Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 08:42 PM EDT

PDB ID	:	5TQZ
Title	:	Frutapin complexed with alpha-D-glucose
Authors	:	Sousa, F.D.; Guo, J.; Coker, A.R.; Monteiro-Moreira, A.C.O.; Moreira, R.A.
Deposited on	:	2016-10-25
Resolution	:	1.60 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 (i)) were used in the production of this report:

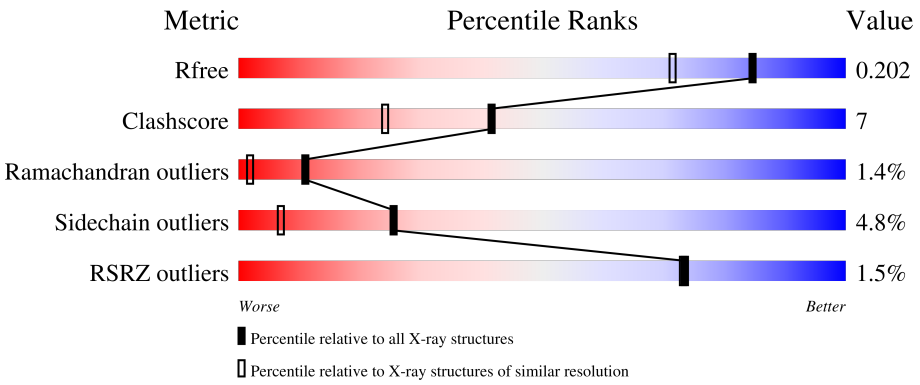
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	150	% 72% 20% 7% •
1	B	150	% 73% 24% • •
1	C	150	3% 75% 19% 5% •
1	D	150	% 71% 24% • •

2 Entry composition (i)

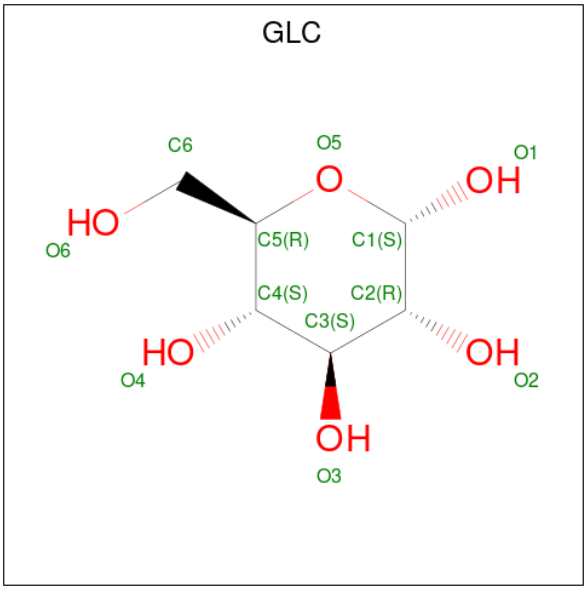
There are 3 unique types of molecules in this entry. The entry contains 5248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Frutapin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1210	781	193	233	3	0	9	0
1	B	150	1170	753	188	227	2	0	4	0
1	C	150	1213	776	197	238	2	0	8	0
1	D	150	1190	763	194	230	3	0	6	0

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0
2	B	1	12	6	6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	C	1	12	6	6	0	0
			Total	C	O		
2	D	1	12	6	6	0	0

- Molecule 3 is water.

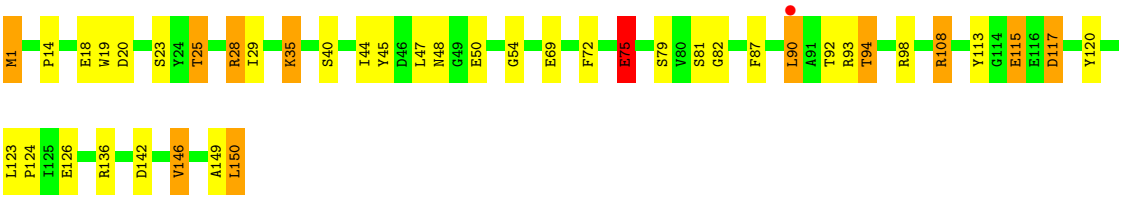
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	113	113	113	0	0
			Total	O		
3	B	109	109	109	0	0
			Total	O		
3	C	98	98	98	0	0
			Total	O		
3	D	97	97	97	0	0

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.

