Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2023 – 02:20 AM EDT

PDB ID	:	3L01
Title	:	Crystal structure of monomeric glycogen synthase from Pyrococcus abyssi
Authors	:	Diaz, A.; Martinez-Pons, C.; Fita, I.; Ferrer, J.C.; Guinovart, J.J.
Deposited on	:	2009-12-09
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

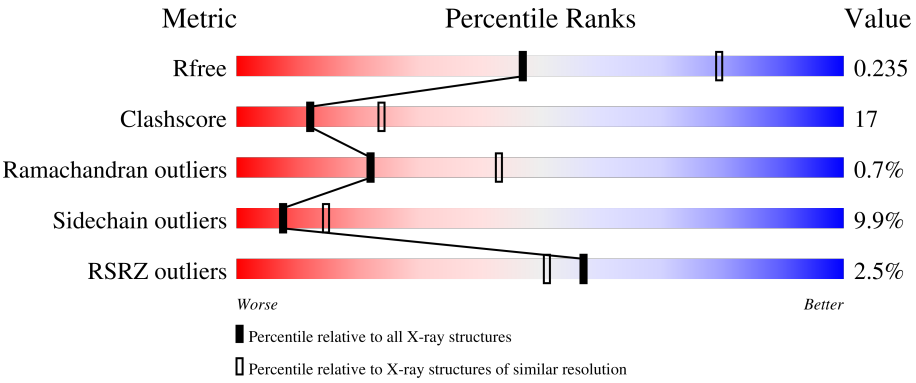
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 >=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 <=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	428	2% 71% 23% 5%
1	B	428	3% 75% 19% 7%
2	C	4	25% 75%
2	D	4	100%

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	GOL	A	6500	-	-	X	-
5	GOL	A	6502	-	-	X	-
5	GOL	B	6501	-	-	X	-
5	GOL	B	6503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7011 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	428	Total	C	N	O	S	0	0	0
			3394	2198	571	615	10			
1	B	428	Total	C	N	O	S	0	0	0
			3394	2198	571	615	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP Q9V2J8
A	0	HIS	-	expression tag	UNP Q9V2J8
A	426	ALA	THR	engineered mutation	UNP Q9V2J8
B	-1	ARG	-	expression tag	UNP Q9V2J8
B	0	HIS	-	expression tag	UNP Q9V2J8
B	426	ALA	THR	engineered mutation	UNP Q9V2J8

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	O		0	0	0
			45	24	21				
2	D	4	Total	C	O		0	0	0
			45	24	21				

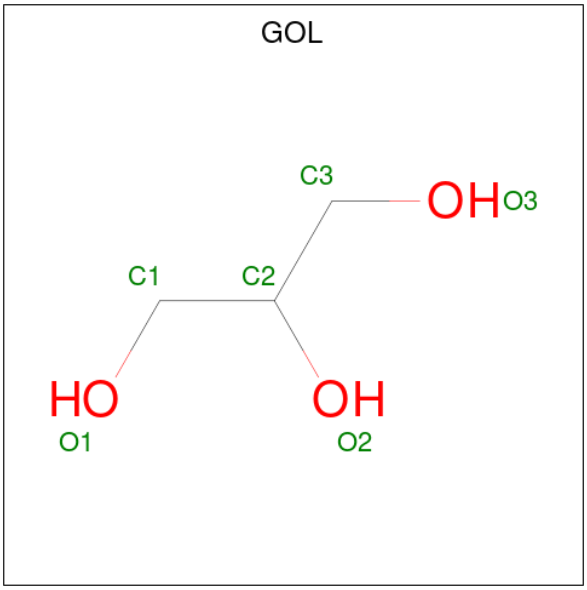
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total K 3 3	0	0
3	B	3	Total K 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	3	Total Cl 3 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

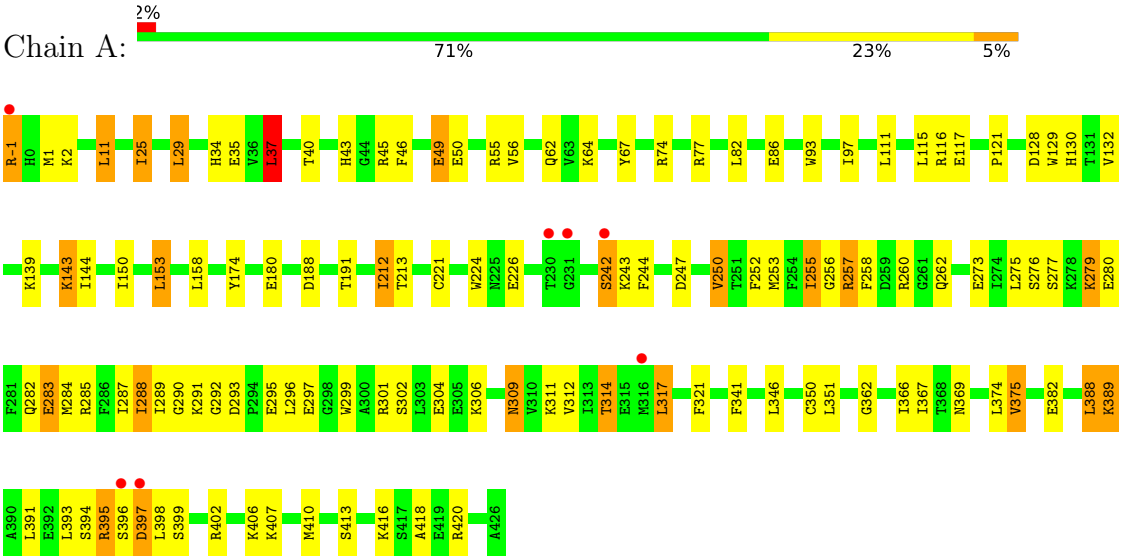
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	48	Total O 48 48	0	0
6	B	49	Total O 49 49	0	0

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 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.

