



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:38 PM UTC

PDB ID : 5TQZ / pdb_00005tqz
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

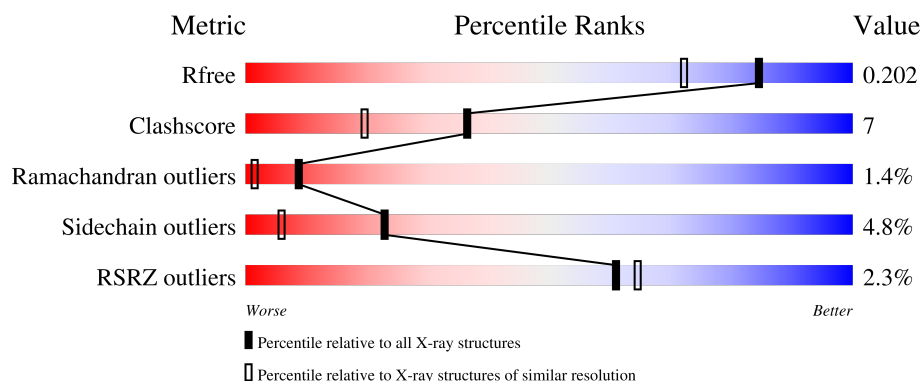
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 $\leq 5\%$. 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	150	% 64% 31% 5%
1	B	150	2% 64% 30% 5%
1	C	150	4% 69% 24%
1	D	150	3% 57% 37% 5%

2 Entry composition [i](#)

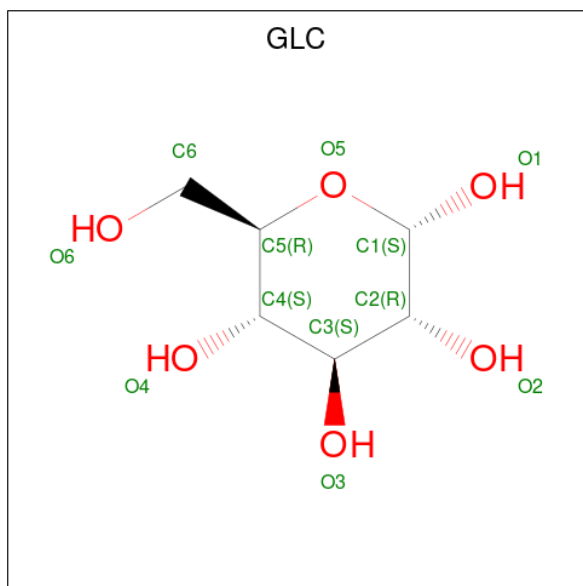
There are 3 unique types of molecules in this entry. The entry contains 5248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



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

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

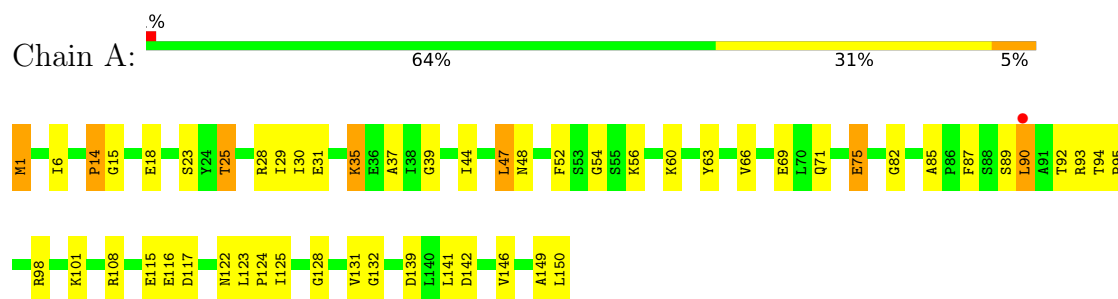
- Molecule 3 is water.