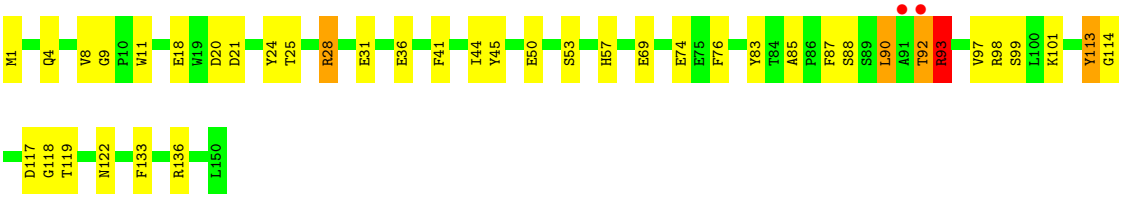
- Molecule 1: Frutapin

Chain A:



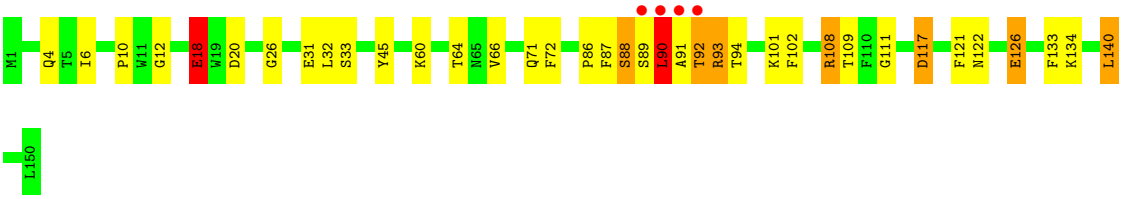
- Molecule 1: Frutapin

Chain B:



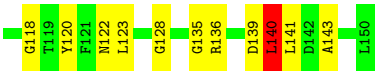
- Molecule 1: Frutapin

Chain C:



- Molecule 1: Frutapin

Chain D:


G118
T119
Y120
F121
N122
L123
G128
G135
R136
D139
L140
L141
D142
A143
L150

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	74.02Å 74.02Å 185.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.11 – 1.60 64.11 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.11-1.60) 99.8 (64.11-1.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.149 , 0.192 0.159 , 0.202	Depositor DCC
R_{free} test set	3914 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.23% 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 (i)

5.1 Standard geometry (i)

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

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	1.76	19/1252 (1.5%)	1.54	18/1697 (1.1%)
1	B	1.77	13/1209 (1.1%)	1.62	20/1640 (1.2%)
1	C	1.60	10/1243 (0.8%)	1.49	13/1683 (0.8%)
1	D	1.72	17/1226 (1.4%)	1.46	7/1660 (0.4%)
All	All	1.71	59/4930 (1.2%)	1.53	58/6680 (0.9%)