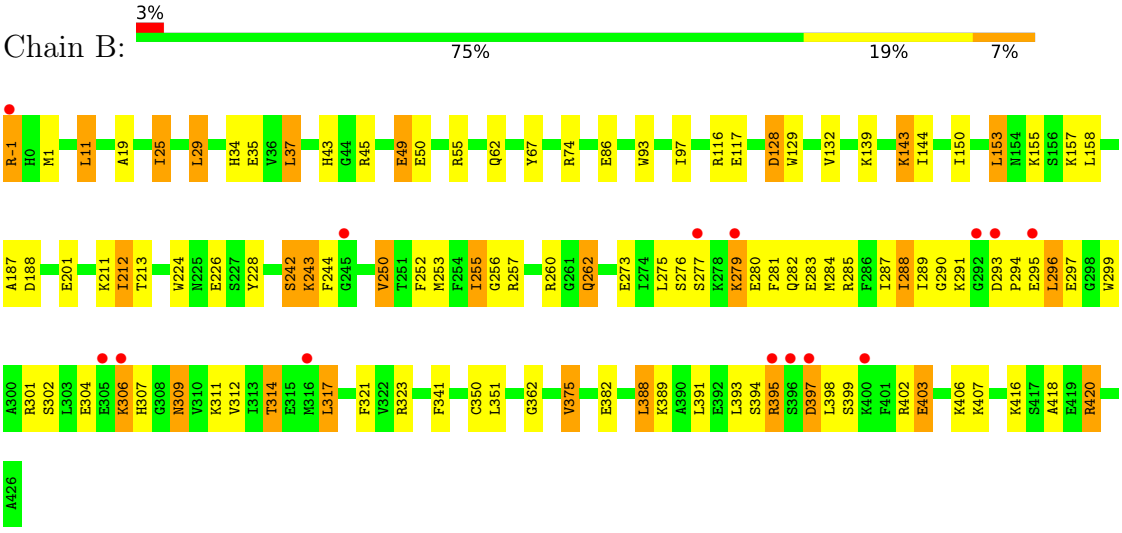
• Molecule 1: GlgA glycogen synthase

Chain A:



• Molecule 1: GlgA glycogen synthase

Chain B:

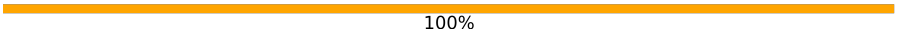


• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.60Å 119.02Å 141.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.60 24.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.7 (24.91-2.60) 82.5 (24.76-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.198 , 0.228 0.210 , 0.235	Depositor DCC
R_{free} test set	2023 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7011	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, CL, K

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	0.74	0/3473	0.74	1/4683 (0.0%)
1	B	0.72	0/3473	0.73	1/4683 (0.0%)
All	All	0.73	0/6946	0.73	2/9366 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	37	LEU	CA-CB-CG	5.11	127.06	115.30

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	3394	0	3405	111	0
1	B	3394	0	3403	109	0
2	C	45	0	39	4	0
2	D	45	0	39	5	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
5	A	12	0	16	8	0
5	B	12	0	16	6	0
6	A	48	0	0	1	0
6	B	49	0	0	2	0
All	All	7011	0	6918	235	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 17.

