



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 02:49 PM EST

PDB ID : 3I4Z  
Title : Crystal structure of the dimethylallyl tryptophan synthase FgaPT2 from *Aspergillus fumigatus*  
Authors : Schall, C.; Zocher, G.; Stehle, T.  
Deposited on : 2009-07-03  
Resolution : 1.76 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

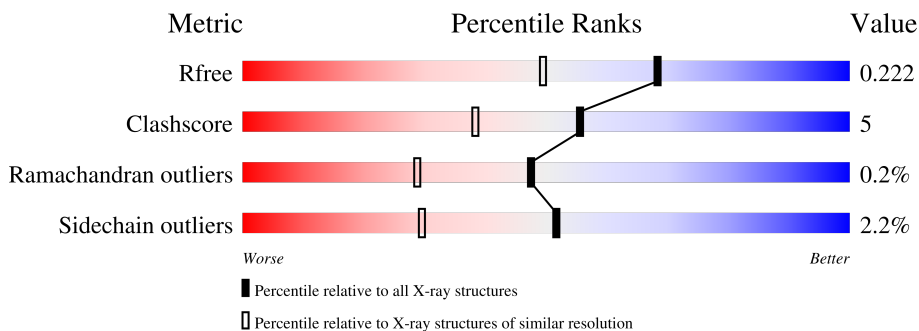
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	465	83% 11% 6%
1	B	465	82% 8% 9%

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	GOL	A	469	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7991 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.

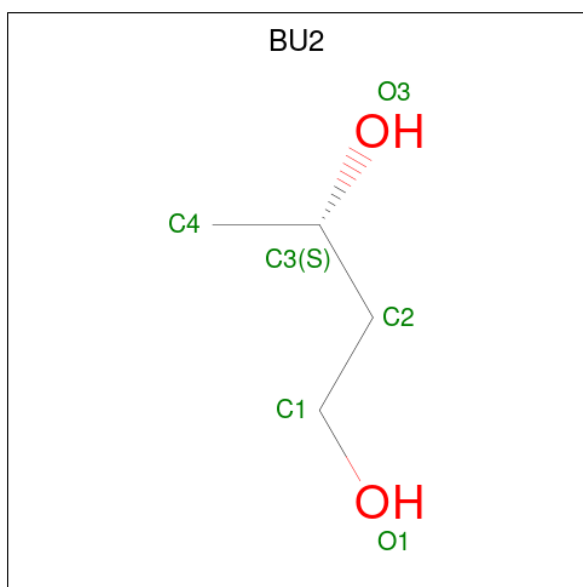
- Molecule 1 is a protein called Tryptophan dimethylallyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	Total	C	N	O	S	0	34	0
			3728	2404	626	681	17			
1	B	421	Total	C	N	O	S	0	20	0
			3507	2257	590	644	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q50EL0
A	-4	SER	-	expression tag	UNP Q50EL0
A	-3	HIS	-	expression tag	UNP Q50EL0
A	-2	GLY	-	expression tag	UNP Q50EL0
A	-1	GLY	-	expression tag	UNP Q50EL0
A	0	SER	-	expression tag	UNP Q50EL0
A	443	ALA	SER	SEE REMARK 999	UNP Q50EL0
B	-5	GLY	-	expression tag	UNP Q50EL0
B	-4	SER	-	expression tag	UNP Q50EL0
B	-3	HIS	-	expression tag	UNP Q50EL0
B	-2	GLY	-	expression tag	UNP Q50EL0
B	-1	GLY	-	expression tag	UNP Q50EL0
B	0	SER	-	expression tag	UNP Q50EL0
B	443	ALA	SER	SEE REMARK 999	UNP Q50EL0

- Molecule 2 is 1,3-BUTANEDIOL (three-letter code: BU2) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C O 6 4 2	0	0
2	A	1	Total C O 6 4 2	0	0
2	B	1	Total C O 6 4 2	0	0
2	B	1	Total C O 6 4 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

