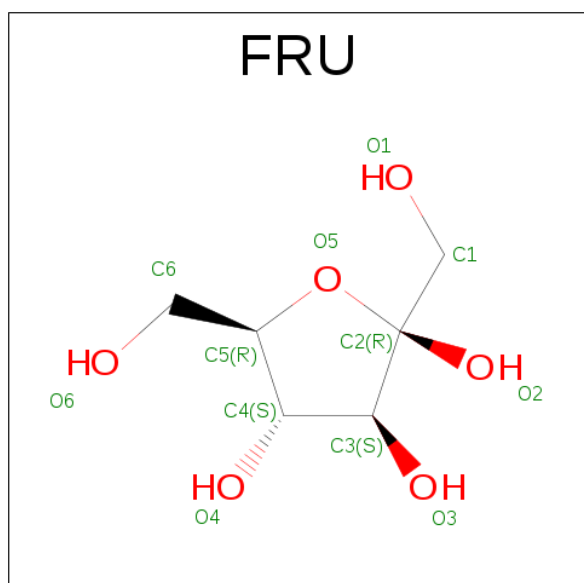
- Molecule 1 is a protein called BETA-FRUCTOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			
1	B	624	Total	C	N	O	S	0	1	0
			4805	3063	784	951	7			

There are 6 discrepancies between the modelled and reference sequences:

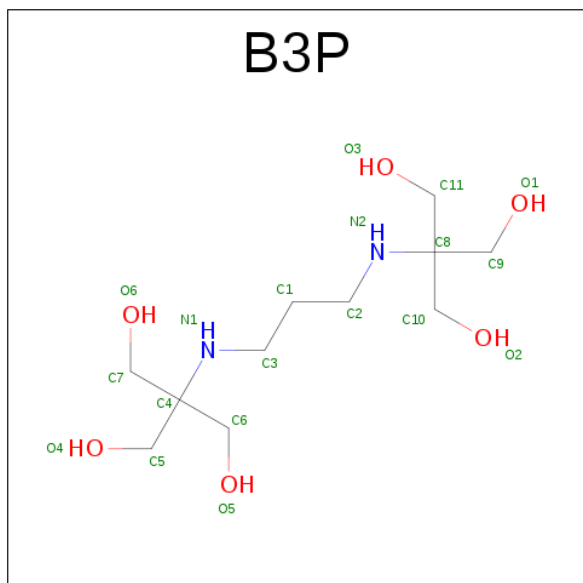
Chain	Residue	Modelled	Actual	Comment	Reference
A	663	ALA	SER	CONFLICT	UNP J7HDY4
A	665	TYR	ARG	CONFLICT	UNP J7HDY4
A	80	ALA	ASP	ENGINEERED MUTATION	UNP J7HDY4
B	663	ALA	SER	CONFLICT	UNP J7HDY4
B	665	TYR	ARG	CONFLICT	UNP J7HDY4
B	80	ALA	ASP	ENGINEERED MUTATION	UNP J7HDY4

- Molecule 2 is SUGAR (FRUCTOSE) (three-letter code: FRU) (formula:  $C_6H_{12}O_6$ ).



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-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	11	2	6		
3	B	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 6 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	10	Total	C	N	O	0	0
			116	64	2	50		
6	B	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total	C	N	O	0	0
			28	16	2	10		
7	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is water.

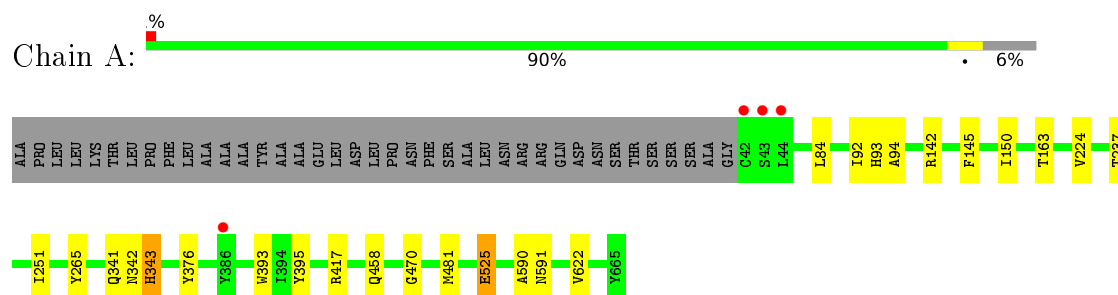
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	852	Total	O	0	0
			852	852		
9	B	640	Total	O	0	0
			640	640		