All (235) 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:279:LYS:HD3	1:B:279:LYS:H	1.08	1.18
1:A:279:LYS:H	1:A:279:LYS:HD3	1.13	1.13
5:A:6500:GOL:H11	5:A:6502:GOL:H31	1.24	1.10
1:B:395:ARG:NE	1:B:395:ARG:HA	1.71	1.04
5:A:6500:GOL:C1	5:A:6502:GOL:H31	1.86	1.04
1:B:279:LYS:HD3	1:B:279:LYS:N	1.78	0.96
1:A:279:LYS:HD3	1:A:279:LYS:N	1.83	0.94
1:A:130:HIS:CE1	5:A:6502:GOL:H32	2.03	0.93
1:A:291:LYS:HD3	1:A:314:THR:O	1.70	0.91
5:A:6500:GOL:H11	5:A:6502:GOL:C3	2.01	0.91
1:B:1:MET:H	1:B:34:HIS:HD2	1.10	0.89
1:A:1:MET:H	1:A:34:HIS:HD2	1.17	0.89
1:B:291:LYS:HD3	1:B:314:THR:O	1.73	0.89
1:A:279:LYS:H	1:A:279:LYS:CD	1.86	0.88
1:B:301:ARG:HH21	1:B:314:THR:CG2	1.91	0.84
1:A:395:ARG:HA	1:A:395:ARG:NE	1.92	0.83
1:B:279:LYS:H	1:B:279:LYS:CD	1.82	0.82
1:B:301:ARG:HH21	1:B:314:THR:HG23	1.46	0.81
1:B:1:MET:H	1:B:34:HIS:CD2	1.98	0.78
1:B:49:GLU:N	1:B:49:GLU:OE2	2.17	0.77
1:A:130:HIS:NE2	5:A:6502:GOL:H32	2.00	0.75
1:B:309:ASN:ND2	1:B:309:ASN:O	2.20	0.74
1:B:395:ARG:HH11	1:B:395:ARG:HG3	1.51	0.74
1:B:323:ARG:HD2	6:B:459:HOH:O	1.87	0.74
1:A:301:ARG:HH21	1:A:314:THR:HG23	1.52	0.74
1:A:301:ARG:HH21	1:A:314:THR:CG2	2.01	0.73
1:B:284:MET:O	1:B:309:ASN:ND2	2.21	0.73
1:B:301:ARG:NH2	1:B:314:THR:HG23	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:MET:O	1:A:309:ASN:ND2	2.25	0.69
1:B:226:GLU:OE1	1:B:406:LYS:NZ	2.26	0.67
2:D:1:GLC:H5	2:D:2:GLC:O5	1.95	0.67
1:A:301:ARG:NH2	1:A:314:THR:HG23	2.10	0.66
1:A:284:MET:HG3	1:A:391:LEU:HD12	1.77	0.66
1:B:139:LYS:NZ	1:B:188:ASP:OD2	2.28	0.66
1:A:221:CYS:SG	1:A:410:MET:HG2	2.36	0.65
2:D:3:GLC:HO6	2:D:4:GLC:C1	2.10	0.65
1:B:393:LEU:O	1:B:395:ARG:N	2.29	0.65
1:B:157:LYS:HE2	2:D:3:GLC:O2	1.97	0.65
1:A:-1:ARG:HG2	1:A:-1:ARG:HH11	1.62	0.64
1:A:280:GLU:HG3	1:A:388:LEU:HD11	1.78	0.64
1:B:243:LYS:CG	1:B:243:LYS:O	2.45	0.64
1:A:317:LEU:HG	1:A:321:PHE:HD2	1.63	0.64
1:B:243:LYS:O	1:B:243:LYS:HG3	1.98	0.63
1:A:395:ARG:O	1:A:397:ASP:N	2.32	0.63
1:A:288:ILE:N	1:A:288:ILE:CD1	2.63	0.61
1:A:1:MET:H	1:A:34:HIS:CD2	2.07	0.61
2:C:3:GLC:HO6	2:C:4:GLC:C1	2.14	0.61
1:B:288:ILE:N	1:B:288:ILE:CD1	2.62	0.61
1:B:301:ARG:NH2	1:B:314:THR:CG2	2.62	0.61
1:A:395:ARG:C	1:A:397:ASP:H	2.03	0.60
1:B:280:GLU:HG3	1:B:388:LEU:HD11	1.83	0.60
1:B:150:ILE:HG21	1:B:153:LEU:HD13	1.83	0.60
1:A:309:ASN:ND2	1:A:309:ASN:O	2.30	0.60
1:B:49:GLU:OE2	1:B:49:GLU:CA	2.50	0.60
1:A:284:MET:CG	1:A:391:LEU:HD12	2.32	0.59
1:A:285:ARG:HA	1:A:309:ASN:ND2	2.17	0.59
1:B:306:LYS:O	1:B:307:HIS:HD2	1.84	0.59
1:B:287:ILE:C	1:B:288:ILE:HD12	2.22	0.59
1:B:306:LYS:C	1:B:307:HIS:CD2	2.76	0.59
1:B:306:LYS:HB3	1:B:307:HIS:CD2	2.39	0.58
1:B:43:HIS:O	1:B:45:ARG:NH1	2.33	0.57
5:B:6501:GOL:H11	5:B:6503:GOL:C3	2.34	0.57
5:A:6500:GOL:O1	5:A:6502:GOL:H31	2.04	0.57
1:A:49:GLU:OE2	1:A:49:GLU:N	2.37	0.57
1:A:293:ASP:HB3	1:A:296:LEU:HD12	1.87	0.57
1:A:391:LEU:C	1:A:391:LEU:HD23	2.25	0.57
1:B:280:GLU:C	1:B:282:GLN:H	2.08	0.56
1:A:287:ILE:C	1:A:288:ILE:HD12	2.26	0.56
1:A:150:ILE:HG21	1:A:153:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:N	1:B:34:HIS:HD2	1.93	0.56
1:B:285:ARG:HA	1:B:309:ASN:ND2	2.20	0.56
1:B:128:ASP:OD2	5:B:6501:GOL:O2	2.23	0.55
1:A:393:LEU:O	1:A:395:ARG:N	2.40	0.55
1:A:-1:ARG:HG2	1:A:-1:ARG:NH1	2.20	0.55
1:B:255:ILE:HG23	1:B:255:ILE:O	2.07	0.55
1:B:97:ILE:HD13	1:B:158:LEU:HD22	1.88	0.54
1:B:341:PHE:O	1:B:362:GLY:HA3	2.07	0.54
1:B:288:ILE:N	1:B:288:ILE:HD12	2.22	0.54
1:A:243:LYS:O	1:A:243:LYS:HG3	2.07	0.54
2:C:3:GLC:O6	2:C:4:GLC:C1	2.56	0.54