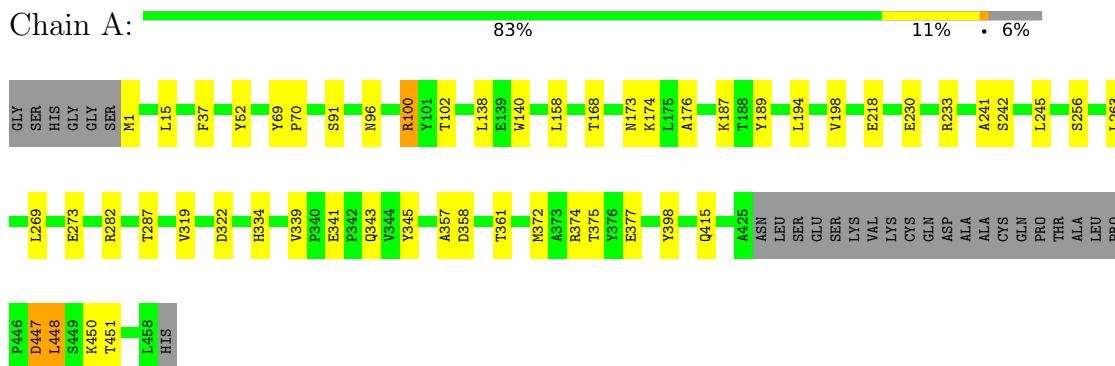
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	359	Total O 361 361	0	2
4	B	323	Total O 323 323	0	0

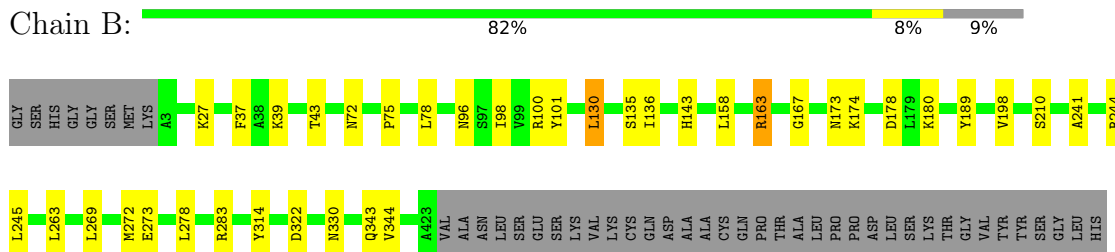
### 3 Residue-property plots [i](#)

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. 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. 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: Tryptophan dimethylallyltransferase



- Molecule 1: Tryptophan dimethylallyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.06Å 98.79Å 125.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.71 – 1.76 24.71 – 1.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.71-1.76) 99.7 (24.71-1.76)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.151 , 0.183 0.195 , 0.222	Depositor DCC
$R_{free}$ test set	2471 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtrriage
Anisotropy	0.812	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BU2, GOL

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	0.72	0/3922	0.74	0/5334
1	B	0.65	0/3660	0.67	0/4980
All	All	0.69	0/7582	0.71	0/10314

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3728	0	3747	43	0
1	B	3507	0	3495	30	0
2	A	36	0	60	6	0
2	B	12	0	20	3	0
3	A	24	0	32	6	0
4	A	361	0	0	7	0
4	B	323	0	0	2	0
All	All	7991	0	7354	74	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 5.



