



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 02:08 am BST

PDB ID : 2BIS / pdb\_00002bis  
Title : Structure of glycogen synthase from *Pyrococcus abyssi*  
Authors : Horcajada, C.; Guinovart, J.J.; Fita, I.; Ferrer, J.C.  
Deposited on : 2005-01-25  
Resolution : 2.80 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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

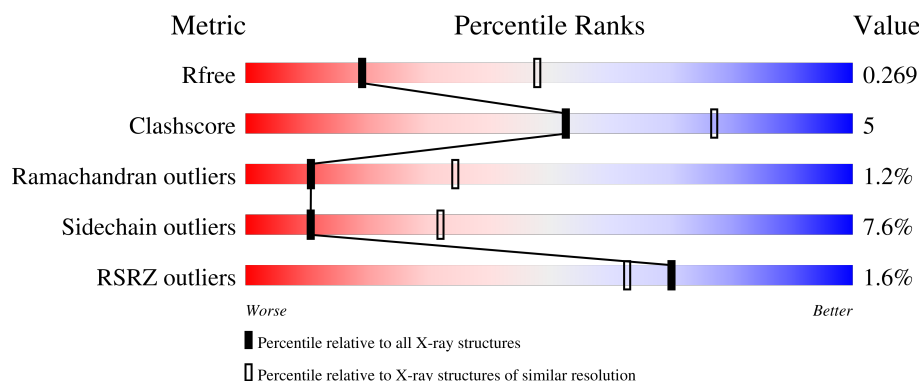
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 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  $\leq 5\%$ . 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	440	 86% 12% .
1	B	440	 85% 13% .
1	C	440	 80% 17% .

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
5	UDP	C	603	-	X	-	-

## 2 Entry composition [i](#)

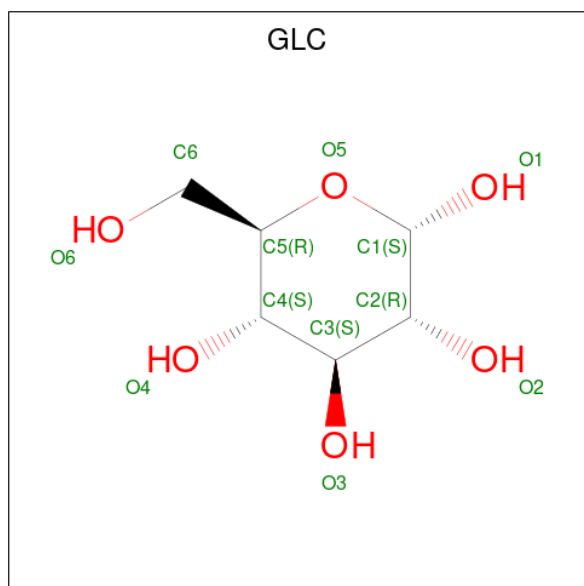
There are 5 unique types of molecules in this entry. The entry contains 10581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLGA GLYCOGEN SYNTHASE.

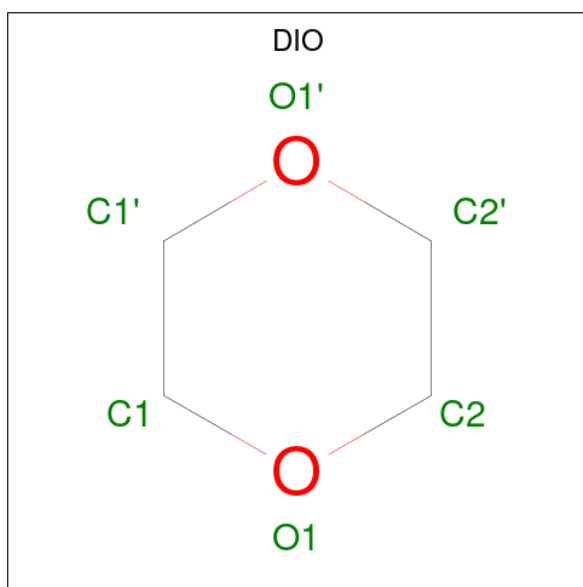
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3483	2256	583	634	10			
1	B	440	Total	C	N	O	S	0	0	0
			3483	2256	583	634	10			
1	C	440	Total	C	N	O	S	11	0	0
			3483	2256	583	634	10			

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (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
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



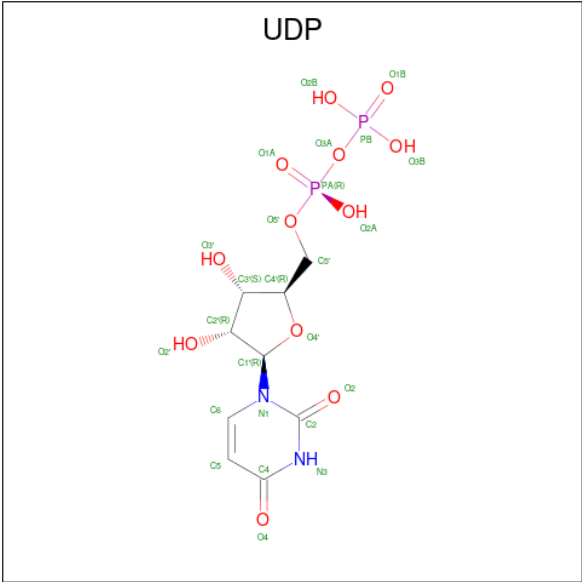
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).