1:A:97:ILE:HD13	1:A:158:LEU:HD22	1.89	0.54
1:B:35:GLU:OE2	1:B:74:ARG:NH1	2.40	0.54
1:A:256:GLY:O	1:A:290:GLY:HA3	2.08	0.53
1:B:45:ARG:NH1	1:B:86:GLU:HG2	2.24	0.53
1:B:129:TRP:N	6:B:466:HOH:O	2.39	0.53
1:B:155:LYS:NZ	1:B:201:GLU:OE1	2.41	0.53
1:B:253:MET:HE2	1:B:289:ILE:HD12	1.91	0.53
1:A:116:ARG:C	1:A:117:GLU:HG2	2.29	0.53
1:B:67:TYR:OH	1:B:74:ARG:HG2	2.08	0.53
1:A:174:TYR:CD2	2:C:1:GLC:H5	2.43	0.53
1:A:255:ILE:HG23	1:A:255:ILE:O	2.08	0.53
1:A:413:SER:OG	1:A:416:LYS:HG3	2.09	0.53
1:A:35:GLU:OE2	1:A:74:ARG:NH1	2.43	0.52
1:A:288:ILE:N	1:A:288:ILE:HD12	2.25	0.52
1:B:253:MET:CE	1:B:289:ILE:HD12	2.39	0.52
1:A:191:THR:HA	1:A:213:THR:O	2.09	0.52
1:A:250:VAL:HG13	1:A:283:GLU:O	2.10	0.52
1:A:50:GLU:HB3	1:A:62:GLN:HE21	1.74	0.52
1:B:-1:ARG:HH11	1:B:-1:ARG:HG2	1.75	0.52
1:B:317:LEU:HG	1:B:321:PHE:HD2	1.75	0.52
1:A:243:LYS:O	1:A:243:LYS:CG	2.58	0.52
1:B:29:LEU:HD13	1:B:418:ALA:HB1	1.91	0.52
1:A:391:LEU:HD23	1:A:391:LEU:O	2.10	0.52
1:B:294:PRO:HA	1:B:297:GLU:HG3	1.92	0.52
1:A:284:MET:SD	1:A:391:LEU:HD12	2.50	0.51
1:A:45:ARG:NH1	1:A:86:GLU:HG2	2.25	0.51
1:B:395:ARG:HG3	1:B:395:ARG:NH1	2.21	0.51
1:A:285:ARG:HA	1:A:309:ASN:HD21	1.74	0.51
1:B:116:ARG:C	1:B:117:GLU:HG2	2.30	0.51
1:A:341:PHE:O	1:A:362:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:HIS:O	1:A:45:ARG:NH1	2.43	0.50
1:B:398:LEU:O	1:B:402:ARG:HG3	2.11	0.50
1:B:187:ALA:O	1:B:211:LYS:NZ	2.38	0.50
1:B:293:ASP:HB3	1:B:296:LEU:HB2	1.93	0.50
5:B:6501:GOL:H11	5:B:6503:GOL:H31	1.93	0.50
1:A:280:GLU:C	1:A:282:GLN:H	2.15	0.50
1:A:67:TYR:OH	1:A:74:ARG:HG2	2.12	0.49
1:A:29:LEU:HD13	1:A:418:ALA:HB1	1.94	0.49
1:B:43:HIS:O	1:B:86:GLU:HA	2.12	0.49
1:B:284:MET:CE	1:B:391:LEU:CD1	2.90	0.49
1:B:285:ARG:HA	1:B:309:ASN:HD21	1.77	0.49
1:B:391:LEU:C	1:B:391:LEU:HD23	2.33	0.49
1:A:374:LEU:HD12	6:A:462:HOH:O	2.12	0.49
1:B:397:ASP:N	1:B:397:ASP:OD1	2.46	0.49
1:A:224:TRP:O	1:A:350:CYS:HB3	2.12	0.48
1:B:50:GLU:HB3	1:B:62:GLN:HE21	1.79	0.48
1:B:281:PHE:CG	1:B:281:PHE:O	2.65	0.48
1:B:242:SER:C	1:B:244:PHE:H	2.17	0.48
1:B:273:GLU:OE2	1:B:299:TRP:NE1	2.42	0.48
1:B:403:GLU:OE1	1:B:403:GLU:HA	2.13	0.48
1:B:306:LYS:O	1:B:307:HIS:CD2	2.67	0.48
1:A:253:MET:CE	1:A:289:ILE:HD12	2.44	0.48
1:A:293:ASP:OD1	1:A:295:GLU:HB3	2.14	0.48
1:A:301:ARG:NH2	1:A:314:THR:CG2	2.70	0.48
1:A:82:LEU:HD23	1:B:228:TYR:OH	2.14	0.47
1:B:25:ILE:HA	1:B:25:ILE:HD13	1.61	0.47
1:B:293:ASP:OD1	1:B:293:ASP:C	2.53	0.47
1:A:130:HIS:HE1	5:A:6502:GOL:H32	1.73	0.47
1:A:389:LYS:HZ2	1:A:389:LYS:HB3	1.79	0.47
1:B:283:GLU:HG2	1:B:283:GLU:O	2.15	0.47
1:B:50:GLU:HB3	1:B:62:GLN:NE2	2.29	0.47
1:A:397:ASP:N	1:A:397:ASP:OD1	2.47	0.46
1:B:293:ASP:OD1	1:B:295:GLU:N	2.48	0.46
1:A:128:ASP:OD2	5:A:6500:GOL:O2	2.29	0.46
1:B:93:TRP:CE2	1:B:97:ILE:HD11	2.51	0.46
2:D:3:GLC:O6	2:D:4:GLC:O5	2.33	0.46
1:A:398:LEU:O	1:A:402:ARG:HG3	2.15	0.46
1:A:395:ARG:C	1:A:397:ASP:N	2.66	0.46
5:B:6501:GOL:C1	5:B:6503:GOL:H31	2.46	0.46
1:A:111:LEU:O	1:A:115:LEU:HG	2.15	0.45
1:A:49:GLU:OE2	1:A:49:GLU:CA	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:OD1	1:A:295:GLU:N	2.49	0.45
1:B:275:LEU:C	1:B:277:SER:H	2.20	0.45
2:D:3:GLC:O6	2:D:4:GLC:C1	2.65	0.45
1:B:-1:ARG:HG2	1:B:-1:ARG:NH1	2.32	0.45
1:B:25:ILE:HD12	1:B:25:ILE:HG23	1.74	0.45
1:B:250:VAL:HG13	1:B:283:GLU:O	2.15	0.45
1:B:280:GLU:C	1:B:282:GLN:N	2.69	0.45
1:B:284:MET:HE3	1:B:391:LEU:CD1	2.47	0.45
1:A:129:TRP:HB3	1:A:180:GLU:HG3	1.98	0.45
1:B:212:ILE:HG13	1:B:213:THR:N	2.32	0.45
1:A:242:SER:C	1:A:244:PHE:H	2.20	0.45
1:A:139:LYS:NZ	1:A:188:ASP:OD2	2.50	0.45
