



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 02:03 pm GMT

PDB ID : 1V3L  
Title : Crystal structure of F283L mutant cyclodextrin glycosyltransferase complexed with a pseudo-tetraose derived from acarbose  
Authors : Kanai, R.; Haga, K.; Akiba, T.; Yamane, K.; Harata, K.  
Deposited on : 2003-11-03  
Resolution : 2.10 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

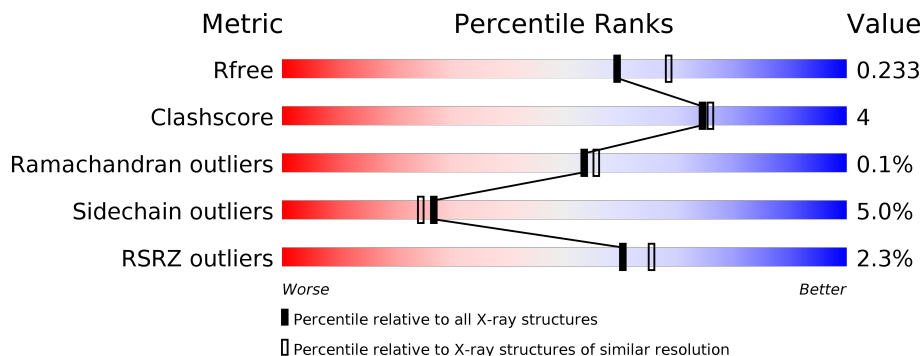
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	686	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	686	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>

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
2	GLC	B	801	-	-	-	X
3	ACI	A	702	-	-	-	X
3	ACI	B	802	-	-	-	X
4	GLD	A	703	-	-	-	X
5	GAL	A	704	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11214 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.

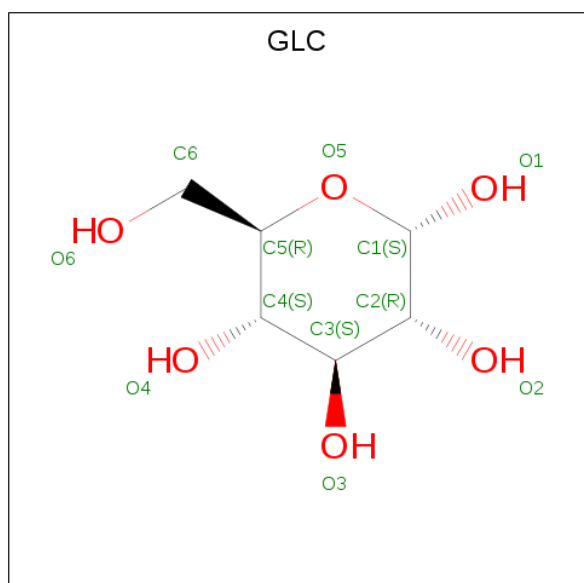
- Molecule 1 is a protein called Cyclomaltodextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5309	3351	906	1036	16			
1	B	686	Total	C	N	O	S	0	0	0
			5309	3351	906	1036	16			

There are 6 discrepancies between the modelled and reference sequences:

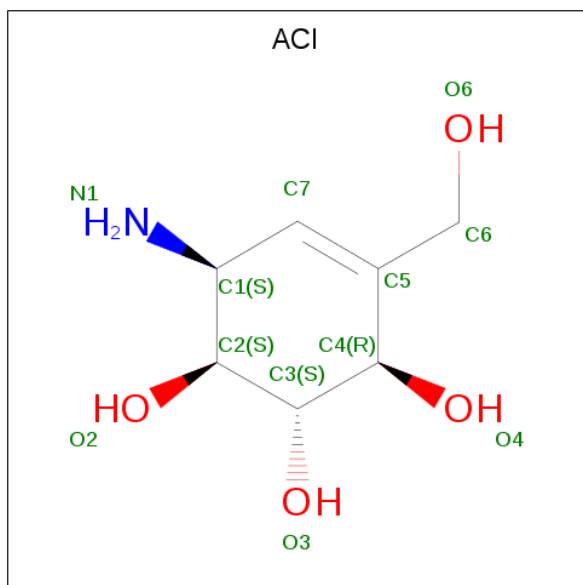
Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LEU	PHE	ENGINEERED	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	283	LEU	PHE	ENGINEERED	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	UNP P05618

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



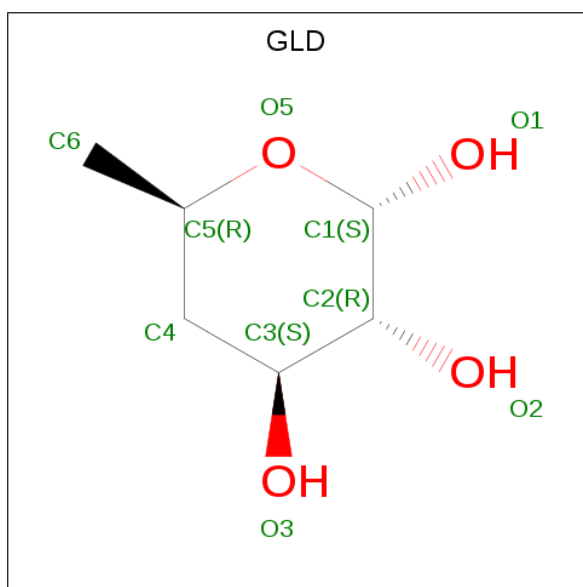
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 6-AMINO-4-HYDROXYMETHYL-CYCLOHEX-4-ENE-1,2,3-TRIOL (three-letter code: ACI) (formula:  $C_7H_{13}NO_4$ ).