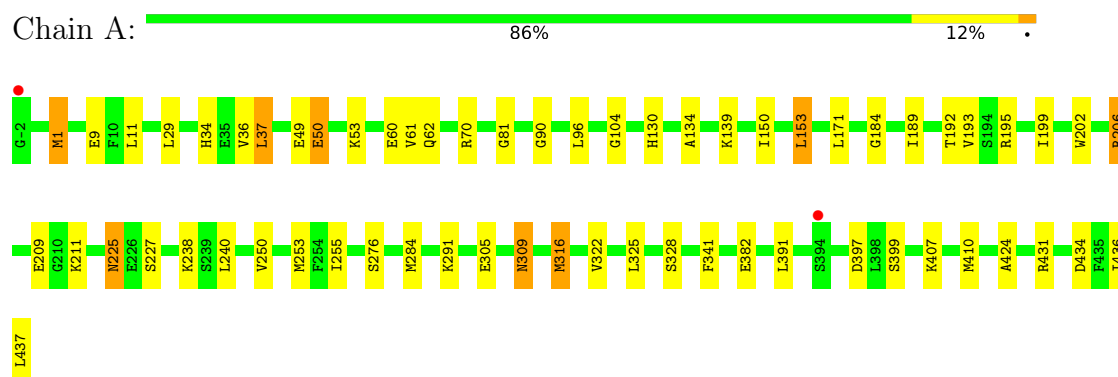


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			8	4	2	2		

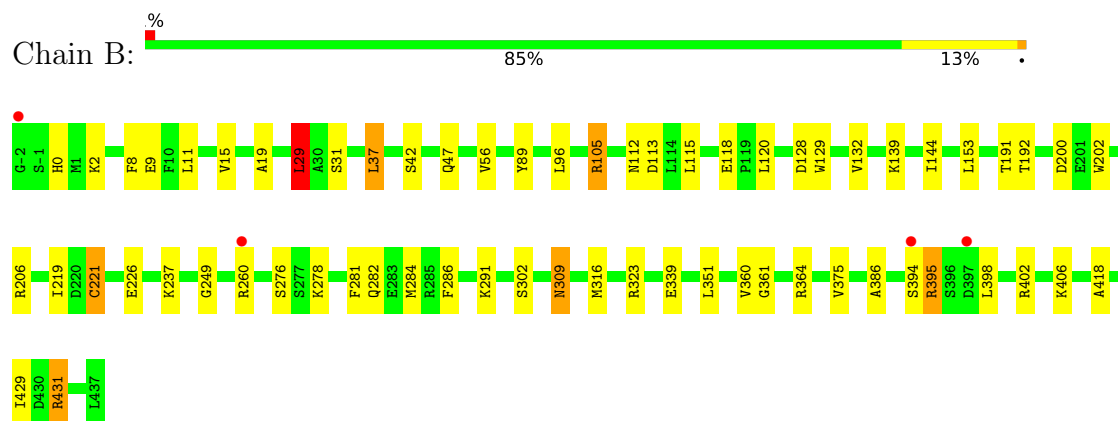
### 3 Residue-property plots [i](#)

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 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.

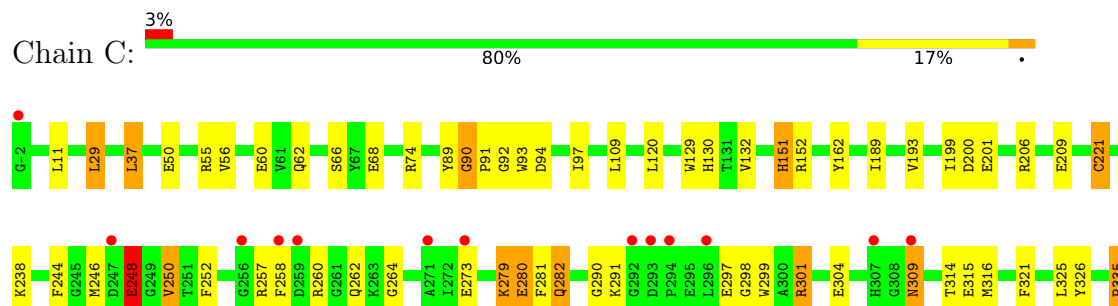
#### • Molecule 1: GLGA GLYCOGEN SYNTHASE