1:A:301:ARG:NH1	1:A:304:GLU:OE1	2.44	0.45
1:A:46:PHE:CD1	1:A:77:ARG:HD3	2.52	0.45
1:A:226:GLU:OE1	1:A:406:LYS:NZ	2.45	0.45
1:A:280:GLU:C	1:A:282:GLN:N	2.70	0.44
2:C:3:GLC:O6	2:C:4:GLC:O5	2.35	0.44
1:A:2:LYS:HG2	1:A:121:PRO:HA	1.99	0.44
1:A:253:MET:HE2	1:A:289:ILE:HD12	1.99	0.44
1:A:301:ARG:HA	1:A:301:ARG:HD3	1.80	0.44
1:B:143:LYS:HA	1:B:143:LYS:HD2	1.41	0.44
1:A:116:ARG:O	1:A:117:GLU:HG2	2.18	0.44
1:B:45:ARG:HH12	1:B:86:GLU:HA	1.82	0.44
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.77	0.44
1:A:49:GLU:O	1:A:64:LYS:HA	2.17	0.44
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.69	0.44
1:B:116:ARG:O	1:B:117:GLU:HG2	2.17	0.44
1:A:293:ASP:O	1:A:297:GLU:HG3	2.18	0.44
1:B:129:TRP:HA	1:B:132:VAL:HG23	2.00	0.44
1:B:290:GLY:O	1:B:314:THR:HA	2.18	0.44
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.75	0.43
1:A:290:GLY:O	1:A:314:THR:HA	2.18	0.43
1:B:-1:ARG:HD2	1:B:-1:ARG:HA	1.81	0.43
1:A:143:LYS:HD2	1:A:143:LYS:HA	1.50	0.43
1:B:224:TRP:O	1:B:350:CYS:HB3	2.18	0.43
1:A:284:MET:HB2	1:A:284:MET:HE2	1.92	0.43
1:A:311:LYS:HG3	1:A:312:VAL:N	2.33	0.43
1:B:293:ASP:OD1	1:B:295:GLU:CB	2.67	0.43
1:A:375:VAL:HG22	1:A:382:GLU:HB3	2.01	0.43
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.84	0.43
1:B:375:VAL:HG22	1:B:382:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:HA	1:A:25:ILE:HD13	1.65	0.42
1:A:46:PHE:CE1	1:A:77:ARG:HD3	2.54	0.42
1:B:311:LYS:HG3	1:B:312:VAL:N	2.34	0.42
1:A:273:GLU:OE2	1:A:299:TRP:NE1	2.46	0.42
1:B:37:LEU:HD23	1:B:37:LEU:N	2.34	0.42
1:B:284:MET:CE	1:B:391:LEU:HD13	2.49	0.42
1:B:284:MET:HE2	1:B:391:LEU:CD1	2.49	0.42
1:A:212:ILE:HG13	1:A:213:THR:N	2.33	0.42
1:B:262:GLN:HE21	1:B:262:GLN:HB2	1.67	0.42
1:B:284:MET:HG3	1:B:391:LEU:HD12	2.01	0.42
5:B:6501:GOL:H11	5:B:6503:GOL:H32	2.01	0.42
1:B:403:GLU:OE1	1:B:403:GLU:O	2.38	0.42
1:A:50:GLU:HB3	1:A:62:GLN:NE2	2.34	0.42
1:A:367:ILE:HG22	1:A:367:ILE:O	2.19	0.42
1:B:301:ARG:NH1	1:B:304:GLU:OE1	2.48	0.42
1:B:256:GLY:O	1:B:290:GLY:HA3	2.20	0.41
1:B:301:ARG:HH21	1:B:314:THR:HG21	1.80	0.41
1:A:1:MET:N	1:A:34:HIS:HD2	1.99	0.41
1:A:40:THR:O	1:A:77:ARG:HA	2.21	0.41
1:A:43:HIS:O	1:A:86:GLU:HA	2.21	0.41
1:A:247:ASP:C	1:A:247:ASP:OD1	2.58	0.41
1:A:275:LEU:C	1:A:277:SER:H	2.23	0.41
1:B:45:ARG:NH1	1:B:86:GLU:HA	2.35	0.41
1:B:242:SER:C	1:B:244:PHE:N	2.74	0.41
1:B:11:LEU:HD13	1:B:19:ALA:HB1	2.01	0.41
1:B:284:MET:HE2	1:B:391:LEU:HD12	2.03	0.41
1:B:403:GLU:OE1	1:B:403:GLU:CA	2.68	0.41
1:A:-1:ARG:HD2	1:A:-1:ARG:HA	1.77	0.41
1:A:37:LEU:N	1:A:37:LEU:HD23	2.36	0.41
1:A:257:ARG:NH2	1:A:292:GLY:HA2	2.35	0.41
1:B:250:VAL:HG22	1:B:252:PHE:CE1	2.56	0.41
1:A:257:ARG:HG3	1:A:258:PHE:N	2.36	0.41
1:B:293:ASP:HA	1:B:294:PRO:HD3	1.90	0.41
1:A:129:TRP:HA	1:A:132:VAL:HG23	2.03	0.40
1:A:346:LEU:HG	1:A:366:ILE:HD13	2.02	0.40
1:A:242:SER:C	1:A:244:PHE:N	2.74	0.40
1:A:250:VAL:HG22	1:A:252:PHE:CE1	2.57	0.40
1:A:293:ASP:OD1	1:A:295:GLU:CB	2.69	0.40
1:B:275:LEU:O	1:B:277:SER:N	2.54	0.40
1:A:93:TRP:CE2	1:A:97:ILE:HD11	2.56	0.40
1:B:416:LYS:O	1:B:420:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HG	1:A:321:PHE:CD2	2.50	0.40
5:B:6501:GOL:C1	5:B:6503:GOL:C3	2.98	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	426/428 (100%)	403 (95%)	20 (5%)	3 (1%)	22	43
1	B	426/428 (100%)	404 (95%)	19 (4%)	3 (1%)	22	43
All	All	852/856 (100%)	807 (95%)	39 (5%)	6 (1%)	22	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	SER
1	B	394	SER
1	A	396	SER
1	A	276	SER
1	B	276	SER
1	B	243	LYS

