



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:42 pm GMT

PDB ID : 2INV  
Title : Crystal structure of insulin fructotransferase in the presence of di-fructose  
Authors : Rhee, S.; Jung, W.S.  
Deposited on : 2006-10-09  
Resolution : 1.80 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

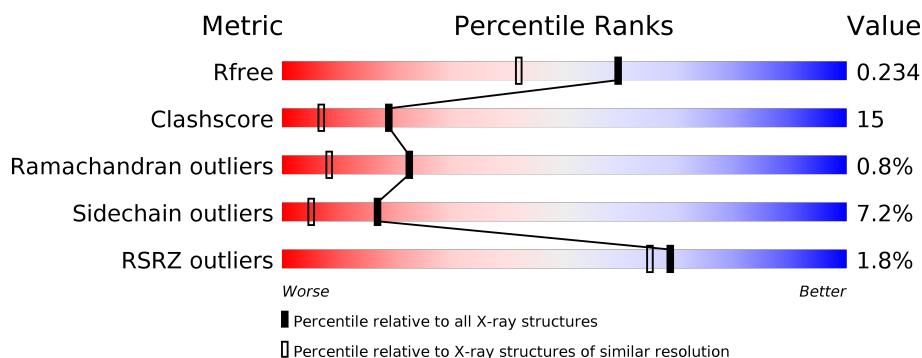
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	410	<div> <div>2%</div> <div>67%26% . .</div> </div>
1	B	410	<div> <div>2%</div> <div>67%27% . .</div> </div>
1	C	410	<div> <div>2%</div> <div>69%26% . .</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	2PO	A	1002	-	-	-	X
3	2PO	B	1001	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9648 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.

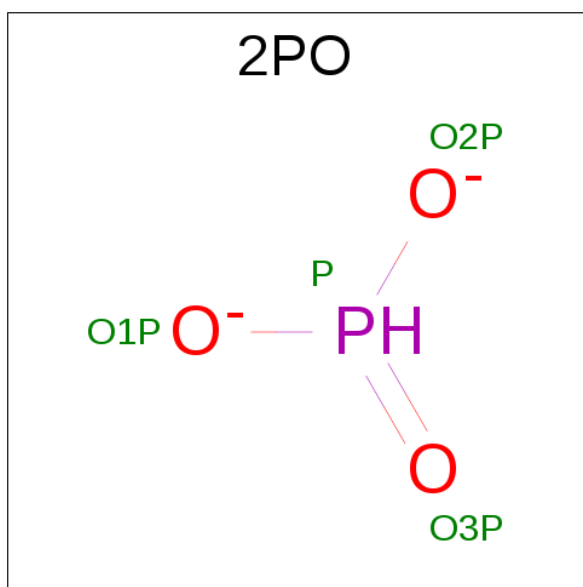
- Molecule 1 is a protein called Insulin Fructotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			
1	B	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			
1	C	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			23	12	11		
2	B	2	Total	C	O	0	0
			23	12	11		
2	C	2	Total	C	O	0	0
			23	12	11		

- Molecule 3 is PHOSPHONATE (three-letter code: 2PO) (formula: HO<sub>3</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			4	3	1		
3	B	1	Total	O	P	0	0
			4	3	1		