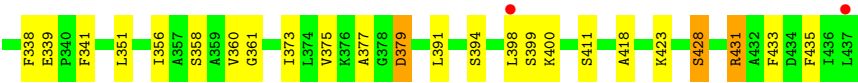
#### • Molecule 1: GLGA GLYCOGEN SYNTHASE



#### • Molecule 1: GLGA GLYCOGEN SYNTHASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.99Å 73.97Å 148.22Å 90.00° 131.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 99.7 (20.00-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.266 0.210 , 0.269	Depositor DCC
$R_{free}$ test set	2060 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 25.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: GLC, DIO, UDP, 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	0.60	0/3564	0.73	1/4806 (0.0%)
1	B	0.58	1/3564 (0.0%)	0.73	2/4806 (0.0%)
1	C	0.83	2/3564 (0.1%)	0.81	5/4806 (0.1%)
All	All	0.68	3/10692 (0.0%)	0.76	8/14418 (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	C	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	ARG	C-N	-29.97	0.65	1.34
1	B	221	CYS	CB-SG	6.34	1.93	1.82
1	C	221	CYS	CB-SG	5.16	1.91	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	HIS	O-C-N	-12.48	102.73	122.70
1	C	152	ARG	O-C-N	11.33	140.83	122.70
1	C	152	ARG	CA-C-N	-10.36	94.41	117.20
1	C	151	HIS	CA-C-N	7.55	133.82	117.20
1	B	316	MET	CG-SD-CE	7.42	112.08	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	LEU	CA-CB-CG	5.86	128.79	115.30
1	B	29	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	316	MET	CG-SD-CE	5.07	108.32	100.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	THR	Peptide
1	C	151	HIS	Mainchain
1	C	89	TYR	Peptide
1	C	90	GLY	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	3483	0	3485	30	0
1	B	3483	0	3485	30	0
1	C	3483	0	3484	50	0
2	A	11	0	10	0	0
2	C	11	0	10	0	0
3	A	24	0	32	1	0
3	B	18	0	24	1	0
3	C	18	0	24	2	0
4	A	18	0	24	5	0
4	B	18	0	24	1	0
4	C	6	0	8	3	0
5	C	8	0	3	0	0
All	All	10581	0	10613	103	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 (103) 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:C:339:GLU:O	1:C:361:GLY:HA3	1.86	0.76
1:C:93:TRP:O	1:C:97:ILE:HD12	1.87	0.74
1:A:341:PHE:H	4:A:614:GOL:H31	1.54	0.72
1:C:299:TRP:O	1:C:299:TRP:CD1	2.46	0.68
1:A:309:ASN:ND2	1:A:309:ASN:O	2.27	0.67
1:C:358:SER:HB3	1:C:377:ALA:HB2	1.75	0.67
1:A:50:GLU:HB2	1:A:62:GLN:NE2	2.10	0.66
1:B:112:ASN:HD21	1:C:431:ARG:HG2	1.62	0.64
1:A:341:PHE:H	4:A:614:GOL:C3	2.11	0.63
1:B:200:ASP:OD2	1:B:360:VAL:O	2.18	0.62
1:A:37:LEU:HD23	1:A:37:LEU:N	2.15	0.62
1:C:411:SER:O	3:C:611:DIO:H22	2.00	0.62
1:C:264:GLY:HA3	1:C:335:PRO:O	2.00	0.61
1:B:284:MET:O	1:B:309:ASN:ND2	2.32	0.59
1:C:321:PHE:CE1	1:C:325:LEU:HD21	2.40	0.57
1:B:284:MET:HE3	1:B:286:PHE:HZ	1.70	0.56
1:B:394:SER:OG	1:B:395:ARG:N	2.39	0.56
1:B:29:LEU:HD13	1:B:418:ALA:HB1	1.88	0.56
1:B:339:GLU:OE1	4:B:617:GOL:C3	2.54	0.55
1:A:189:ILE:HD11	1:A:424:ALA:HB1	1.88	0.55
1:B:237:LYS:HE3	1:B:249:GLY:O	2.06	0.55
1:C:129:TRP:HE1	4:C:620:GOL:C3	2.20	0.54
1:B:284:MET:HE3	1:B:286:PHE:CZ	2.43	0.54
1:B:398:LEU:O	1:B:402:ARG:HG3	2.08	0.54
1:C:37:LEU:N	1:C:37:LEU:HD23	2.24	0.52
1:A:1:MET:H	1:A:34:HIS:HD2	1.56	0.52
1:A:184:GLY:O	1:A:211:LYS:NZ	2.42	0.52
1:C:298:GLY:HA2	1:C:301:ARG:NH1	2.25	0.52
1:C:193:VAL:CG1	1:C:341:PHE:HB2	2.40	0.51
1:B:112:ASN:HD21	1:C:431:ARG:H	1.58	0.51
1:C:29:LEU:HD13	1:C:418:ALA:HB1	1.92	0.50
1:C:379:ASP:OD1	1:C:379:ASP:O	2.30	0.50
1:A:225:ASN:ND2	1:A:227:SER:OG	2.45	0.49
1:B:200:ASP:OD1	1:B:364:ARG:NH2	2.46	0.49
1:B:89:TYR:HA	1:B:96:LEU:HD13	1.93	0.49
1:A:193:VAL:HG12	1:A:341:PHE:HB2	1.94	0.49