All (74) 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:138:LEU:H	3:A:469:GOL:H11	1.09	1.17
1:A:415:GLN:NE2	2:A:464:BU2:HC42	1.90	0.86
1:B:163:ARG:HD3	1:B:163:ARG:H	1.40	0.85
1:B:330:ASN:HD21	1:B:343:GLN:HE21	1.23	0.84
1:A:448:LEU:HD23	1:A:448:LEU:N	1.91	0.84
1:A:91[B]:SER:OG	1:A:100[B]:ARG:HG2	1.79	0.82
1:A:138:LEU:N	3:A:469:GOL:H11	1.94	0.78
1:A:138:LEU:HB2	3:A:469:GOL:H2	1.65	0.76
1:A:102[A]:THR:HG22	1:A:176:ALA:HB2	1.69	0.74
1:B:330:ASN:HD21	1:B:343:GLN:NE2	1.85	0.74
1:A:174:LYS:HG2	1:A:189:TYR:HB2	1.75	0.67
1:A:447:ASP:OD1	1:A:450:LYS:HE2	1.95	0.67
1:A:448:LEU:HD23	1:A:448:LEU:H	1.60	0.65
3:A:468:GOL:H11	4:A:493:HOH:O	1.97	0.65
1:A:187[A]:LYS:HG3	4:A:748:HOH:O	1.97	0.64
1:A:448:LEU:N	1:A:448:LEU:CD2	2.61	0.62
1:A:102[A]:THR:HG22	1:A:176:ALA:CB	2.29	0.61
1:A:282[B]:ARG:HG3	1:A:339:VAL:HG11	1.82	0.60
1:A:102[B]:THR:HG21	1:A:174:LYS:HE3	1.82	0.60
1:B:163:ARG:H	1:B:163:ARG:CD	2.11	0.59
1:A:415:GLN:HE22	2:A:464:BU2:HC42	1.63	0.59
1:B:244:ARG:HH21	2:B:460:BU2:HC41	1.68	0.58
1:A:361[B]:THR:HG23	4:A:724:HOH:O	2.04	0.58
1:B:174[B]:LYS:HG2	1:B:189:TYR:HB2	1.85	0.57
1:A:334[A]:HIS:HE1	1:A:341:GLU:OE1	1.87	0.57
1:A:158:LEU:HG	1:A:198[A]:VAL:CG1	2.34	0.57
1:B:244:ARG:HE	2:B:460:BU2:HC3	1.71	0.55
1:A:241:ALA:HA	1:A:263:LEU:O	2.07	0.55
1:B:244:ARG:HG3	1:B:263:LEU:HB2	1.89	0.55
1:A:15:LEU:HD21	1:A:52[B]:TYR:HD1	1.72	0.54
1:A:282[B]:ARG:NH1	1:A:287:THR:HG23	2.24	0.53
1:A:91[B]:SER:OG	1:A:100[B]:ARG:CG	2.53	0.53
1:B:135:SER:OG	4:B:624:HOH:O	2.19	0.52
1:A:158:LEU:HG	1:A:198[A]:VAL:HG12	1.93	0.51
2:A:463:BU2:HC21	1:B:314:TYR:CZ	2.46	0.50
1:B:244:ARG:HB3	2:B:460:BU2:HC3	1.93	0.49
1:A:345[A]:TYR:HD2	1:A:398:TYR:CD1	2.31	0.49
1:B:27:LYS:NZ	4:B:660:HOH:O	2.39	0.49
1:A:357:ALA:HB1	1:A:377[A]:GLU:HG2	1.95	0.48
1:A:358[B]:ASP:HA	1:A:361[B]:THR:HG22	1.95	0.48

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:469:GOL:H12	4:A:489:HOH:O	2.13	0.48
1:A:343:GLN:NE2	4:A:799:HOH:O	2.47	0.47
1:A:140:TRP:HZ2	1:A:218[B]:GLU:HG2	1.80	0.46
1:B:241:ALA:HA	1:B:263:LEU:O	2.16	0.46
1:A:140:TRP:CZ3	1:A:256[B]:SER:HB2	2.51	0.46
2:A:462:BU2:HC11	4:A:712:HOH:O	2.17	0.45
1:A:269:LEU:O	1:A:273:GLU:HG3	2.16	0.45
1:B:78:LEU:HD13	1:B:314:TYR:CE2	2.52	0.45
1:B:158:LEU:HG	1:B:198[B]:VAL:CG1	2.47	0.45
1:B:330:ASN:ND2	1:B:343:GLN:HE21	2.02	0.44
1:B:178[B]:ASP:HB3	1:B:180:LYS:HE2	1.99	0.44
1:B:130:LEU:HD12	1:B:136:ILE:HG21	2.00	0.43
1:A:174:LYS:HE2	1:A:189:TYR:CG	2.53	0.43
1:B:272[A]:MET:SD	1:B:344:VAL:HB	2.59	0.43
1:A:230:GLU:HG2	1:A:233[B]:ARG:HH12	1.83	0.42
1:A:69:TYR:HA	1:A:70:PRO:HD3	1.95	0.42
1:B:100:ARG:HG2	1:B:101:TYR:N	2.34	0.42
1:A:448:LEU:HD22	1:B:75:PRO:HD3	2.02	0.42
1:A:322:ASP:HB3	2:A:463:BU2:HC3	2.02	0.42
1:A:415:GLN:NE2	2:A:464:BU2:C4	2.72	0.42
1:A:374[B]:ARG:HG3	1:A:375:THR:HG23	2.02	0.42
3:A:468:GOL:C1	4:A:493:HOH:O	2.62	0.42
1:B:39:LYS:O	1:B:43:THR:HG23	2.20	0.42
1:B:98:ILE:HD12	1:B:180:LYS:HB3	2.01	0.42
1:B:143:HIS:HE1	1:B:210:SER:O	2.03	0.41
1:A:168[B]:THR:HG21	1:A:194:LEU:HD21	2.03	0.41
1:A:91[B]:SER:HG	1:A:100[B]:ARG:HG2	1.82	0.41
1:B:163:ARG:HD3	1:B:163:ARG:N	2.21	0.41
1:A:319:VAL:HG22	1:B:72:ASN:HB3	2.03	0.41
1:B:269:LEU:O	1:B:273:GLU:HG3	2.21	0.40
1:A:187[A]:LYS:HE3	1:A:187[A]:LYS:HB3	1.76	0.40
1:A:451:THR:HG21	1:B:75:PRO:HB3	2.03	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	468/465 (101%)	462 (99%)	5 (1%)	1 (0%)	47 29
1	B	439/465 (94%)	429 (98%)	9 (2%)	1 (0%)	47 29
All	All	907/930 (98%)	891 (98%)	14 (2%)	2 (0%)	47 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	GLY
1	A	447	ASP