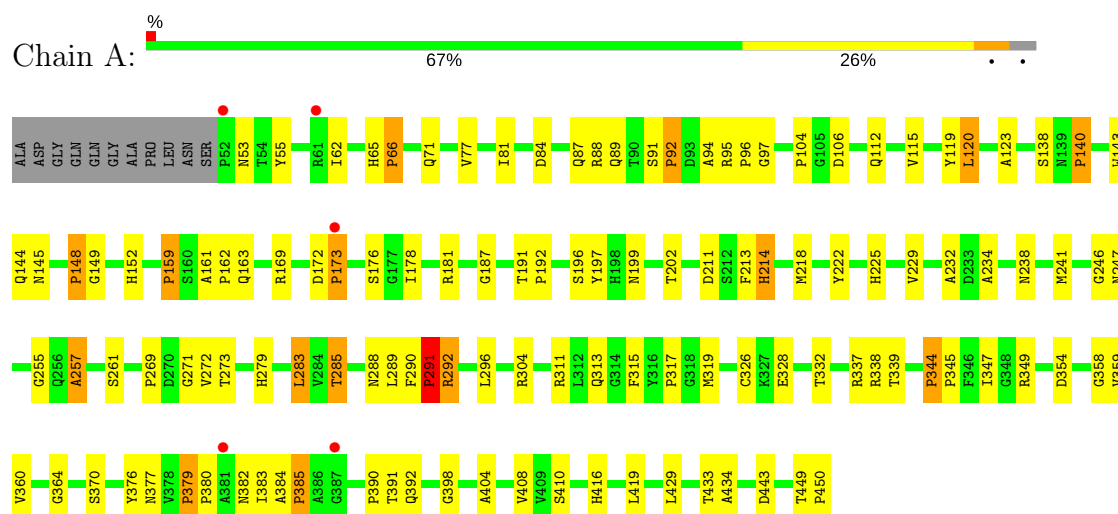
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	210	Total	O	0	0
			210	210		
4	C	212	Total	O	0	0
			212	212		

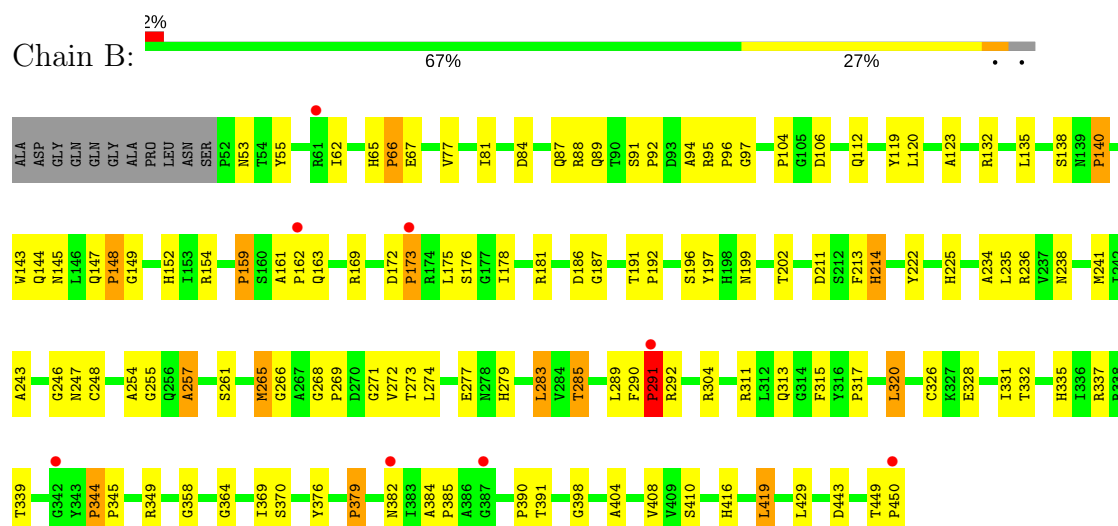
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Insulin Fructotransferase