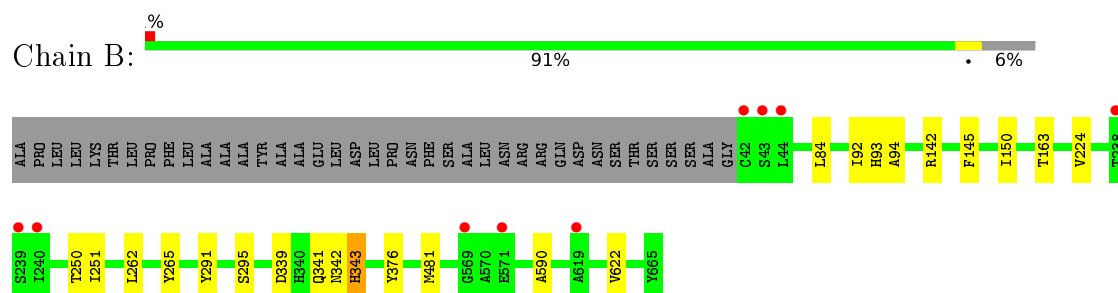
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: BETA-FRUCTOFURANOSIDASE



#### • Molecule 1: BETA-FRUCTOFURANOSIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.43Å 204.74Å 145.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.63 – 1.84 48.29 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (118.63-1.84) 99.8 (48.29-1.84)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.163 , 0.179 0.174 , 0.188	Depositor DCC
$R_{free}$ test set	9596 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 192541 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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: BMA, B3P, NAG, FRU, MAN

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	0.49	4/4940 (0.1%)	0.72	8/6754 (0.1%)
1	B	0.50	3/4940 (0.1%)	0.73	10/6754 (0.1%)
All	All	0.49	7/9880 (0.1%)	0.72	18/13508 (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
5	A	2	0
6	B	1	0
8	B	1	0
All	All	4	0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	590	ALA	C-N	-19.65	0.88	1.34
1	A	590	ALA	C-N	-14.30	1.01	1.34
1	A	93	HIS	C-N	7.79	1.51	1.34
1	A	591	ASN	C-N	-5.48	1.21	1.34
1	B	339	ASP	C-N	-5.32	1.21	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	HIS	O-C-N	12.77	143.13	122.70
1	A	93	HIS	O-C-N	12.61	142.88	122.70
1	B	343	HIS	O-C-N	11.61	141.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	HIS	O-C-N	10.62	139.69	122.70
1	A	342	ASN	C-N-CA	10.10	146.95	121.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1063	MAN	C1
5	A	1064	MAN	C1
8	B	1062	MAN	C1
6	B	1115	MAN	C1

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	4805	0	4496	13	0
1	B	4805	0	4498	9	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	19	0	26	1	0
3	B	19	0	26	1	0
4	A	210	0	195	7	0
4	B	182	0	169	1	0
5	A	83	0	70	1	0
6	A	116	0	97	0	0
6	B	116	0	97	0	0
7	A	28	0	25	0	0
7	B	28	0	25	0	0
8	B	72	0	61	0	0
9	A	852	0	0	5	0
9	B	640	0	0	3	0
All	All	11999	0	9809	30	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 1.

The worst 5 of 30 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)
4:A:1319:NAG:H83	9:A:2457:HOH:O	1.37	1.25
1:A:525:GLU:HB2	4:A:1606:NAG:H81	1.76	0.66
1:A:237:THR:HG23	9:A:2332:HOH:O	2.03	0.58
1:B:150:ILE:HG12	1:B:224:VAL:HG11	1.86	0.57
1:A:150:ILE:HG12	1:A:224:VAL:HG11	1.87	0.56