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	357/357 (100%)	321 (90%)	36 (10%)	7 14
1	B	357/357 (100%)	322 (90%)	35 (10%)	8 15
All	All	714/714 (100%)	643 (90%)	71 (10%)	8 15

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	11	LEU
1	A	25	ILE
1	A	29	LEU
1	A	37	LEU
1	A	49	GLU
1	A	55	ARG
1	A	56	VAL
1	A	143	LYS
1	A	144	ILE
1	A	153	LEU
1	A	212	ILE
1	A	242	SER
1	A	250	VAL
1	A	255	ILE
1	A	257	ARG
1	A	260	ARG
1	A	262	GLN
1	A	279	LYS
1	A	283	GLU
1	A	288	ILE
1	A	302	SER
1	A	306	LYS
1	A	309	ASN
1	A	314	THR
1	A	317	LEU
1	A	351	LEU
1	A	369	ASN
1	A	375	VAL
1	A	388	LEU
1	A	389	LYS
1	A	395	ARG
1	A	397	ASP
1	A	399	SER
1	A	407	LYS

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Mol	Chain	Res	Type
1	A	420	ARG
1	B	-1	ARG
1	B	11	LEU
1	B	25	ILE
1	B	29	LEU
1	B	37	LEU
1	B	49	GLU
1	B	55	ARG
1	B	143	LYS
1	B	144	ILE
1	B	153	LEU
1	B	212	ILE
1	B	242	SER
1	B	250	VAL
1	B	255	ILE
1	B	257	ARG
1	B	260	ARG
1	B	262	GLN
1	B	279	LYS
1	B	288	ILE
1	B	296	LEU
1	B	302	SER
1	B	306	LYS
1	B	309	ASN
1	B	314	THR
1	B	317	LEU
1	B	351	LEU
1	B	375	VAL
1	B	388	LEU
1	B	389	LYS
1	B	395	ARG
1	B	397	ASP
1	B	399	SER
1	B	403	GLU
1	B	407	LYS
1	B	420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	217	ASN

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Mol	Chain	Res	Type
1	A	262	GLN
1	A	307	HIS
1	B	34	HIS
1	B	62	GLN
1	B	207	ASN
1	B	217	ASN
1	B	262	GLN
1	B	307	HIS
1	B	309	ASN
1	B	404	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)

8 monosaccharides 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	GLC	C	1	2	12,12,12	0.77	0	17,17,17	1.51	5 (29%)
2	GLC	C	2	2	11,11,12	0.82	0	15,15,17	2.11	5 (33%)
2	GLC	C	3	2	11,11,12	0.53	0	15,15,17	1.13	2 (13%)
2	GLC	C	4	2	11,11,12	0.49	0	15,15,17	1.46	3 (20%)
2	GLC	D	1	2	12,12,12	0.77	0	17,17,17	1.45	4 (23%)
2	GLC	D	2	2	11,11,12	0.57	0	15,15,17	2.57	8 (53%)
2	GLC	D	3	2	11,11,12	0.30	0	15,15,17	1.63	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	D	4	2	11,11,12	0.53	0	15,15,17	1.25	2 (13%)

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	GLC	C	1	2	-	2/2/22/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	1/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	1/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	GLC	C1-C2-C3	4.43	115.11	109.67
2	D	2	GLC	O5-C5-C6	4.16	113.73	107.20
2	C	2	GLC	C1-C2-C3	4.08	114.69	109.67
2	D	3	GLC	C1-O5-C5	3.94	117.53	112.19
2	D	2	GLC	C1-O5-C5	3.68	117.17	112.19
2	D	2	GLC	O5-C1-C2	-3.36	105.58	110.77
2	C	2	GLC	O5-C1-C2	-3.35	105.60	110.77
2	C	2	GLC	C1-O5-C5	-3.29	107.74	112.19
2	D	2	GLC	C6-C5-C4	-3.25	105.39	113.00
2	C	4	GLC	C1-C2-C3	3.20	113.59	109.67
2	C	1	GLC	C3-C4-C5	-3.13	104.66	110.24
2	D	3	GLC	C1-C2-C3	-3.08	105.88	109.67
2	C	4	GLC	O5-C5-C6	2.95	111.83	107.20
2	D	1	GLC	O3-C3-C2	-2.90	103.64	110.35
2	C	1	GLC	C1-C2-C3	2.82	116.16	110.31
2	D	2	GLC	O6-C6-C5	-2.68	102.11	111.29
2	D	2	GLC	O2-C2-C3	-2.59	104.95	110.14
2	D	3	GLC	O5-C1-C2	-2.59	106.78	110.77
2	C	3	GLC	O5-C1-C2	-2.44	107.00	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GLC	C1-O5-C5	2.40	118.19	113.66
2	D	1	GLC	C4-C3-C2	2.36	114.94	110.82
2	D	1	GLC	C1-O5-C5	-2.31	109.30	113.66
2	C	2	GLC	O5-C5-C6	2.30	110.81	107.20
2	D	4	GLC	O2-C2-C3	-2.26	105.60	110.14
2	D	2	GLC	O3-C3-C4	-2.22	105.22	110.35
2	D	4	GLC	C6-C5-C4	-2.20	107.85	113.00
2	C	1	GLC	C4-C3-C2	2.18	114.62	110.82
2	D	1	GLC	O4-C4-C5	2.16	114.66	109.30
2	D	3	GLC	C2-C3-C4	-2.09	107.28	110.89
2	C	4	GLC	C2-C3-C4	-2.08	107.30	110.89
2	C	3	GLC	C1-O5-C5	2.06	114.98	112.19
2	C	2	GLC	O4-C4-C5	2.05	114.39	109.30
2	C	1	GLC	O1-C1-C2	2.05	114.79	109.03

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	GLC	C4-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
2	C	2	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	1	0
2	C	3	GLC	3	0
2	C	1	GLC	1	0
2	D	1	GLC	1	0
2	D	4	GLC	3	0

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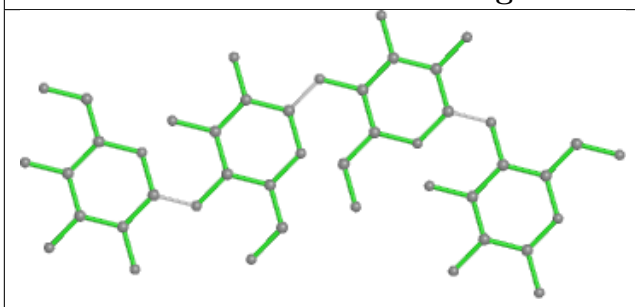
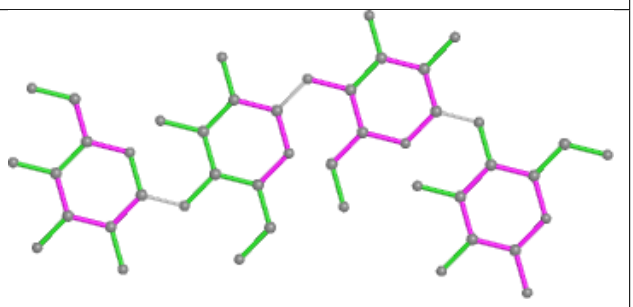
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	GLC	3	0
2	D	3	GLC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