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

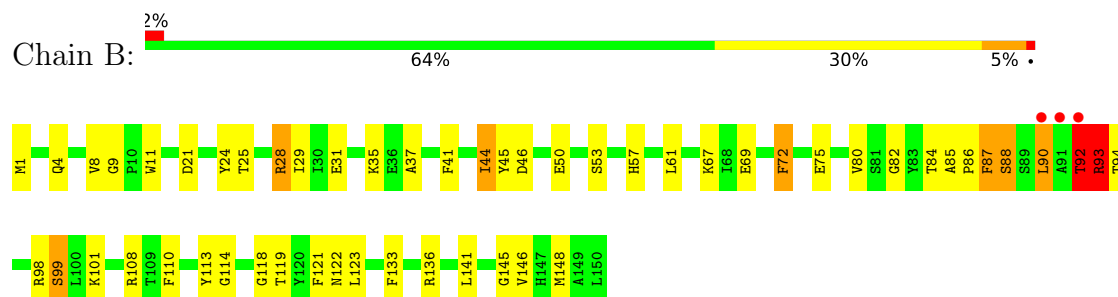
3 Residue-property plots [i](#)

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.

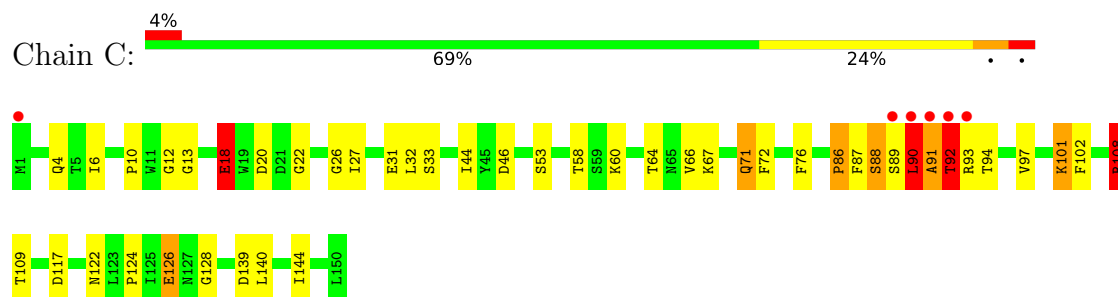
• Molecule 1: Frutapin



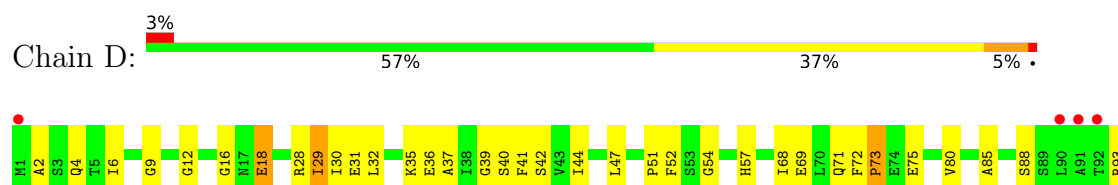
• Molecule 1: Frutapin

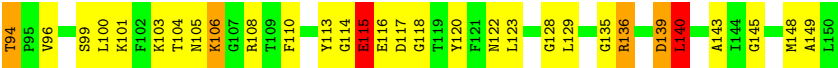


• Molecule 1: Frutapin



• Molecule 1: Frutapin





4 Data and refinement statistics

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) 100.0 (64.11-1.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	2.12	32/1252 (2.6%)	1.57	8/1697 (0.5%)
1	B	2.16	36/1209 (3.0%)	1.71	15/1640 (0.9%)
1	C	1.97	29/1243 (2.3%)	1.67	14/1683 (0.8%)
1	D	2.11	41/1226 (3.3%)	1.67	16/1660 (1.0%)
All	All	2.09	138/4930 (2.8%)	1.65	53/6680 (0.8%)