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	623/663 (94%)	595 (96%)	28 (4%)	0	100	100
1	B	623/663 (94%)	595 (96%)	28 (4%)	0	100	100
All	All	1246/1326 (94%)	1190 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/527 (94%)	497 (100%)	1 (0%)	95	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	498/527 (94%)	497 (100%)	1 (0%)	95	94
All	All	996/1054 (94%)	994 (100%)	2 (0%)	95	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	B	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	B	458	GLN
1	B	268	HIS
1	A	341	GLN
1	B	341	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 ⓘ

37 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
5	NAG	A	1058	1,5	14,14,15	0.36	0	15,19,21	0.99	1 (6%)
5	NAG	A	1059	5	14,14,15	0.61	0	15,19,21	1.36	4 (26%)
5	BMA	A	1060	5	11,11,12	0.39	0	15,15,17	1.95	3 (20%)
5	MAN	A	1061	5	11,11,12	0.63	0	15,15,17	0.87	0
5	MAN	A	1062	5	11,11,12	0.38	0	15,15,17	0.85	0
5	MAN	A	1063	5	11,11,12	0.57	0	15,15,17	1.76	4 (26%)
5	MAN	A	1064	5	11,11,12	0.56	0	15,15,17	1.16	1 (6%)
6	NAG	A	1107	1,6	14,14,15	0.90	1 (7%)	15,19,21	0.70	0
6	NAG	A	1108	6	14,14,15	0.28	0	15,19,21	0.78	0
6	BMA	A	1109	6	11,11,12	0.36	0	15,15,17	1.42	1 (6%)
6	MAN	A	1110	6	11,11,12	0.48	0	15,15,17	0.86	0
6	MAN	A	1111	6	11,11,12	0.38	0	15,15,17	0.73	1 (6%)
6	MAN	A	1112	6	11,11,12	0.45	0	15,15,17	0.67	0
6	MAN	A	1113	6	11,11,12	0.52	0	15,15,17	0.97	1 (6%)
6	MAN	A	1114	6	11,11,12	0.53	0	15,15,17	1.19	1 (6%)
6	MAN	A	1115	6	11,11,12	0.34	0	15,15,17	0.87	1 (6%)
6	MAN	A	1116	6	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
7	NAG	A	1576	1,7	14,14,15	0.29	0	15,19,21	0.98	1 (6%)
7	NAG	A	1577	7	14,14,15	0.46	0	15,19,21	1.74	4 (26%)
8	NAG	B	1058	1,8	14,14,15	0.32	0	15,19,21	0.96	1 (6%)
8	NAG	B	1059	8	14,14,15	0.50	0	15,19,21	0.71	0
8	BMA	B	1060	8	11,11,12	0.36	0	15,15,17	1.68	3 (20%)
8	MAN	B	1061	8	11,11,12	0.35	0	15,15,17	1.02	0
8	MAN	B	1062	8	11,11,12	0.69	0	15,15,17	1.35	2 (13%)
8	MAN	B	1063	8	11,11,12	0.31	0	15,15,17	0.85	1 (6%)
6	NAG	B	1107	1,6	14,14,15	0.83	1 (7%)	15,19,21	0.90	0
6	NAG	B	1108	6	14,14,15	0.41	0	15,19,21	0.87	0
6	BMA	B	1109	6	11,11,12	0.31	0	15,15,17	0.71	0
6	MAN	B	1110	6	11,11,12	0.29	0	15,15,17	0.87	1 (6%)
6	MAN	B	1111	6	11,11,12	0.37	0	15,15,17	1.37	2 (13%)
6	MAN	B	1112	6	11,11,12	0.37	0	15,15,17	0.76	1 (6%)
6	MAN	B	1113	6	11,11,12	0.49	0	15,15,17	0.95	0
6	MAN	B	1114	6	11,11,12	0.35	0	15,15,17	0.58	0
6	MAN	B	1115	6	11,11,12	0.62	0	15,15,17	1.42	2 (13%)
6	MAN	B	1116	6	11,11,12	0.52	0	15,15,17	0.78	0
7	NAG	B	1576	1,7	14,14,15	0.29	0	15,19,21	0.97	1 (6%)
7	NAG	B	1577	7	14,14,15	0.36	0	15,19,21	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1058	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1059	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1060	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1061	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1062	5	-	0/2/19/22	0/1/1/1
5	MAN	A	1063	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	A	1064	5	1/1/4/5	0/2/19/22	1/1/1/1
6	NAG	A	1107	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1108	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1109	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1110	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1111	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1112	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1113	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1114	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1115	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1116	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1576	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1577	7	-	0/6/23/26	0/1/1/1
8	NAG	B	1058	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1059	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1060	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1061	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1062	8	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	B	1063	8	-	0/2/19/22	0/1/1/1
6	NAG	B	1107	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1108	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1109	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1110	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1111	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1112	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1113	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1114	6	-	0/2/19/22	0/1/1/1
6	MAN	B	1115	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	B	1116	6	-	0/2/19/22	0/1/1/1
7	NAG	B	1576	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1577	7	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1107	NAG	C1-C2	2.52	1.56	1.52
6	A	1107	NAG	C1-C2	3.11	1.56	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1109	BMA	O3-C3-C4	-4.45	100.33	110.36
5	A	1060	BMA	O3-C3-C4	-3.38	102.74	110.36
5	A	1063	MAN	O2-C2-C1	-2.82	103.58	109.23
7	A	1576	NAG	O4-C4-C3	-2.32	105.12	110.36
6	B	1115	MAN	O2-C2-C3	-2.12	105.92	110.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	1062	MAN	C1
5	A	1064	MAN	C1
5	A	1063	MAN	C1
6	B	1115	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1064	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1059	NAG	1	0