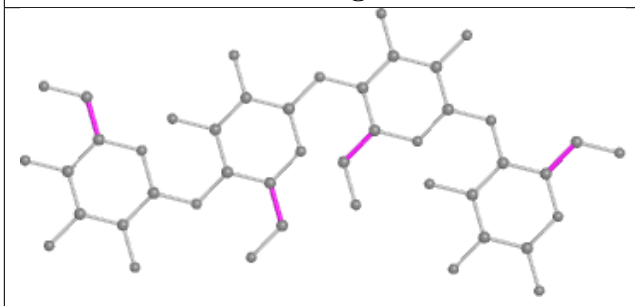
Oligosaccharide Chain C



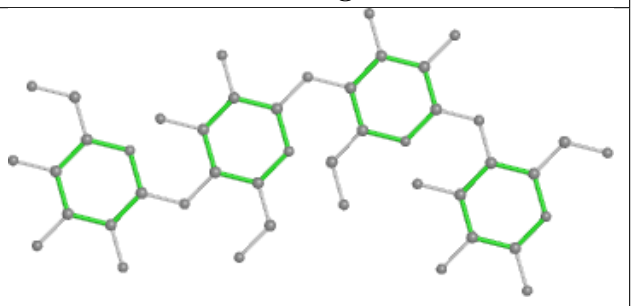
Bond lengths



Bond angles

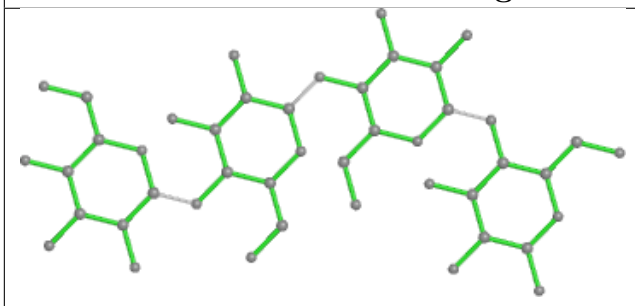


Torsions

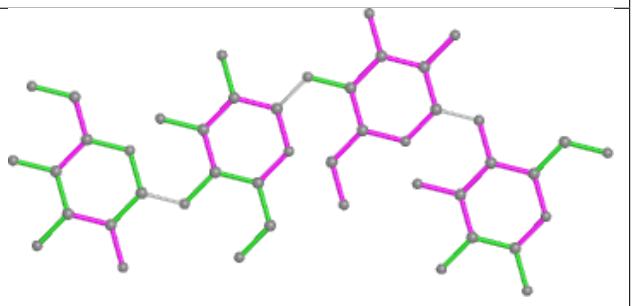


Rings

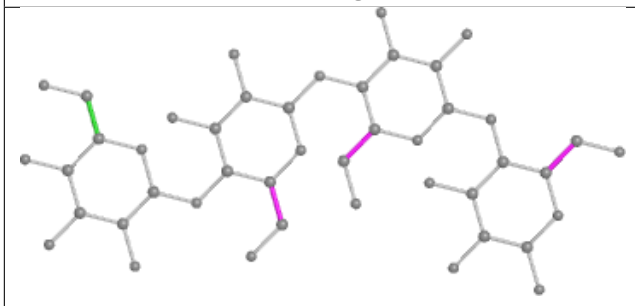
Oligosaccharide Chain D



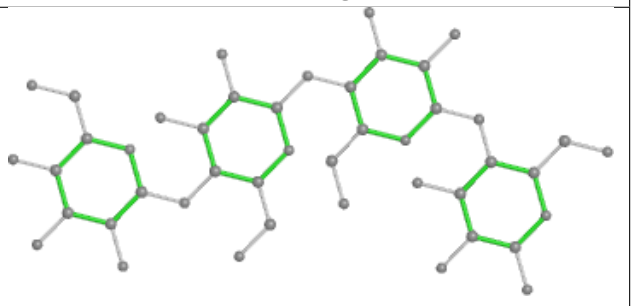
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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	GOL	B	6501	-	5,5,5	0.26	0	5,5,5	0.52	0
5	GOL	B	6503	-	5,5,5	0.49	0	5,5,5	0.50	0
5	GOL	A	6500	-	5,5,5	0.42	0	5,5,5	0.55	0
5	GOL	A	6502	-	5,5,5	0.57	0	5,5,5	0.53	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	GOL	B	6501	-	-	4/4/4/4	-
5	GOL	B	6503	-	-	2/4/4/4	-
5	GOL	A	6500	-	-	4/4/4/4	-
5	GOL	A	6502	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	6500	GOL	C1-C2-C3-O3
5	B	6501	GOL	O1-C1-C2-O2
5	B	6501	GOL	O1-C1-C2-C3
5	B	6501	GOL	C1-C2-C3-O3
5	A	6500	GOL	O1-C1-C2-O2
5	A	6500	GOL	O1-C1-C2-C3
5	B	6503	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	6500	GOL	O2-C2-C3-O3
5	B	6501	GOL	O2-C2-C3-O3
5	B	6503	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	6501	GOL	6	0
5	B	6503	GOL	5	0
5	A	6500	GOL	5	0
5	A	6502	GOL	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	428/428 (100%)	-0.20	7 (1%) 72 68	20, 32, 67, 80	0
1	B	428/428 (100%)	-0.14	14 (3%) 46 39	21, 33, 74, 90	0
All	All	856/856 (100%)	-0.17	21 (2%) 57 51	20, 32, 70, 90	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	ARG	3.6
1	B	316	MET	3.4
1	B	-1	ARG	3.4
1	B	397	ASP	3.1
1	A	316	MET	2.9
1	B	395	ARG	2.8
1	B	396	SER	2.7
1	B	293	ASP	2.6
1	A	396	SER	2.5
1	A	397	ASP	2.4
1	B	279	LYS	2.4
1	A	230	THR	2.3
1	B	306	LYS	2.3
1	A	231	GLY	2.2
1	B	400	LYS	2.2
1	B	245	GLY	2.1
1	B	292	GLY	2.1
1	B	305	GLU	2.0
1	A	242	SER	2.0
1	B	277	SER	2.0
1	B	295	GLU	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)