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 (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	ASN	C-O	8.98	1.34	1.23
1	C	102	PHE	C-O	-8.68	1.13	1.23
1	C	26	GLY	N-CA	8.62	1.54	1.45
1	A	92	THR	N-CA	8.44	1.57	1.46
1	B	28	ARG	N-CA	8.19	1.56	1.46
1	C	92	THR	CA-C	8.12	1.62	1.52
1	A	23	SER	C-N	8.12	1.40	1.33
1	D	71	GLN	CA-C	-7.64	1.45	1.53
1	C	108	ARG	CZ-NH2	7.53	1.43	1.33
1	B	31	GLU	C-O	-7.41	1.15	1.24
1	A	14	PRO	N-CA	7.40	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	28	ARG	N-CA	7.39	1.55	1.46
1	A	66	VAL	C-O	-7.39	1.16	1.24
1	D	104	THR	CA-CB	7.36	1.65	1.53
1	D	120	TYR	C-O	7.36	1.33	1.23
1	B	75	GLU	N-CA	7.29	1.54	1.46
1	C	12	GLY	N-CA	7.25	1.54	1.44
1	A	52	PHE	CA-C	7.17	1.60	1.52
1	B	93	ARG	N-CA	7.15	1.55	1.46
1	B	84	THR	N-CA	-7.15	1.36	1.45
1	A	116	GLU	CA-CB	7.15	1.62	1.52
1	D	135	GLY	C-O	7.13	1.31	1.23
1	A	128	GLY	C-O	7.09	1.29	1.23
1	A	139	ASP	CA-C	-7.08	1.43	1.52
1	B	50	GLU	C-O	-7.04	1.16	1.24
1	D	47	LEU	N-CA	7.03	1.54	1.46
1	D	103	LYS	CA-C	-6.99	1.44	1.52
1	B	123	LEU	CA-CB	-6.96	1.45	1.53
1	B	98	ARG	N-CA	-6.95	1.37	1.46
1	B	86	PRO	CA-C	-6.88	1.44	1.52
1	A	18	GLU	N-CA	6.87	1.54	1.45
1	D	117	ASP	C-O	-6.85	1.15	1.24
1	D	145	GLY	N-CA	6.84	1.51	1.45
1	B	80	VAL	N-CA	6.74	1.54	1.46
1	C	144	ILE	C-O	6.73	1.30	1.24
1	B	145	GLY	N-CA	6.71	1.52	1.45
1	A	142	ASP	C-O	6.70	1.32	1.24
1	A	47	LEU	C-O	-6.66	1.16	1.23
1	A	131	VAL	N-CA	-6.61	1.39	1.46
1	A	93	ARG	CD-NE	-6.59	1.37	1.46
1	D	136[A]	ARG	C-O	-6.59	1.16	1.23
1	D	136[B]	ARG	C-O	-6.59	1.16	1.23
1	C	87	PHE	CA-C	6.55	1.61	1.53
1	D	80	VAL	CA-C	-6.53	1.44	1.52
1	C	58	THR	C-O	-6.41	1.16	1.24
1	D	116	GLU	CA-C	6.35	1.60	1.53
1	B	11	TRP	C-O	6.32	1.31	1.24
1	B	37	ALA	C-O	6.30	1.32	1.24
1	C	20	ASP	C-O	-6.30	1.16	1.24
1	A	93	ARG	CZ-NH2	-6.30	1.25	1.33
1	B	99	SER	N-CA	6.29	1.53	1.45
1	B	9	GLY	N-CA	-6.25	1.36	1.44
1	B	24	TYR	CA-C	6.24	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	LYS	C-O	6.18	1.31	1.23
1	D	100	LEU	C-O	6.17	1.31	1.23
1	B	90	LEU	N-CA	6.17	1.53	1.46
1	A	89	SER	CA-C	6.16	1.61	1.52
1	A	63	TYR	C-O	-6.14	1.15	1.23
1	B	114	GLY	N-CA	6.13	1.54	1.45
1	C	53	SER	N-CA	6.12	1.53	1.46
1	D	18	GLU	N-CA	6.12	1.53	1.46
1	A	141	LEU	N-CA	6.10	1.54	1.46
1	D	29	ILE	C-O	-6.00	1.18	1.24
1	D	105	ASN	CG-ND2	-5.99	1.20	1.33
1	B	136	ARG	CZ-NH2	-5.96	1.25	1.33
1	D	40	SER	CA-CB	5.96	1.63	1.53