## 5.6 Ligand geometry [i](#)

32 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
2	FRU	A	1000	-	11,12,12	0.61	0	10,18,18	0.50	0
3	B3P	A	1001	-	18,18,18	0.64	0	17,23,23	2.08	3 (17%)
4	NAG	A	1052	1	14,14,15	0.24	0	15,19,21	1.04	1 (6%)
4	NAG	A	1125	1	14,14,15	0.46	0	15,19,21	1.06	1 (6%)
4	NAG	A	1215	1	14,14,15	0.51	0	15,19,21	1.08	1 (6%)
4	NAG	A	1236	1	14,14,15	0.41	0	15,19,21	0.72	0
4	NAG	A	1242	1	14,14,15	0.22	0	15,19,21	0.80	0
4	NAG	A	1319	1	14,14,15	0.26	0	15,19,21	0.53	0
4	NAG	A	1357	1	14,14,15	0.37	0	15,19,21	1.26	2 (13%)
4	NAG	A	1444	1	14,14,15	0.42	0	15,19,21	0.98	1 (6%)
4	NAG	A	1471	1	14,14,15	0.35	0	15,19,21	1.20	1 (6%)
4	NAG	A	1483	1	14,14,15	0.33	0	15,19,21	0.78	1 (6%)
4	NAG	A	1512	1	14,14,15	0.30	0	15,19,21	1.20	3 (20%)
4	NAG	A	1539	1	14,14,15	0.68	0	15,19,21	1.24	1 (6%)
4	NAG	A	1555	1	14,14,15	0.33	0	15,19,21	1.10	2 (13%)
4	NAG	A	1606	1	14,14,15	0.72	0	15,19,21	1.90	5 (33%)
4	NAG	A	1644	1	14,14,15	0.32	0	15,19,21	0.78	0
2	FRU	B	1000	-	11,12,12	0.60	0	10,18,18	0.68	0
3	B3P	B	1001	-	18,18,18	0.59	0	17,23,23	1.86	3 (17%)
4	NAG	B	1052	1	14,14,15	0.30	0	15,19,21	0.65	0
4	NAG	B	1125	1	14,14,15	0.45	0	15,19,21	1.07	1 (6%)
4	NAG	B	1215	1	14,14,15	0.35	0	15,19,21	0.86	1 (6%)
4	NAG	B	1236	1	14,14,15	0.35	0	15,19,21	0.82	0
4	NAG	B	1242	1	14,14,15	0.30	0	15,19,21	1.17	2 (13%)
4	NAG	B	1319	1	14,14,15	0.27	0	15,19,21	0.54	0
4	NAG	B	1357	1	14,14,15	0.33	0	15,19,21	0.77	0
4	NAG	B	1444	1	14,14,15	0.38	0	15,19,21	1.46	2 (13%)
4	NAG	B	1471	1	14,14,15	0.36	0	15,19,21	0.71	0
4	NAG	B	1483	1	14,14,15	0.27	0	15,19,21	0.76	0
4	NAG	B	1539	1	14,14,15	0.48	0	15,19,21	1.59	3 (20%)
4	NAG	B	1555	1	14,14,15	0.44	0	15,19,21	0.67	0
4	NAG	B	1644	1	14,14,15	0.38	0	15,19,21	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	A	1000	-	-	0/5/24/24	0/1/1/1
3	B3P	A	1001	-	-	0/28/28/28	0/0/0/0
4	NAG	A	1052	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1125	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1215	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1319	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1357	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1444	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1471	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1512	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1539	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1555	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1606	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
2	FRU	B	1000	-	-	0/5/24/24	0/1/1/1
3	B3P	B	1001	-	-	0/28/28/28	0/0/0/0
4	NAG	B	1052	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1125	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1236	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1242	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1319	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1357	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1444	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1471	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1539	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1555	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1644	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1606	NAG	O7-C7-C8	-2.15	118.11	122.07
3	A	1001	B3P	C7-C4-C5	-2.15	106.21	110.16
3	B	1001	B3P	C7-C4-C5	-2.09	106.33	110.16
4	A	1125	NAG	O5-C5-C4	-2.02	106.80	110.13
4	A	1444	NAG	C3-C4-C5	2.05	113.89	110.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	B3P	1	0
4	A	1319	NAG	3	0
4	A	1471	NAG	1	0
4	A	1606	NAG	3	0
3	B	1001	B3P	1	0
4	B	1319	NAG	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	624/663 (94%)	-0.27	4 (0%) 90 89	12, 19, 30, 51	0
1	B	624/663 (94%)	-0.06	9 (1%) 78 76	15, 26, 41, 50	0
All	All	1248/1326 (94%)	-0.17	13 (1%) 84 83	12, 22, 38, 51	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	CYS	4.2
1	B	240	ILE	3.7
1	A	42	CYS	3.5
1	B	569	GLY	2.9
1	B	571	GLU	2.9