1:C:209:GLU:HG2	1:C:433:PHE:HA	1.95	0.49
1:A:250:VAL:HG21	1:A:391:LEU:HD12	1.95	0.49
1:A:150:ILE:HG21	1:A:153:LEU:CD1	2.43	0.48
1:C:199:ILE:HG12	3:C:612:DIO:H22	1.94	0.48
1:A:171:LEU:HA	3:A:607:DIO:H2'2	1.95	0.48
1:B:115:LEU:O	1:C:423:LYS:NZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:SER:HA	1:B:281:PHE:CG	2.49	0.48
1:A:240:LEU:HD21	1:A:325:LEU:HD23	1.95	0.47
1:A:90:GLY:HA3	1:A:96:LEU:HB2	1.96	0.47
1:B:112:ASN:ND2	1:C:431:ARG:HG2	2.27	0.47
1:C:129:TRP:HA	1:C:132:VAL:HG23	1.96	0.47
1:B:375:VAL:HG11	1:B:386:ALA:HB2	1.97	0.47
1:C:358:SER:CB	1:C:377:ALA:HB2	2.44	0.47
1:C:250:VAL:HG12	1:C:252:PHE:CE1	2.50	0.47
1:B:9:GLU:HB3	1:B:19:ALA:HB2	1.97	0.47
1:A:284:MET:O	1:A:309:ASN:ND2	2.45	0.47
1:B:105:ARG:HG3	1:C:435:PHE:CE1	2.51	0.47
1:C:93:TRP:O	1:C:97:ILE:CD1	2.61	0.46
1:A:202:TRP:O	1:A:206:ARG:HB2	2.15	0.46
1:C:129:TRP:HE1	4:C:620:GOL:H32	1.81	0.46
1:C:356:ILE:HG12	1:C:373:ILE:HD12	1.98	0.46
1:A:407:LYS:HA	1:A:410:MET:CE	2.46	0.46
1:C:50:GLU:HG3	1:C:62:GLN:CG	2.45	0.46
1:C:238:LYS:HG3	1:C:248:GLU:OE2	2.15	0.46
1:C:90:GLY:O	1:C:92:GLY:N	2.49	0.46
1:C:315:GLU:N	1:C:315:GLU:OE1	2.49	0.45
1:A:322:VAL:HG11	4:A:616:GOL:H31	1.98	0.45
1:B:37:LEU:HD23	1:B:37:LEU:N	2.32	0.45
1:A:341:PHE:N	4:A:614:GOL:H31	2.28	0.45
1:C:246:MET:SD	1:C:309:ASN:O	2.75	0.45
1:C:244:PHE:HB2	1:C:246:MET:CE	2.47	0.45
1:C:309:ASN:HD22	1:C:309:ASN:HA	1.65	0.44
1:C:130:HIS:NE2	4:C:620:GOL:H31	2.33	0.44
1:C:298:GLY:HA2	1:C:301:ARG:HH12	1.82	0.44
1:C:258:PHE:CE1	1:C:290:GLY:O	2.70	0.44
1:B:429:ILE:O	1:B:431:ARG:HD3	2.18	0.43
1:A:130:HIS:HE1	4:A:615:GOL:H12	1.82	0.43
1:B:226:GLU:OE1	1:B:406:LYS:NZ	2.51	0.43
1:C:279:LYS:NZ	1:C:279:LYS:HB2	2.33	0.43
1:A:206:ARG:HH11	1:A:206:ARG:HB3	1.83	0.43
1:A:309:ASN:ND2	1:A:309:ASN:C	2.71	0.42
1:A:240:LEU:HD21	1:A:325:LEU:CD2	2.49	0.42
1:B:2:LYS:NZ	1:B:118:GLU:OE1	2.49	0.42
1:B:323:ARG:HG3	1:B:351:LEU:HD11	2.00	0.42
1:C:297:GLU:O	1:C:301:ARG:HD3	2.19	0.42
1:A:53:LYS:NZ	1:A:60:GLU:OE2	2.52	0.42
1:A:195:ARG:O	1:A:199:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ASP:OD2	1:C:360:VAL:O	2.37	0.41
1:C:193:VAL:HG12	1:C:341:PHE:HB2	2.02	0.41
1:C:250:VAL:HG21	1:C:391:LEU:HD12	2.01	0.41
1:B:276:SER:HA	1:B:281:PHE:CD1	2.56	0.41
1:C:97:ILE:HG22	1:C:162:TYR:CD2	2.55	0.41
1:C:280:GLU:C	1:C:282:GLN:H	2.23	0.41
1:A:104:GLY:HA2	1:A:134:ALA:HA	2.02	0.41
1:B:339:GLU:O	1:B:361:GLY:HA3	2.20	0.41
1:C:326:TYR:HB2	1:C:351:LEU:HD13	2.02	0.41
1:B:29:LEU:CD1	1:B:418:ALA:HB1	2.51	0.41
1:C:290:GLY:O	1:C:314:THR:HA	2.21	0.41
1:B:112:ASN:HD21	1:C:431:ARG:N	2.18	0.41
1:B:202:TRP:CE2	3:B:609:DIO:H2'1	2.55	0.41
1:A:250:VAL:HG21	1:A:391:LEU:CD1	2.51	0.41
1:C:280:GLU:C	1:C:282:GLN:N	2.73	0.41
1:A:36:VAL:C	1:A:37:LEU:HD23	2.42	0.40
1:C:423:LYS:HB3	1:C:428:SER:O	2.20	0.40
1:C:301:ARG:HA	1:C:304:GLU:HB3	2.04	0.40
1:A:436:ILE:HG12	1:C:109:LEU:CD1	2.52	0.40
1:B:129:TRP:HA	1:B:132:VAL:HG23	2.04	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	438/440 (100%)	416 (95%)	19 (4%)	3 (1%)	19	48
1	B	438/440 (100%)	410 (94%)	24 (6%)	4 (1%)	14	42
1	C	438/440 (100%)	393 (90%)	36 (8%)	9 (2%)	5	20
All	All	1314/1320 (100%)	1219 (93%)	79 (6%)	16 (1%)	11	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	ARG
1	C	91	PRO
1	C	260	ARG
1	B	128	ASP
1	C	248	GLU
1	C	281	PHE
1	C	428	SER
1	A	209	GLU
1	B	395	ARG
1	C	399	SER
1	A	276	SER
1	C	257	ARG
1	C	335	PRO
1	A	81	GLY
1	B	15	VAL
1	C	250	VAL