1	A	85	ALA	CA-CB	-5.89	1.44	1.53
1	D	80	VAL	N-CA	-5.88	1.39	1.46
1	B	35	LYS	C-O	-5.87	1.16	1.24
1	D	54	GLY	C-O	5.84	1.32	1.23
1	D	51	PRO	C-O	5.81	1.30	1.23
1	C	101[A]	LYS	N-CA	-5.81	1.38	1.46
1	C	101[B]	LYS	N-CA	-5.81	1.38	1.46
1	B	29	ILE	CA-C	-5.80	1.45	1.52
1	B	108	ARG	NE-CZ	5.80	1.39	1.33
1	D	6	ILE	N-CA	5.80	1.53	1.46
1	A	71	GLN	C-O	5.77	1.30	1.23
1	D	30	ILE	N-CA	-5.74	1.39	1.46
1	B	45	TYR	N-CA	-5.69	1.38	1.45
1	D	149	ALA	CA-CB	-5.68	1.44	1.53
1	C	97	VAL	CA-CB	5.67	1.59	1.53
1	B	98	ARG	CZ-NH1	5.66	1.40	1.32
1	A	93	ARG	CA-C	-5.66	1.45	1.52
1	A	122	ASN	C-O	5.65	1.30	1.23
1	A	101	LYS	C-O	5.61	1.30	1.23
1	C	90	LEU	CA-C	5.60	1.60	1.52
1	D	31	GLU	CD-OE1	5.60	1.35	1.25
1	B	67	LYS	C-O	5.57	1.30	1.24
1	C	126	GLU	CD-OE2	5.50	1.35	1.25
1	A	54	GLY	N-CA	-5.50	1.37	1.45
1	D	115	GLU	CA-C	5.49	1.59	1.52
1	A	31	GLU	CA-C	5.49	1.59	1.52
1	A	95	PRO	C-O	-5.47	1.17	1.23
1	D	73	PRO	CA-C	5.47	1.63	1.52
1	C	71	GLN	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	116	GLU	CA-CB	5.45	1.59	1.52
1	B	94	THR	C-O	-5.44	1.16	1.23
1	A	37	ALA	C-O	5.43	1.31	1.23
1	D	117	ASP	CA-CB	5.41	1.61	1.53
1	A	125	ILE	CA-C	-5.41	1.45	1.52
1	C	92	THR	N-CA	5.38	1.52	1.46
1	B	11	TRP	CD1-NE1	5.37	1.49	1.37
1	D	41	PHE	N-CA	5.37	1.52	1.46
1	D	52	PHE	C-O	-5.36	1.17	1.23
1	C	18	GLU	CA-CB	5.32	1.62	1.53
1	C	18	GLU	N-CA	5.31	1.52	1.46
1	C	27	ILE	N-CA	-5.30	1.40	1.46
1	A	39	GLY	C-O	5.30	1.31	1.23
1	D	32	LEU	CA-C	-5.27	1.46	1.52
1	C	67	LYS	C-O	-5.27	1.18	1.24
1	B	90	LEU	CA-CB	5.25	1.60	1.53
1	B	87	PHE	C-O	-5.23	1.18	1.24
1	A	15	GLY	N-CA	5.23	1.51	1.45
1	B	98	ARG	NE-CZ	-5.23	1.27	1.33
1	C	44	ILE	CA-CB	-5.23	1.48	1.54
1	B	141	LEU	CA-C	-5.22	1.46	1.52
1	D	113	TYR	C-O	-5.22	1.17	1.24
1	C	128	GLY	C-O	-5.22	1.18	1.23
1	A	63	TYR	N-CA	5.20	1.51	1.45
1	D	4	GLN	N-CA	5.20	1.51	1.45
1	D	39	GLY	C-O	-5.18	1.18	1.24
1	D	6	ILE	CA-CB	5.18	1.59	1.54
1	D	51	PRO	N-CA	5.18	1.53	1.47
1	C	91	ALA	N-CA	5.16	1.52	1.46
1	C	10	PRO	N-CA	5.16	1.56	1.47
1	C	46	ASP	CG-OD2	5.15	1.35	1.25
1	C	76	PHE	C-O	5.14	1.30	1.23
1	D	101	LYS	N-CA	5.13	1.52	1.46
1	D	12	GLY	N-CA	5.12	1.52	1.45
1	B	44	ILE	N-CA	5.12	1.52	1.46
1	B	148	MET	CA-C	5.08	1.58	1.52
1	A	30	ILE	N-CA	-5.08	1.40	1.46
1	D	99	SER	CA-C	5.07	1.58	1.52
1	C	124	PRO	C-O	5.04	1.29	1.23
1	B	121	PHE	N-CA	5.01	1.52	1.45
1	D	37	ALA	CA-CB	5.01	1.62	1.53