### 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
8	MAN	B	1063	11/12	0.82	0.39	22.58	60,61,63,63	0
5	NAG	A	1058	14/15	0.94	0.10	3.19	17,19,24,24	0
8	NAG	B	1058	14/15	0.97	0.09	-0.17	22,25,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	1108	14/15	0.97	0.08	-0.49	19,19,22,22	0
6	NAG	B	1107	14/15	0.97	0.08	-0.71	17,18,20,20	0
6	NAG	A	1108	14/15	0.96	0.08	-0.77	16,17,18,19	0
6	NAG	A	1107	14/15	0.97	0.08	-1.05	14,15,16,16	0
6	MAN	A	1113	11/12	0.83	0.17	-	53,56,61,62	0
8	MAN	B	1062	11/12	0.81	0.38	-	56,59,61,61	0
6	MAN	B	1112	11/12	0.76	0.57	-	79,84,87,90	0
6	MAN	B	1110	11/12	0.91	0.16	-	38,42,48,49	0
8	BMA	B	1060	11/12	0.91	0.15	-	36,43,51,52	0
6	MAN	A	1114	11/12	0.88	0.15	-	36,43,47,52	0
7	NAG	A	1576	14/15	0.90	0.14	-	37,41,48,59	0
5	MAN	A	1062	11/12	0.82	0.35	-	46,48,51,52	0
6	MAN	A	1115	11/12	0.81	0.26	-	53,57,60,69	0
6	MAN	A	1112	11/12	0.91	0.11	-	33,36,39,45	0
7	NAG	B	1577	14/15	0.73	0.38	-	70,81,86,87	0
8	NAG	B	1059	14/15	0.95	0.13	-	25,26,27,31	0
5	MAN	A	1064	11/12	0.49	0.44	-	81,85,90,94	0
6	MAN	A	1111	11/12	0.98	0.08	-	14,15,15,16	0
6	MAN	B	1114	11/12	0.98	0.09	-	16,18,18,18	0
5	BMA	A	1060	11/12	0.92	0.13	-	28,32,41,43	0
7	NAG	B	1576	14/15	0.88	0.17	-	46,51,58,68	0
5	MAN	A	1063	11/12	0.79	0.30	-	54,62,69,70	0
6	MAN	A	1110	11/12	0.96	0.08	-	16,19,25,29	0
6	BMA	A	1109	11/12	0.95	0.08	-	20,21,23,29	0
6	MAN	B	1116	11/12	0.71	0.20	-	52,56,58,60	0
5	MAN	A	1061	11/12	0.83	0.36	-	46,48,52,57	0
6	BMA	B	1109	11/12	0.96	0.07	-	22,23,26,31	0
6	MAN	B	1115	11/12	0.84	0.13	-	37,39,41,46	0
6	MAN	B	1111	11/12	0.81	0.25	-	57,61,65,70	0
6	MAN	A	1116	11/12	0.67	0.53	-	79,84,90,91	0
8	MAN	B	1061	11/12	0.63	0.39	-	61,67,71,71	0
6	MAN	B	1113	11/12	0.94	0.09	-	19,21,27,33	0
5	NAG	A	1059	14/15	0.96	0.09	-	19,21,24,31	0
7	NAG	A	1577	14/15	0.64	0.37	-	69,74,80,80	0