### 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	419/408 (103%)	408 (97%)	11 (3%)	46 23
1	B	391/408 (96%)	383 (98%)	8 (2%)	55 34
All	All	810/816 (99%)	791 (98%)	19 (2%)	52 28

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	37	PHE
1	A	96	ASN
1	A	100[A]	ARG
1	A	100[B]	ARG
1	A	173	ASN
1	A	242[A]	SER
1	A	242[B]	SER
1	A	245	LEU
1	A	372	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	448	LEU
1	B	37	PHE
1	B	96	ASN
1	B	130	LEU
1	B	163	ARG
1	B	173	ASN
1	B	245	LEU
1	B	278	LEU
1	B	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	127	GLN
1	B	26	GLN
1	B	96	ASN
1	B	143	HIS
1	B	265	GLN
1	B	335	GLN
1	B	343	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 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	BU2	A	461	-	5,5,5	0.60	0	5,5,5	0.75	0
3	GOL	A	469	-	5,5,5	0.57	0	5,5,5	0.75	0
2	BU2	B	461	-	5,5,5	0.42	0	5,5,5	0.54	0
2	BU2	A	464	-	5,5,5	0.40	0	5,5,5	0.36	0
3	GOL	A	468	-	5,5,5	0.38	0	5,5,5	0.41	0
2	BU2	A	462	-	5,5,5	0.34	0	5,5,5	0.76	0
3	GOL	A	466	-	5,5,5	0.31	0	5,5,5	0.45	0
3	GOL	A	467	-	5,5,5	0.33	0	5,5,5	0.91	0
2	BU2	A	463	-	5,5,5	0.46	0	5,5,5	1.18	0
2	BU2	A	465	-	5,5,5	0.27	0	5,5,5	0.81	0
2	BU2	B	460	-	5,5,5	0.46	0	5,5,5	0.53	0
2	BU2	A	460	-	5,5,5	0.38	0	5,5,5	0.67	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	BU2	A	461	-	-	1/3/3/3	-
3	GOL	A	469	-	-	2/4/4/4	-
2	BU2	B	461	-	-	1/3/3/3	-
2	BU2	A	464	-	-	1/3/3/3	-
3	GOL	A	468	-	-	2/4/4/4	-
2	BU2	A	462	-	-	0/3/3/3	-
3	GOL	A	466	-	-	2/4/4/4	-
3	GOL	A	467	-	-	0/4/4/4	-
2	BU2	A	463	-	-	3/3/3/3	-
2	BU2	A	465	-	-	2/3/3/3	-
2	BU2	B	460	-	-	1/3/3/3	-
2	BU2	A	460	-	-	3/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	460	BU2	O1-C1-C2-C3
2	A	460	BU2	C1-C2-C3-C4
2	A	463	BU2	O1-C1-C2-C3
2	A	464	BU2	O1-C1-C2-C3
2	A	465	BU2	C1-C2-C3-C4
2	B	460	BU2	O1-C1-C2-C3
3	A	468	GOL	O1-C1-C2-O2
3	A	468	GOL	O1-C1-C2-C3
3	A	469	GOL	O2-C2-C3-O3
3	A	469	GOL	C1-C2-C3-O3
2	A	463	BU2	C1-C2-C3-O3
2	A	463	BU2	C1-C2-C3-C4
2	A	465	BU2	C1-C2-C3-O3
3	A	466	GOL	O1-C1-C2-O2
2	A	460	BU2	C1-C2-C3-O3
3	A	466	GOL	O1-C1-C2-C3
2	A	461	BU2	C1-C2-C3-O3
2	B	461	BU2	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	469	GOL	4	0
2	A	464	BU2	3	0
3	A	468	GOL	2	0
2	A	462	BU2	1	0
2	A	463	BU2	2	0
2	B	460	BU2	3	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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.