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	3
1	B	0	1
1	C	0	2
All	All	0	6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	31	GLU	CD-OE1	9.40	1.35	1.25
1	C	126	GLU	CD-OE2	9.22	1.35	1.25
1	C	18	GLU	CG-CD	8.40	1.64	1.51
1	C	108	ARG	CZ-NH2	7.83	1.43	1.33
1	D	19	TRP	CG-CD1	6.95	1.46	1.36
1	D	40	SER	CA-CB	6.84	1.63	1.52
1	D	18	GLU	CD-OE1	6.69	1.33	1.25
1	A	120	TYR	CG-CD2	6.68	1.47	1.39
1	B	74	GLU	CD-OE1	-6.63	1.18	1.25
1	B	9	GLY	N-CA	-6.61	1.36	1.46
1	A	81	SER	CB-OG	6.59	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	TRP	CD1-NE1	6.57	1.49	1.38
1	A	45	TYR	CD1-CE1	-6.48	1.29	1.39
1	D	19	TRP	CE3-CZ3	-6.21	1.27	1.38
1	D	18	GLU	CG-CD	6.14	1.61	1.51
1	A	23	SER	CB-OG	6.08	1.50	1.42
1	C	121	PHE	CE2-CZ	-6.07	1.25	1.37
1	A	120	TYR	CE2-CZ	-6.03	1.30	1.38
1	A	120	TYR	CD2-CE2	-6.02	1.30	1.39
1	B	24	TYR	CE2-CZ	6.01	1.46	1.38
1	B	45	TYR	CE1-CZ	-6.01	1.30	1.38
1	D	11	TRP	CZ3-CH2	-6.00	1.30	1.40
1	A	93	ARG	CZ-NH2	-5.99	1.25	1.33
1	C	12	GLY	N-CA	5.90	1.54	1.46
1	B	122	ASN	C-O	5.88	1.34	1.23
1	B	98	ARG	CZ-NH1	5.87	1.40	1.33
1	A	19	TRP	CD1-NE1	-5.82	1.28	1.38
1	A	113	TYR	CZ-OH	5.72	1.47	1.37
1	B	136	ARG	CZ-NH2	-5.65	1.25	1.33
1	A	54	GLY	N-CA	-5.60	1.37	1.46
1	A	40	SER	CB-OG	-5.56	1.35	1.42
1	A	93	ARG	CD-NE	-5.55	1.37	1.46
1	D	63	TYR	CG-CD1	5.51	1.46	1.39
1	D	54	GLY	C-O	5.49	1.32	1.23
1	B	114	GLY	N-CA	5.48	1.54	1.46
1	D	73	PRO	CA-C	5.47	1.63	1.52
1	A	92	THR	N-CA	5.43	1.57	1.46
1	C	26	GLY	N-CA	5.33	1.54	1.46
1	B	76	PHE	CG-CD1	5.31	1.46	1.38
1	A	81	SER	CA-CB	-5.30	1.45	1.52
1	B	113	TYR	CG-CD1	-5.30	1.32	1.39
1	A	115	GLU	CA-CB	-5.28	1.42	1.53
1	B	45	TYR	CZ-OH	5.26	1.46	1.37
1	C	102	PHE	C-O	-5.26	1.13	1.23
1	A	150	LEU	C-OXT	5.24	1.33	1.23
1	D	75	GLU	CD-OE2	5.23	1.31	1.25
1	D	50	GLU	CD-OE2	5.18	1.31	1.25
1	D	120	TYR	C-O	5.18	1.33	1.23
1	C	10	PRO	N-CA	5.16	1.56	1.47
1	B	28	ARG	N-CA	5.14	1.56	1.46
1	D	24	TYR	CG-CD1	5.14	1.45	1.39
1	A	72	PHE	CG-CD1	5.13	1.46	1.38
1	A	79	SER	CB-OG	5.11	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	ARG	CZ-NH2	5.11	1.39	1.33
1	D	69	GLU	CD-OE2	5.07	1.31	1.25
1	A	50	GLU	CG-CD	-5.06	1.44	1.51
1	C	133	PHE	CG-CD2	-5.06	1.31	1.38
1	D	135	GLY	C-O	5.06	1.31	1.23
1	C	111	GLY	N-CA	-5.03	1.38	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	108	ARG	NE-CZ-NH2	11.36	125.98	120.30
1	B	28	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	B	93	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	D	46	ASP	CB-CG-OD1	-9.50	109.75	118.30
1	C	108	ARG	NE-CZ-NH1	-9.47	115.57	120.30
1	A	117	ASP	CB-CG-OD1	9.19	126.57	118.30
1	D	140	LEU	CB-CG-CD1	-9.18	95.40	111.00
1	A	108	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	28	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	B	18	GLU	OE1-CD-OE2	8.56	133.57	123.30
1	A	98	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	136	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	31	GLU	OE1-CD-OE2	-7.51	114.28	123.30
1	B	90	LEU	CA-CB-CG	7.51	132.57	115.30
1	D	93	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	36	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	C	87	PHE	CB-CA-C	7.11	124.62	110.40
1	D	28	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	A	1	MET	CB-CG-SD	-6.75	92.16	112.40
1	B	93	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	45	TYR	CG-CD1-CE1	-6.55	116.06	121.30
1	C	18	GLU	OE1-CD-OE2	-6.52	115.47	123.30
1	B	31	GLU	CG-CD-OE1	6.50	131.31	118.30
1	C	140	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	C	20	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	45	TYR	CD1-CE1-CZ	6.33	125.50	119.80
1	C	121	PHE	CB-CG-CD1	6.32	125.22	120.80
1	B	24	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	A	18	GLU	CG-CD-OE2	6.20	130.70	118.30
1	A	75	GLU	OE1-CD-OE2	-6.11	115.97	123.30
1	A	108	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	98	ARG	NE-CZ-NH2	-6.01	117.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	123	LEU	C-N-CD	5.84	140.66	128.40
1	B	20	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	D	141	LEU	CB-CG-CD1	5.73	120.74	111.00
1	A	126	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	B	50	GLU	CG-CD-OE1	5.71	129.72	118.30
1	A	142	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	A	20	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	102	PHE	CB-CG-CD1	-5.62	116.87	120.80
1	B	83	TYR	CZ-CE2-CD2	-5.59	114.77	119.80
1	C	72	PHE	CB-CG-CD2	5.49	124.64	120.80
1	B	117	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	45	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	D	122	ASN	N-CA-CB	-5.38	100.91	110.60
1	A	117	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	101	LYS	CG-CD-CE	5.29	127.77	111.90
1	A	94	THR	CA-CB-CG2	-5.25	105.05	112.40
1	B	28	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	146[A]	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	A	146[B]	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	A	93	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	117[A]	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	117[B]	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	28	ARG	CA-CB-CG	-5.13	102.12	113.40
1	B	97	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	C	122	ASN	N-CA-CB	-5.07	101.48	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	GLU	Mainchain
1	A	82	GLY	Mainchain
1	A	87	PHE	Peptide
1	B	28	ARG	Sidechain
1	C	90	LEU	Peptide
1	C	92	THR	Peptide