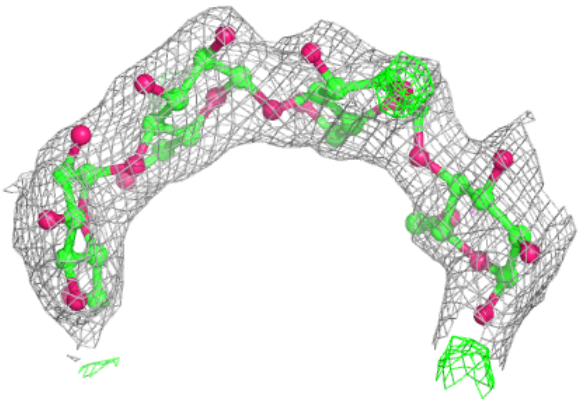
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

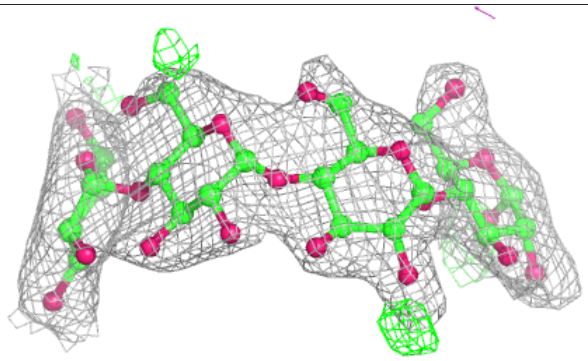
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	12/12	0.87	0.32	44,57,84,122	0
2	GLC	C	1	12/12	0.89	0.30	42,55,93,120	0
2	GLC	C	2	11/12	0.94	0.21	31,45,54,54	0
2	GLC	D	2	11/12	0.95	0.20	33,42,55,55	0
2	GLC	C	4	11/12	0.96	0.12	15,28,53,60	0
2	GLC	D	3	11/12	0.97	0.20	25,37,45,46	0
2	GLC	D	4	11/12	0.97	0.13	18,29,40,55	0
2	GLC	C	3	11/12	0.98	0.16	15,24,38,48	0

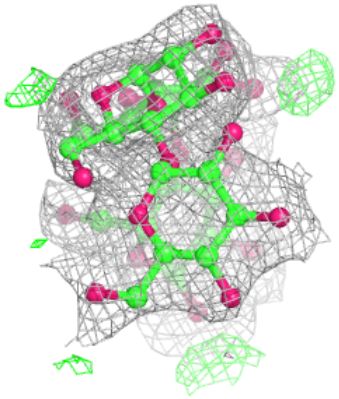
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

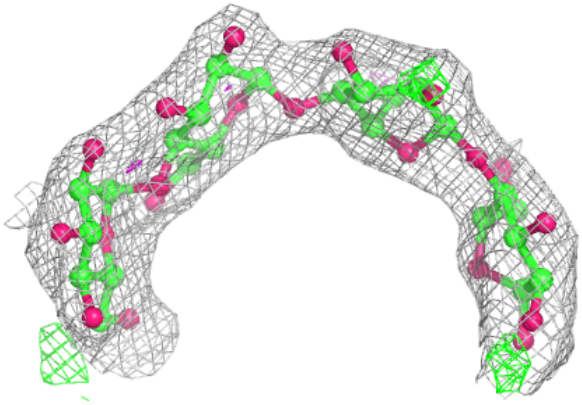


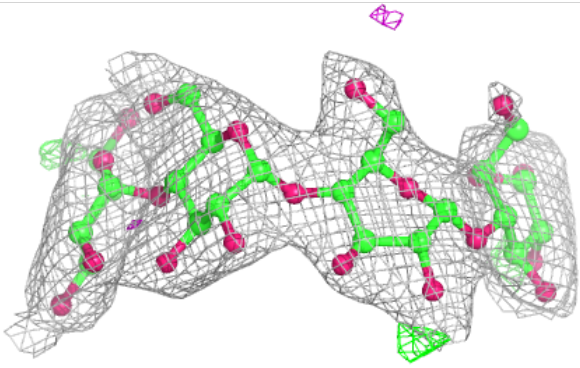


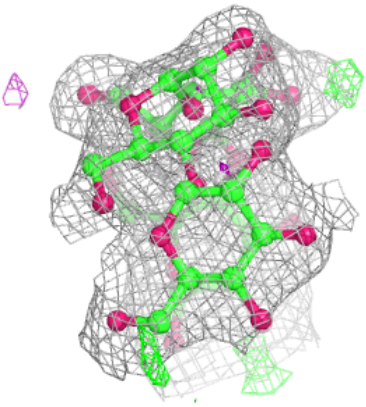


Electron density around Chain D:

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







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^{th} 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(Å^2)	Q<0.9
3	K	B	5606	1/1	0.94	0.09	58,58,58,58	0
5	GOL	A	6502	6/6	0.94	0.25	33,38,48,50	0
5	GOL	A	6500	6/6	0.95	0.14	27,39,41,44	0
4	CL	A	5700	1/1	0.95	0.20	31,31,31,31	0
5	GOL	B	6501	6/6	0.95	0.14	32,37,57,59	0
4	CL	B	5705	1/1	0.96	0.15	32,32,32,32	0
4	CL	B	5701	1/1	0.96	0.15	36,36,36,36	0
3	K	B	5605	1/1	0.97	0.06	46,46,46,46	0
4	CL	A	5703	1/1	0.97	0.13	45,45,45,45	0
3	K	A	5607	1/1	0.97	0.09	63,63,63,63	0
4	CL	B	5702	1/1	0.97	0.16	54,54,54,54	0
5	GOL	B	6503	6/6	0.97	0.20	17,35,53,56	0
3	K	B	5601	1/1	0.98	0.23	38,38,38,38	0
4	CL	A	5704	1/1	0.98	0.24	25,25,25,25	0
3	K	A	5602	1/1	0.98	0.06	24,24,24,24	0
3	K	A	5600	1/1	0.99	0.25	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.