## 6.4 Ligands ⓘ

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
4	NAG	A	1539	14/15	0.80	0.25	9.12	39,46,49,52	0
4	NAG	B	1236	14/15	0.79	0.41	7.46	76,82,88,89	0
4	NAG	A	1606	14/15	0.69	0.31	6.80	50,56,57,60	0
4	NAG	B	1539	14/15	0.72	0.29	6.52	55,61,65,69	0
4	NAG	B	1471	14/15	0.89	0.15	3.54	31,35,38,38	0
4	NAG	A	1236	14/15	0.85	0.15	2.64	28,33,36,36	0
4	NAG	B	1644	14/15	0.93	0.14	2.54	26,28,34,39	0
4	NAG	A	1644	14/15	0.94	0.12	2.18	22,24,33,35	0
3	B3P	A	1001	19/19	0.87	0.12	2.13	32,36,39,40	0
3	B3P	B	1001	19/19	0.85	0.13	2.00	39,41,46,47	0
4	NAG	A	1483	14/15	0.92	0.15	1.91	35,39,42,45	0
4	NAG	B	1555	14/15	0.85	0.19	1.56	39,40,43,44	0
4	NAG	B	1357	14/15	0.94	0.15	1.50	39,42,46,48	0
4	NAG	A	1471	14/15	0.91	0.12	1.16	29,31,37,40	0
4	NAG	A	1357	14/15	0.95	0.09	0.10	31,33,36,38	0
4	NAG	A	1444	14/15	0.95	0.08	-0.18	23,24,28,32	0
2	FRU	B	1000	12/12	0.98	0.09	-0.40	18,18,19,20	0
2	FRU	A	1000	12/12	0.99	0.10	-0.61	13,13,15,15	0
4	NAG	B	1444	14/15	0.93	0.10	-0.67	32,35,37,37	0
4	NAG	B	1319	14/15	0.76	0.43	-	72,79,81,82	0
4	NAG	A	1512	14/15	0.80	0.23	-	47,54,67,68	0
4	NAG	A	1052	14/15	0.87	0.26	-	45,50,54,54	0
4	NAG	A	1215	14/15	0.77	0.44	-	62,74,75,79	0
4	NAG	B	1125	14/15	0.49	0.32	-	56,63,65,66	0
4	NAG	A	1125	14/15	0.69	0.29	-	54,62,66,66	0
4	NAG	B	1215	14/15	0.62	0.52	-	74,83,86,89	0
4	NAG	B	1483	14/15	0.84	0.21	-	53,57,61,63	0
4	NAG	B	1052	14/15	0.75	0.35	-	64,71,76,76	0
4	NAG	A	1319	14/15	0.78	0.45	-	55,62,68,68	0
4	NAG	B	1242	14/15	0.76	0.44	-	67,70,74,76	0
4	NAG	A	1242	14/15	0.79	0.33	-	50,56,59,59	0
4	NAG	A	1555	14/15	0.74	0.26	-	55,63,68,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.