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	1210	0	1198	24	2
1	B	1170	0	1153	19	0
1	C	1213	0	1180	15	2
1	D	1190	0	1168	16	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	2	0
3	A	113	0	0	2	0
3	B	109	0	0	4	0
3	C	98	0	0	5	0
3	D	97	0	0	2	0
All	All	5248	0	4747	67	2

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 7.

All (67) 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:29[B]:ILE:HD13	1:A:44[B]:ILE:HB	1.55	0.88
1:A:29[B]:ILE:HD13	1:A:44[B]:ILE:CB	2.05	0.87
1:B:87:PHE:H	1:B:90:LEU:HD22	1.41	0.85
1:A:29[B]:ILE:CD1	1:A:44[B]:ILE:HB	2.08	0.84
1:C:94:THR:HG23	3:C:321:HOH:O	1.82	0.78
1:C:18:GLU:HG2	3:C:314:HOH:O	1.87	0.75
1:B:25[A]:THR:HG22	1:B:25[A]:THR:O	1.87	0.75
1:C:109[B]:THR:HG23	3:C:309:HOH:O	1.87	0.74
1:A:25[B]:THR:CG2	1:A:48:ASN:H	2.02	0.71
1:A:25[B]:THR:HG21	1:A:48:ASN:H	1.56	0.68
1:D:96:VAL:HG11	1:D:140:LEU:HD11	1.76	0.68
1:A:29[B]:ILE:HD13	1:A:44[B]:ILE:CG1	2.25	0.66
1:B:87:PHE:O	1:B:90:LEU:HB2	1.97	0.65
1:A:90:LEU:H	1:A:90:LEU:HD12	1.63	0.64
1:B:85:ALA:HB2	1:B:118:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:THR:O	1:B:93:ARG:HB3	1.98	0.63
1:A:69:GLU:OE2	3:A:301:HOH:O	2.16	0.61
1:A:29[B]:ILE:HD13	1:A:44[B]:ILE:HG13	1.81	0.61
1:D:42[B]:SER:OG	3:D:301:HOH:O	2.16	0.60
1:A:35:LYS:HD3	3:A:314:HOH:O	2.04	0.58
1:A:123:LEU:HD12	1:B:8[B]:VAL:HG11	1.87	0.57
1:D:136[B]:ARG:HE	1:D:143:ALA:HB3	1.71	0.56
1:C:89:SER:O	1:C:90:LEU:HD22	2.06	0.55
1:B:25[A]:THR:HG22	1:D:2:ALA:HB1	1.88	0.54
1:A:29[B]:ILE:HD12	1:A:44[B]:ILE:HB	1.90	0.52
1:A:29[B]:ILE:HD12	1:A:29[B]:ILE:N	2.23	0.52
1:C:71:GLN:CD	1:C:108:ARG:HH12	2.13	0.51
1:D:85:ALA:HB2	1:D:118:GLY:HA3	1.93	0.51
1:C:86:PRO:HB3	1:C:93:ARG:HG3	1.91	0.51
1:D:29:ILE:HG12	1:D:69:GLU:HG3	1.93	0.50
1:C:6:ILE:HD13	1:D:128:GLY:HA3	1.94	0.49
1:A:150:LEU:HD12	1:A:150:LEU:N	2.26	0.49
1:D:140:LEU:CD1	2:D:201:GLC:H62	2.43	0.49
1:B:4:GLN:NE2	3:B:304:HOH:O	2.45	0.48
1:B:25[A]:THR:O	1:B:25[A]:THR:CG2	2.60	0.48
1:C:109[A]:THR:HG22	3:C:309:HOH:O	2.12	0.48
1:C:33:SER:HA	1:C:64:THR:O	2.14	0.47
1:A:123:LEU:CD1	1:B:8[B]:VAL:HG11	2.44	0.47
1:B:92:THR:O	1:B:93:ARG:CB	2.63	0.46
1:A:150:LEU:HD11	1:C:4:GLN:H	1.81	0.46
1:D:75:GLU:HG3	1:D:106:LYS:HG2	1.97	0.46