### 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	367/367 (100%)	340 (93%)	27 (7%)	11	33
1	B	367/367 (100%)	341 (93%)	26 (7%)	12	35
1	C	367/367 (100%)	336 (92%)	31 (8%)	9	28
All	All	1101/1101 (100%)	1017 (92%)	84 (8%)	11	32

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	GLU
1	A	11	LEU
1	A	29	LEU
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	49	GLU
1	A	50	GLU
1	A	61	VAL
1	A	70	ARG
1	A	139	LYS
1	A	153	LEU
1	A	206	ARG
1	A	225	ASN
1	A	238	LYS
1	A	253	MET
1	A	255	ILE
1	A	291	LYS
1	A	305	GLU
1	A	309	ASN
1	A	316	MET
1	A	328	SER
1	A	382	GLU
1	A	397	ASP
1	A	399	SER
1	A	431	ARG
1	A	434	ASP
1	A	437	LEU
1	B	0	HIS
1	B	8	PHE
1	B	11	LEU
1	B	29	LEU
1	B	31	SER
1	B	37	LEU
1	B	42	SER
1	B	47	GLN
1	B	56	VAL
1	B	105	ARG
1	B	113	ASP
1	B	120	LEU
1	B	139	LYS
1	B	144	ILE
1	B	153	LEU
1	B	191	THR
1	B	192	THR
1	B	206	ARG
1	B	219	ILE
1	B	221	CYS

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Mol	Chain	Res	Type
1	B	278	LYS
1	B	282	GLN
1	B	291	LYS
1	B	302	SER
1	B	309	ASN
1	B	431	ARG
1	C	11	LEU
1	C	29	LEU
1	C	37	LEU
1	C	55	ARG
1	C	56	VAL
1	C	60	GLU
1	C	66	SER
1	C	68	GLU
1	C	74	ARG
1	C	94	ASP
1	C	120	LEU
1	C	189	ILE
1	C	201	GLU
1	C	206	ARG
1	C	221	CYS
1	C	248	GLU
1	C	262	GLN
1	C	273	GLU
1	C	279	LYS
1	C	280	GLU
1	C	282	GLN
1	C	291	LYS
1	C	301	ARG
1	C	309	ASN
1	C	316	MET
1	C	338	PHE
1	C	375	VAL
1	C	379	ASP
1	C	394	SER
1	C	400	LYS
1	C	431	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS

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Mol	Chain	Res	Type
1	A	130	HIS
1	A	217	ASN
1	A	225	ASN
1	A	309	ASN
1	B	34	HIS
1	B	112	ASN
1	B	154	ASN
1	B	217	ASN
1	B	309	ASN
1	B	369	ASN
1	B	385	ASN
1	C	62	GLN
1	C	151	HIS
1	C	207	ASN
1	C	309	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

20 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	DIO	A	607	-	6,6,6	0.60	0	6,6,6	0.58	0
4	GOL	A	615	-	5,5,5	0.46	0	5,5,5	0.40	0
3	DIO	C	613	-	6,6,6	0.43	0	6,6,6	0.87	0
4	GOL	B	617	-	5,5,5	0.35	0	5,5,5	0.50	0
2	GLC	A	601	-	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
2	GLC	C	602	-	11,11,12	0.42	0	15,15,17	1.69	4 (26%)
3	DIO	A	604	-	6,6,6	0.61	0	6,6,6	0.69	0
3	DIO	B	608	-	6,6,6	0.52	0	6,6,6	0.66	0
5	UDP	C	603	-	8,8,26	2.20	4 (50%)	9,10,40	3.96	6 (66%)
3	DIO	A	606	-	6,6,6	0.53	0	6,6,6	1.00	0
4	GOL	C	620	-	5,5,5	0.29	0	5,5,5	0.51	0
4	GOL	B	618	-	5,5,5	0.35	0	5,5,5	0.48	0
4	GOL	A	614	1	5,5,5	0.37	0	5,5,5	0.33	0
4	GOL	B	619	-	5,5,5	0.44	0	5,5,5	0.68	0
3	DIO	C	612	-	6,6,6	0.45	0	6,6,6	0.61	0
3	DIO	A	605	-	6,6,6	0.50	0	6,6,6	0.43	0
3	DIO	B	610	-	6,6,6	0.51	0	6,6,6	0.84	0
3	DIO	B	609	-	6,6,6	0.51	0	6,6,6	0.40	0
4	GOL	A	616	-	5,5,5	0.34	0	5,5,5	0.24	0
3	DIO	C	611	-	6,6,6	0.54	0	6,6,6	0.34	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
3	DIO	A	607	-	-	-	0/1/1/1
4	GOL	A	615	-	-	2/4/4/4	-
3	DIO	C	613	-	-	-	0/1/1/1
4	GOL	B	617	-	-	4/4/4/4	-
2	GLC	A	601	-	-	0/2/19/22	0/1/1/1
2	GLC	C	602	-	-	1/2/19/22	0/1/1/1
3	DIO	A	604	-	-	-	0/1/1/1
3	DIO	B	608	-	-	-	0/1/1/1
5	UDP	C	603	-	-	-	0/1/1/2
3	DIO	A	606	-	-	-	0/1/1/1
4	GOL	C	620	-	-	4/4/4/4	-
4	GOL	B	618	-	-	2/4/4/4	-
4	GOL	A	614	1	-	0/4/4/4	-
4	GOL	B	619	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DIO	C	612	-	-	-	0/1/1/1
3	DIO	A	605	-	-	-	0/1/1/1
3	DIO	B	610	-	-	-	0/1/1/1
3	DIO	B	609	-	-	-	0/1/1/1
4	GOL	A	616	-	-	2/4/4/4	-
3	DIO	C	611	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	UDP	C4-N3	-3.23	1.32	1.38
5	C	603	UDP	C2-N1	3.13	1.41	1.36
5	C	603	UDP	C2-N3	-2.76	1.32	1.37
5	C	603	UDP	C5-C4	-2.10	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	603	UDP	C4-N3-C2	-6.40	119.36	125.70
5	C	603	UDP	N1-C2-N3	5.83	121.73	115.13
5	C	603	UDP	C6-N1-C2	-5.17	119.23	122.40
5	C	603	UDP	C5-C4-N3	4.19	121.10	114.84
2	C	602	GLC	C1-O5-C5	3.91	117.48	112.19
5	C	603	UDP	O4-C4-C5	-2.95	119.98	125.16
2	A	601	GLC	C1-O5-C5	2.81	116.01	112.19
2	C	602	GLC	O3-C3-C4	2.63	116.44	110.35
5	C	603	UDP	O2-C2-N1	-2.58	119.95	122.79
2	A	601	GLC	C1-C2-C3	2.33	112.53	109.67
2	C	602	GLC	C2-C3-C4	-2.14	107.19	110.89
2	A	601	GLC	O3-C3-C2	2.07	113.96	109.99
2	C	602	GLC	O5-C5-C6	2.02	110.38	107.20