1	B	82	GLY	N-CA	5.01	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	GLU	CG-CD	5.00	1.64	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	GLY	CA-C-N	10.06	131.28	120.12
1	C	13	GLY	C-N-CA	10.06	131.28	120.12
1	D	123	LEU	CA-C-N	-8.45	108.85	120.25
1	D	123	LEU	C-N-CA	-8.45	108.85	120.25
1	C	72	PHE	CA-C-O	-8.01	111.97	120.70
1	C	87	PHE	CB-CA-C	7.79	124.62	111.22
1	C	108	ARG	NE-CZ-NH2	7.53	125.98	119.20
1	D	94	THR	N-CA-C	-7.22	100.97	110.07
1	B	101	LYS	CG-CD-CE	7.16	127.77	111.30
1	D	104	THR	N-CA-C	6.94	120.43	109.81
1	A	1	MET	CB-CG-SD	-6.84	92.16	112.70
1	C	18	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	90	LEU	N-CA-C	-6.36	98.15	108.52
1	D	47	LEU	CA-C-O	6.27	127.10	120.33
1	D	114	GLY	N-CA-C	-6.12	103.17	112.84
1	B	28	ARG	CA-CB-CG	-5.99	102.12	114.10
1	D	44	ILE	N-CA-C	-5.94	98.58	107.37
1	C	108	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	A	132	GLY	O-C-N	5.87	129.80	123.87
1	A	14	PRO	CB-CA-C	5.85	116.56	110.00
1	B	88	SER	N-CA-C	5.82	123.19	110.80
1	B	28	ARG	CA-C-N	-5.71	114.14	122.58
1	B	28	ARG	C-N-CA	-5.71	114.14	122.58
1	B	146	VAL	N-CA-CB	5.71	120.82	111.58
1	D	122	ASN	N-CA-CB	-5.71	100.91	110.32
1	A	6	ILE	O-C-N	-5.69	116.86	122.67
1	A	98	ARG	N-CA-C	5.67	119.38	112.23
1	B	31	GLU	CG-CD-OE1	5.61	131.31	118.40
1	B	72	PHE	N-CA-C	-5.52	103.09	109.93
1	C	122	ASN	N-CA-CB	-5.36	101.48	110.32
1	A	18	GLU	CG-CD-OE2	5.35	130.70	118.40
1	C	92	THR	CA-C-O	5.34	126.25	120.43
1	D	94	THR	CB-CA-C	5.34	116.39	108.87
1	D	129	LEU	CA-C-O	-5.33	114.53	120.66
1	A	131	VAL	N-CA-C	5.32	119.23	113.43
1	B	61	LEU	CA-C-N	5.32	126.49	119.84
1	B	61	LEU	C-N-CA	5.32	126.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	GLY	CA-C-O	-5.30	118.50	122.37
1	C	22	GLY	N-CA-C	-5.29	103.19	112.77
1	B	122	ASN	N-CA-CB	-5.28	101.87	110.59
1	D	108	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	B	110	PHE	N-CA-C	-5.23	99.88	108.41
1	C	139	ASP	N-CA-C	-5.21	106.18	112.54
1	D	28	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	B	92	THR	CA-C-O	-5.13	113.17	120.51
1	D	140	LEU	CB-CG-CD1	-5.10	95.40	110.70
1	B	67	LYS	CA-CB-CG	5.06	124.23	114.10
1	A	128	GLY	O-C-N	5.06	128.16	123.35
1	D	139	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	57	HIS	N-CA-C	-5.04	100.17	108.49
1	D	106	LYS	N-CA-C	5.03	119.40	113.16
1	C	86	PRO	CA-C-N	-5.02	115.72	123.14
1	C	86	PRO	C-N-CA	-5.02	115.72	123.14