1:C:126:GLU:HG3	1:D:9:GLY:O	2.16	0.46
1:A:75:GLU:OE2	1:A:108:ARG:CD	2.64	0.46
1:D:140:LEU:HD12	2:D:201:GLC:C6	2.45	0.46
1:A:14:PRO:HD2	1:A:94:THR:HB	1.98	0.45
1:A:25[B]:THR:HG23	1:A:48:ASN:H	1.80	0.45
1:D:68:ILE:HG23	1:D:110:PHE:CD1	2.51	0.45
1:A:75:GLU:OE2	1:A:108:ARG:HD3	2.17	0.45
1:C:32:LEU:C	1:C:32:LEU:HD12	2.37	0.45
1:A:149:ALA:O	1:A:150:LEU:HB2	2.16	0.45
1:C:101[B]:LYS:HE3	1:C:109[B]:THR:OG1	2.17	0.45
1:A:124:PRO:O	1:B:8[B]:VAL:HG13	2.17	0.45
1:B:92:THR:HG21	3:B:338:HOH:O	2.16	0.44
1:D:18:GLU:HG2	1:D:136[A]:ARG:NH2	2.33	0.44
1:C:18:GLU:CG	3:C:314:HOH:O	2.54	0.44
1:B:99:SER:HA	1:B:113:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:O	1:B:57:HIS:HB2	2.18	0.43
1:A:25[B]:THR:HG23	1:A:47:LEU:HA	2.01	0.43
1:B:92:THR:N	3:B:307:HOH:O	2.51	0.43
1:D:96:VAL:HG11	1:D:140:LEU:CD1	2.47	0.43
1:B:21:ASP:HB2	1:B:133:PHE:O	2.19	0.42
1:B:119:THR:HA	3:B:317:HOH:O	2.18	0.42
1:D:115:GLU:HG3	3:D:391:HOH:O	2.19	0.41
1:D:72:PHE:CD1	1:D:73:PRO:HA	2.55	0.41
1:C:108:ARG:HH11	1:C:108:ARG:HD3	1.69	0.41
1:A:28:ARG:CB	1:A:29[B]:ILE:HD12	2.51	0.40
1:B:44:ILE:HD12	1:B:53:SER:OG	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:OE1	1:C:117[A]:ASP:OD2[1_655]	1.67	0.53
1:A:117:ASP:OD2	1:C:117[A]:ASP:OD2[1_655]	1.93	0.27

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	157/150 (105%)	150 (96%)	6 (4%)	1 (1%)	25 8
1	B	152/150 (101%)	143 (94%)	8 (5%)	1 (1%)	22 7
1	C	156/150 (104%)	146 (94%)	7 (4%)	3 (2%)	8 1
1	D	154/150 (103%)	147 (96%)	4 (3%)	3 (2%)	8 1
All	All	619/600 (103%)	586 (95%)	25 (4%)	8 (1%)	11 2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	ARG
1	C	88	SER
1	D	16	GLY
1	C	91	ALA
1	C	90	LEU
1	D	35	LYS
1	D	88	SER
1	A	35	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	133/124 (107%)	127 (96%)	6 (4%)	27 8
1	B	128/124 (103%)	124 (97%)	4 (3%)	40 15
1	C	132/124 (106%)	121 (92%)	11 (8%)	11 2
1	D	130/124 (105%)	124 (95%)	6 (5%)	27 8
All	All	523/496 (105%)	496 (95%)	27 (5%)	25 6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	25[A]	THR
1	A	25[B]	THR
1	A	90	LEU
1	A	146[A]	VAL
1	A	146[B]	VAL
1	B	1	MET
1	B	69	GLU
1	B	88	SER
1	B	92	THR
1	C	18	GLU
1	C	31	GLU
1	C	60	LYS
1	C	66	VAL