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	618	GOL	O1-C1-C2-C3
4	C	620	GOL	C1-C2-C3-O3
4	B	618	GOL	O1-C1-C2-O2
4	B	617	GOL	C1-C2-C3-O3
4	C	620	GOL	O1-C1-C2-C3

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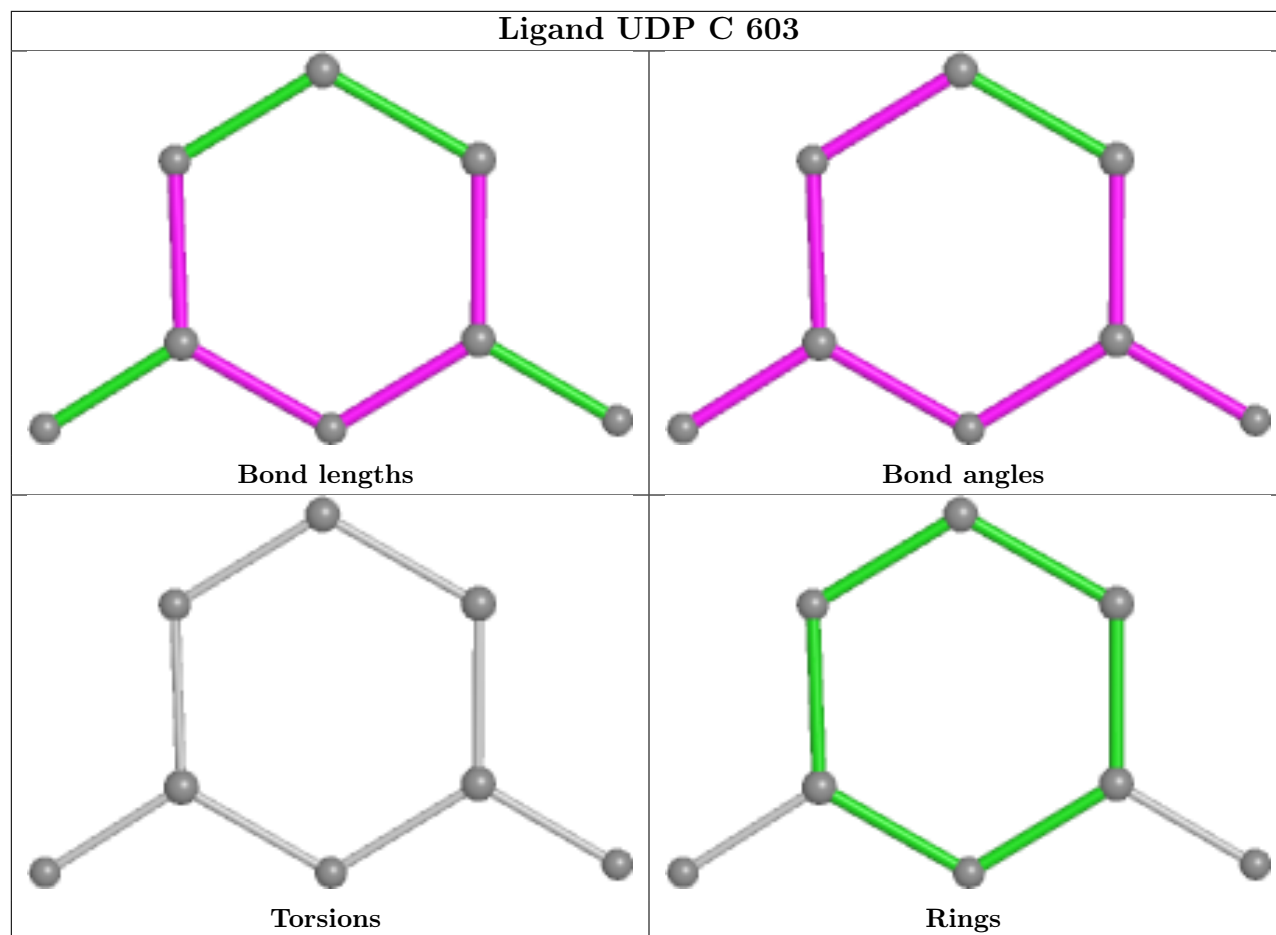
Mol	Chain	Res	Type	Atoms
4	C	620	GOL	O1-C1-C2-O2
4	C	620	GOL	O2-C2-C3-O3
4	B	617	GOL	O2-C2-C3-O3
4	B	617	GOL	O1-C1-C2-O2
4	A	615	GOL	O2-C2-C3-O3
4	A	616	GOL	O1-C1-C2-O2
2	C	602	GLC	C4-C5-C6-O6
4	A	615	GOL	C1-C2-C3-O3
4	B	617	GOL	O1-C1-C2-C3
4	A	616	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	607	DIO	1	0
4	A	615	GOL	1	0
4	B	617	GOL	1	0
4	C	620	GOL	3	0
4	A	614	GOL	3	0
3	C	612	DIO	1	0
3	B	609	DIO	1	0
4	A	616	GOL	1	0
3	C	611	DIO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	152:ARG	C	153:LEU	N	0.65