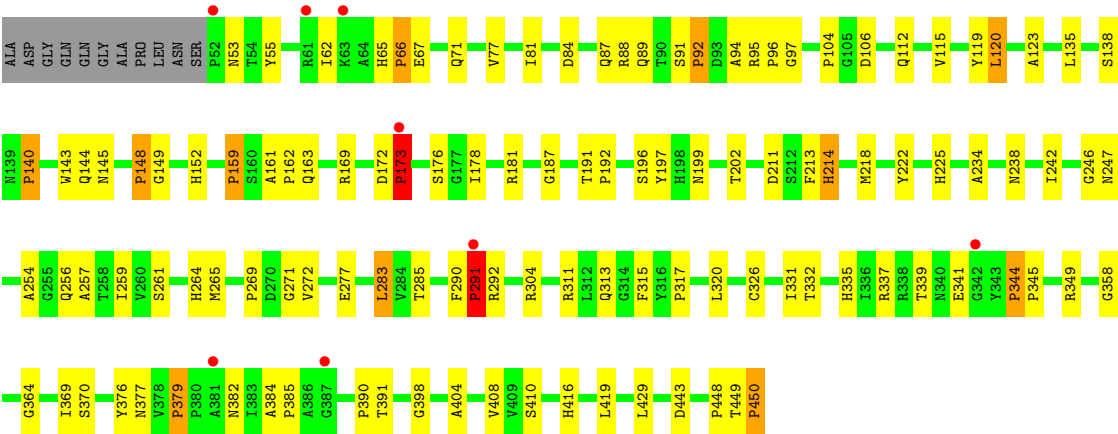


#### • Molecule 1: Insulin Fructotransferase



#### • Molecule 1: Insulin Fructotransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.17Å 91.90Å 92.92Å 90.00° 124.82° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 46.45 – 1.80	Depositor EDS
% Data completeness (in resolution range)	82.4 (50.00-1.80) 98.1 (46.45-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.207 , 0.227 0.214 , 0.234	Depositor DCC
$R_{free}$ test set	9984 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.012 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.013 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.019 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.019 for $-h+k-l, -l, -k$ 0.005 for $-h-k-l, l, k$ 0.019 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.005 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.487 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.487 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.013 for $-h-2^*l, -k, l$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

<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.



Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, 2PO

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	0.54	4/3042 (0.1%)	1.05	9/4143 (0.2%)
1	B	0.52	2/3042 (0.1%)	1.07	11/4143 (0.3%)
1	C	0.49	1/3042 (0.0%)	1.07	10/4143 (0.2%)
All	All	0.52	7/9126 (0.1%)	1.06	30/12429 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	C-N	11.36	1.60	1.34
1	B	291	PRO	C-N	10.70	1.58	1.34
1	C	291	PRO	C-N	9.93	1.56	1.34
1	B	285	THR	CB-OG1	7.35	1.57	1.43
1	A	285	THR	CB-OG1	7.27	1.57	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	PRO	O-C-N	-29.27	75.86	122.70
1	C	291	PRO	O-C-N	-28.55	77.02	122.70
1	A	291	PRO	O-C-N	-28.07	77.78	122.70
1	C	172	ASP	C-N-CD	-20.71	75.03	120.60
1	B	172	ASP	C-N-CD	-20.41	75.70	120.60

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	2982	0	2905	105	0
1	B	2982	0	2905	102	0
1	C	2982	0	2905	99	0
2	A	23	0	21	3	0
2	B	23	0	21	4	0
2	C	23	0	21	3	0
3	A	4	0	1	0	0
3	B	4	0	1	0	0
4	A	203	0	0	1	0
4	B	210	0	0	0	0
4	C	212	0	0	2	0
All	All	9648	0	8780	261	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 15.

The worst 5 of 261 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:265:MSE:HE3	1:B:273:THR:HG22	1.32	1.10
1:A:319:MSE:HE1	1:A:338:ARG:HB2	1.39	1.01
1:C:291:PRO:HB2	2:C:1:FRU:O6	1.67	0.93
1:A:291:PRO:HB2	2:A:1:FRU:O6	1.70	0.90
1:B:291:PRO:HB2	2:B:1:FRU:O6	1.73	0.89

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	397/410 (97%)	369 (93%)	25 (6%)	3 (1%)	22	8
1	B	397/410 (97%)	369 (93%)	25 (6%)	3 (1%)	22	8
1	C	397/410 (97%)	368 (93%)	26 (6%)	3 (1%)	22	8
All	All	1191/1230 (97%)	1106 (93%)	76 (6%)	9 (1%)	22	8

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	PRO
1	A	199	ASN
1	B	199	ASN
1	C	199	ASN
1	B	257	ALA