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Mol	Chain	Res	Type
1	C	88	SER
1	C	90	LEU
1	C	92	THR
1	C	93	ARG
1	C	134[A]	LYS
1	C	134[B]	LYS
1	C	140	LEU
1	D	36	GLU
1	D	93	ARG
1	D	94	THR
1	D	115	GLU
1	D	139	ASP
1	D	140	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	127	ASN
1	B	4	GLN
1	B	17	ASN
1	C	65	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	GLC	C	201	-	12,12,12	0.80	0	17,17,17	1.49	2 (11%)
2	GLC	B	201	-	12,12,12	0.47	0	17,17,17	2.56	6 (35%)
2	GLC	A	201	-	12,12,12	0.91	0	17,17,17	2.65	6 (35%)
2	GLC	D	201	-	12,12,12	1.02	1 (8%)	17,17,17	1.90	4 (23%)

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	201	-	-	0/2/22/22	0/1/1/1
2	GLC	B	201	-	-	0/2/22/22	0/1/1/1
2	GLC	A	201	-	-	0/2/22/22	0/1/1/1
2	GLC	D	201	-	-	1/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	GLC	O5-C1	2.08	1.48	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	201	GLC	C1-O5-C5	7.66	128.12	113.66
2	A	201	GLC	O1-C1-C2	6.23	126.57	109.03
2	A	201	GLC	C1-O5-C5	5.56	124.15	113.66
2	D	201	GLC	C1-O5-C5	4.75	122.62	113.66
2	A	201	GLC	O2-C2-C1	3.82	118.01	109.16
2	C	201	GLC	C1-O5-C5	3.72	120.68	113.66
2	B	201	GLC	C1-C2-C3	3.58	117.75	110.31
2	B	201	GLC	O5-C5-C6	-3.36	98.08	106.44
2	D	201	GLC	O5-C5-C4	3.32	115.73	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	GLC	O5-C5-C4	3.18	115.46	109.69
2	D	201	GLC	O5-C1-C2	3.10	115.82	110.28
2	B	201	GLC	C6-C5-C4	3.00	120.02	113.00
2	D	201	GLC	C1-C2-C3	2.94	116.41	110.31
2	A	201	GLC	O1-C1-O5	-2.83	101.88	110.38
2	A	201	GLC	C3-C4-C5	-2.77	105.30	110.24
2	B	201	GLC	C3-C4-C5	-2.51	105.76	110.24
2	C	201	GLC	O5-C5-C4	2.20	113.69	109.69
2	B	201	GLC	O3-C3-C2	-2.07	105.55	110.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	GLC	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	150/150 (100%)	-0.43	1 (0%)	87	87	11, 18, 29, 47	1 (0%)
1	B	150/150 (100%)	-0.35	2 (1%)	77	77	11, 17, 31, 55	2 (1%)
1	C	150/150 (100%)	-0.27	4 (2%)	54	52	12, 19, 41, 92	0
1	D	150/150 (100%)	-0.37	2 (1%)	77	77	12, 21, 37, 62	2 (1%)
All	All	600/600 (100%)	-0.35	9 (1%)	73	73	11, 19, 36, 92	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	THR	7.2
1	C	90	LEU	6.8
1	B	91	ALA	6.4
1	C	92	THR	5.5
1	C	91	ALA	4.8
1	C	89	SER	4.0
1	D	91	ALA	2.8
1	A	90	LEU	2.1
1	D	1	MET	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, 95th 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	201	12/12	0.91	0.09	26,31,34,35	0
2	GLC	C	201	12/12	0.94	0.08	28,32,42,45	0
2	GLC	A	201	12/12	0.95	0.06	18,25,31,32	0
2	GLC	B	201	12/12	0.96	0.06	15,19,24,36	0

6.5 Other polymers (i)

There are no such residues in this entry.