## 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	440/440 (100%)	-0.24	2 (0%) 87 83	33, 48, 67, 78	0
1	B	440/440 (100%)	-0.27	4 (0%) 81 75	36, 48, 67, 76	0
1	C	439/440 (99%)	-0.01	15 (3%) 48 40	34, 48, 72, 92	0
All	All	1319/1320 (99%)	-0.17	21 (1%) 70 63	33, 48, 68, 92	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-2	GLY	5.5
1	A	-2	GLY	4.4
1	B	260	ARG	3.0
1	C	258	PHE	2.9
1	C	294	PRO	2.8
1	C	437	LEU	2.6
1	B	397	ASP	2.6
1	C	247	ASP	2.6
1	C	271	ALA	2.5
1	C	273	GLU	2.5
1	B	-2	GLY	2.4
1	C	307	HIS	2.4
1	C	309	ASN	2.3
1	C	296	LEU	2.3
1	C	256	GLY	2.3
1	A	394	SER	2.2
1	C	292	GLY	2.1
1	C	259	ASP	2.1
1	C	293	ASP	2.1
1	C	398	LEU	2.1
1	B	394	SER	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](#)

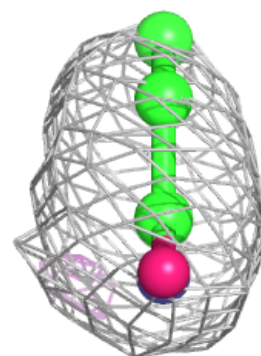
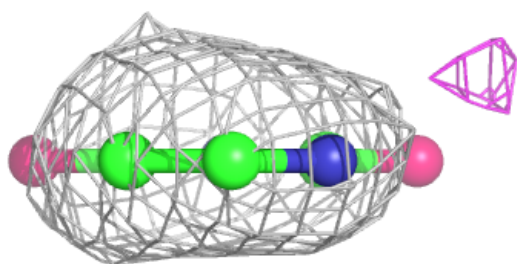
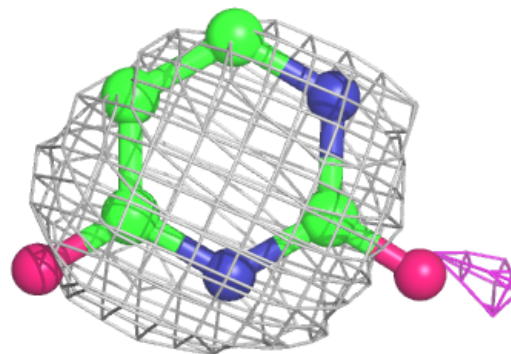
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	GOL	B	617	6/6	0.66	0.17	83,84,85,85	0
4	GOL	A	614	6/6	0.69	0.19	73,73,74,75	0
2	GLC	C	602	11/12	0.74	0.16	75,76,78,78	0
2	GLC	A	601	11/12	0.75	0.15	73,75,76,77	0
3	DIO	A	607	6/6	0.77	0.21	72,72,72,72	0
3	DIO	A	605	6/6	0.78	0.19	59,59,60,60	0
4	GOL	C	620	6/6	0.78	0.20	78,79,79,79	0
4	GOL	A	615	6/6	0.80	0.20	71,71,71,72	0
3	DIO	B	609	6/6	0.80	0.18	69,69,70,70	0
4	GOL	B	619	6/6	0.80	0.19	83,84,85,85	0
3	DIO	A	606	6/6	0.80	0.18	63,63,64,65	0
4	GOL	B	618	6/6	0.83	0.16	79,79,79,80	0
3	DIO	B	608	6/6	0.84	0.16	65,66,67,68	0
3	DIO	C	612	6/6	0.85	0.17	71,71,72,72	0
4	GOL	A	616	6/6	0.85	0.14	82,83,83,83	0
3	DIO	B	610	6/6	0.86	0.20	74,75,76,76	0
3	DIO	C	611	6/6	0.87	0.16	71,71,71,72	0
3	DIO	C	613	6/6	0.88	0.17	73,74,74,74	0
3	DIO	A	604	6/6	0.91	0.12	55,56,56,57	0
5	UDP	C	603	8/25	0.91	0.21	80,80,81,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around UDP C 603:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.