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	20	0
1	C	1213	0	1180	15	2
1	D	1190	0	1168	17	0
2	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	69	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 (69) 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
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:C:71:GLN:CD	1:C:108:ARG:HH12	2.13	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29[B]:ILE:HD12	1:A:29[B]:ILE:N	2.23	0.52
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:32:LEU:C	1:C:32:LEU:HD12	2.37	0.49
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: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:D:148[B]:MET:HE3	1:D:148[B]:MET:HB2	1.89	0.43
1:B:99:SER:HA	1:B:113:TYR:O	2.19	0.43
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:B:46:ASP:CG	1:B:72:PHE:CZ	2.98	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	21	7
1	B	152/150 (101%)	143 (94%)	8 (5%)	1 (1%)	18	6
1	C	156/150 (104%)	146 (94%)	7 (4%)	3 (2%)	6	1
1	D	154/150 (103%)	147 (96%)	4 (3%)	3 (2%)	6	1
All	All	619/600 (103%)	586 (95%)	25 (4%)	8 (1%)	9	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

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Mol	Chain	Res	Type
1	A	35	LYS

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	133/124 (107%)	126 (95%)	7 (5%)	20	4
1	B	128/124 (103%)	124 (97%)	4 (3%)	35	13
1	C	132/124 (106%)	123 (93%)	9 (7%)	14	3
1	D	130/124 (105%)	124 (95%)	6 (5%)	24	6
All	All	523/496 (105%)	497 (95%)	26 (5%)	23	5

All (26) 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	60	LYS
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
1	C	88	SER
1	C	90	LEU
1	C	92	THR
1	C	108	ARG
1	C	140	LEU

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Mol	Chain	Res	Type
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	122	ASN
1	B	4	GLN
1	C	122	ASN
1	C	127	ASN
1	D	4	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	201	-	12,12,12	0.47	0	17,17,17	2.51	6 (35%)
2	GLC	A	201	-	12,12,12	0.91	1 (8%)	17,17,17	2.60	6 (35%)
2	GLC	D	201	-	12,12,12	1.03	1 (8%)	17,17,17	1.89	4 (23%)
2	GLC	C	201	-	12,12,12	0.80	0	17,17,17	1.48	2 (11%)

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	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
2	GLC	C	201	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	GLC	O5-C1	2.14	1.48	1.42
2	A	201	GLC	O1-C1	2.02	1.45	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	GLC	C1-O5-C5	7.48	128.12	113.65
2	A	201	GLC	O1-C1-C2	6.06	126.57	108.98
2	A	201	GLC	C1-O5-C5	5.42	124.15	113.65
2	D	201	GLC	C1-O5-C5	4.63	122.62	113.65
2	A	201	GLC	O2-C2-C1	3.80	118.01	109.25
2	C	201	GLC	C1-O5-C5	3.63	120.68	113.65
2	B	201	GLC	C1-C2-C3	3.62	117.75	110.36
2	B	201	GLC	O5-C5-C6	-3.37	98.08	106.44
2	D	201	GLC	O5-C5-C4	3.35	115.73	109.70
2	A	201	GLC	O5-C5-C4	3.20	115.46	109.70
2	D	201	GLC	O5-C1-C2	3.14	115.82	110.30
2	D	201	GLC	C1-C2-C3	2.97	116.41	110.36
2	A	201	GLC	O1-C1-O5	-2.87	101.88	110.41
2	B	201	GLC	C6-C5-C4	2.85	120.02	113.02
2	A	201	GLC	C3-C4-C5	-2.72	105.30	110.23
2	B	201	GLC	C3-C4-C5	-2.47	105.76	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	GLC	O5-C5-C4	2.21	113.69	109.70
2	B	201	GLC	O3-C3-C2	-2.05	105.55	110.38

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%)	-0.23	1 (0%) 84 87	7, 18, 29, 47	10 (6%)
1	B	150/150 (100%)	-0.25	3 (2%) 65 69	6, 17, 31, 45	6 (4%)
1	C	150/150 (100%)	0.01	6 (4%) 42 44	6, 19, 41, 92	8 (5%)
1	D	150/150 (100%)	-0.02	4 (2%) 56 59	6, 21, 37, 62	8 (5%)
All	All	600/600 (100%)	-0.12	14 (2%) 61 64	6, 18, 35, 92	32 (5%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	7.7
1	B	91	ALA	6.5
1	C	91	ALA	5.4
1	B	92	THR	5.0
1	C	92	THR	4.4
1	D	92	THR	3.1
1	D	91	ALA	3.0
1	C	89	SER	2.8
1	A	90	LEU	2.8
1	D	90	LEU	2.5
1	C	1	MET	2.5
1	D	1	MET	2.5
1	C	93	ARG	2.4
1	B	90	LEU	2.4

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	GLC	C	201	12/12	0.92	0.09	28,32,42,45	0
2	GLC	D	201	12/12	0.93	0.07	26,31,34,35	0
2	GLC	A	201	12/12	0.96	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.