### 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	322/325 (99%)	299 (93%)	23 (7%)	17	5
1	B	322/325 (99%)	298 (92%)	24 (8%)	16	5
1	C	322/325 (99%)	299 (93%)	23 (7%)	17	5
All	All	966/975 (99%)	896 (93%)	70 (7%)	17	5

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	PRO
1	B	344	PRO
1	C	377	ASN
1	B	214	HIS
1	B	291	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	214	HIS
1	B	324	ASN
1	C	377	ASN
1	B	264	HIS
1	B	335	HIS

### 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 ⓘ

6 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	1	2	11,11,12	1.11	1 (9%)	15,15,18	2.47	4 (26%)
2	FRU	A	2	2	11,12,12	3.98	3 (27%)	10,18,18	2.43	2 (20%)
2	FRU	B	1	2	11,11,12	1.11	1 (9%)	15,15,18	2.48	4 (26%)
2	FRU	B	2	2	11,12,12	3.39	3 (27%)	10,18,18	2.89	3 (30%)
2	FRU	C	1	2	11,11,12	1.11	1 (9%)	15,15,18	2.48	4 (26%)
2	FRU	C	2	2	11,12,12	3.20	3 (27%)	10,18,18	1.97	2 (20%)

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	1	2	-	0/4/20/24	0/1/1/1
2	FRU	A	2	2	-	0/5/24/24	0/1/1/1
2	FRU	B	1	2	-	0/4/20/24	0/1/1/1
2	FRU	B	2	2	-	0/5/24/24	0/1/1/1
2	FRU	C	1	2	-	0/4/20/24	0/1/1/1
2	FRU	C	2	2	-	0/5/24/24	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	FRU	O1-C1	-9.04	1.13	1.42
2	A	2	FRU	O1-C1	-9.04	1.13	1.42
2	B	2	FRU	O1-C1	-9.04	1.13	1.42
2	A	2	FRU	O6-C6	-8.29	1.07	1.42
2	B	2	FRU	O6-C6	-4.29	1.24	1.42

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	FRU	O5-C2-C1	-3.28	102.16	109.16
2	B	1	FRU	O5-C2-C1	-3.26	102.19	109.16
2	A	1	FRU	O5-C2-C1	-3.26	102.20	109.16
2	A	1	FRU	C6-C5-C4	-2.70	108.52	115.05
2	C	1	FRU	C6-C5-C4	-2.69	108.54	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	FRU	3	0
2	B	1	FRU	4	0
2	B	2	FRU	1	0
2	C	1	FRU	3	0

## 5.6 Ligand geometry ⓘ

2 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	2PO	A	1002	-	0,3,3	0.00	-	0,3,3	0.00	-
3	2PO	B	1001	-	0,3,3	0.00	-	0,3,3	0.00	-

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	2PO	A	1002	-	-	0/0/0/0	0/0/0/0
3	2PO	B	1001	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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, 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	395/410 (96%)	0.03	5 (1%) 77 74	10, 14, 25, 31	0
1	B	395/410 (96%)	0.02	8 (2%) 65 61	10, 14, 25, 30	0
1	C	395/410 (96%)	0.02	8 (2%) 65 61	10, 14, 25, 30	0
All	All	1185/1230 (96%)	0.02	21 (1%) 69 65	10, 14, 25, 31	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	GLY	3.8
1	C	173	PRO	3.1
1	C	342	GLY	3.0
1	C	291	PRO	3.0
1	B	450	PRO	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
2	FRU	A	2	12/12	0.72	0.20	1.94	27,29,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FRU	C	2	12/12	0.80	0.17	1.65	26,29,30,31	0
2	FRU	B	2	12/12	0.78	0.16	1.39	28,29,30,32	0
2	FRU	A	1	11/12	0.86	0.14	0.85	22,23,25,25	0
2	FRU	B	1	11/12	0.83	0.14	0.60	24,25,26,26	0
2	FRU	C	1	11/12	0.80	0.14	0.47	22,24,25,25	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	2PO	A	1002	4/4	0.85	0.13	3.66	45,45,46,47	0
3	2PO	B	1001	4/4	0.86	0.16	3.35	33,33,33,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.