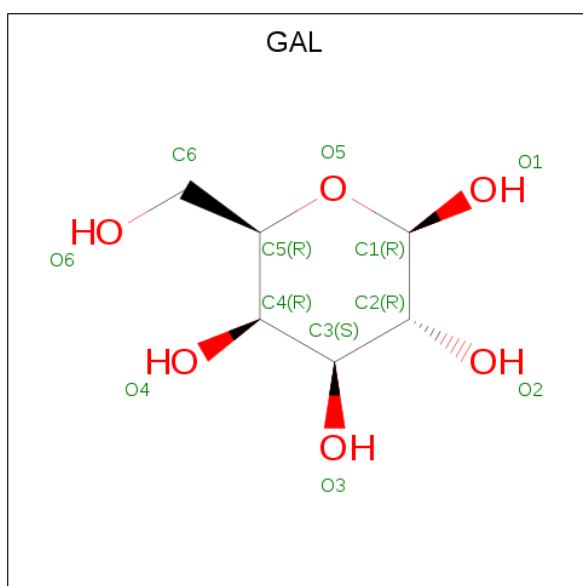
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is 4,6-DIDEOXYGLUCOSE (three-letter code: GLD) (formula:  $C_6H_{12}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		
4	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Ca 2	0	0
6	A	2	Total 2	Ca 2	0	0

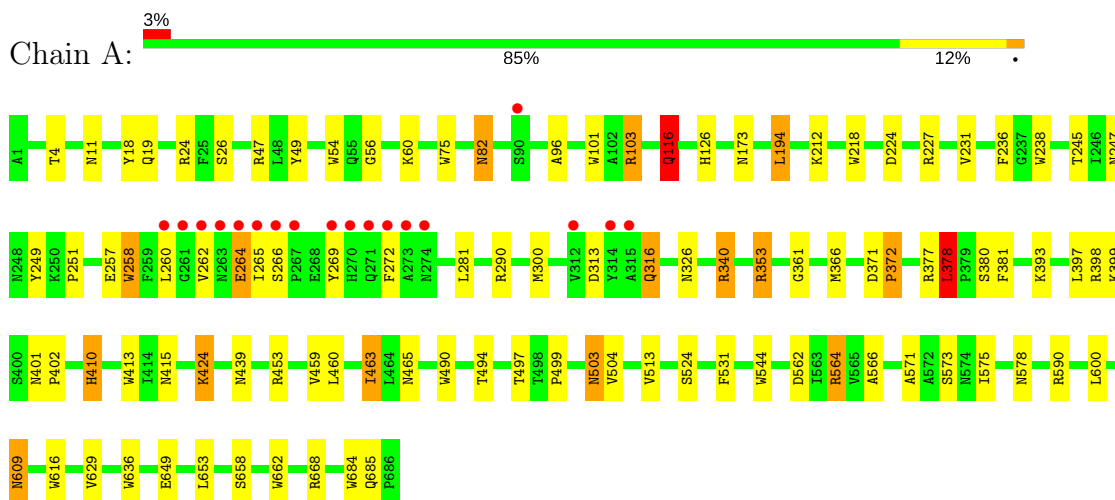
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	267	Total 267	O 267	0	0
7	B	237	Total 237	O 237	0	0

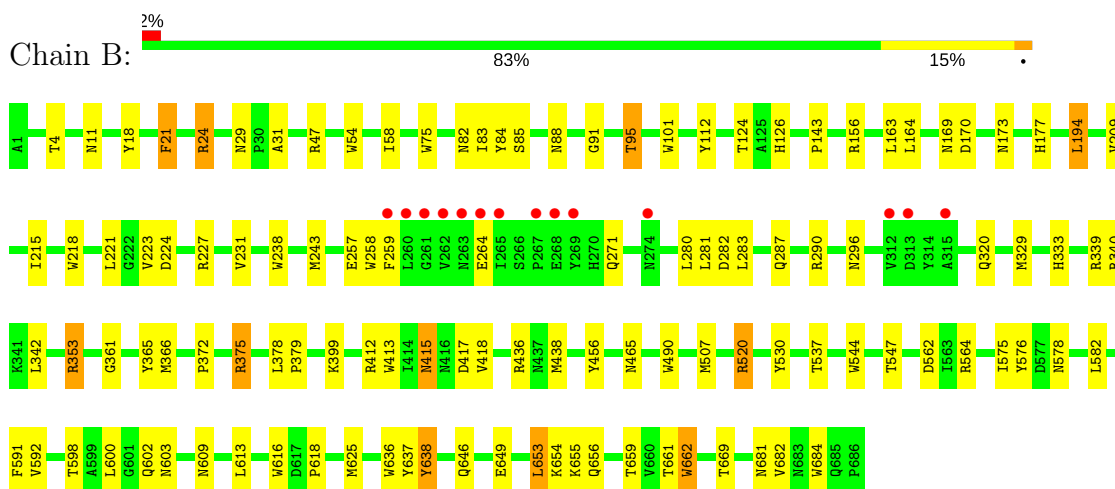
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Cyclomaltodextrin glucanotransferase



#### • Molecule 1: Cyclomaltodextrin glucanotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.97Å 73.71Å 80.08Å 85.47° 105.53° 101.43°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	82.8 (10.00-2.10) 82.8 (10.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.169 , 0.232 0.169 , 0.233	Depositor DCC
$R_{free}$ test set	4087 reflections (6.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 68.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: ACI, GLC, GLD, GAL, CA

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	0.78	0/5442	1.44	64/7424 (0.9%)
1	B	0.76	0/5442	1.44	71/7424 (1.0%)
All	All	0.77	0/10884	1.44	135/14848 (0.9%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	NE-CZ-NH2	-15.04	112.78	120.30
1	A	398	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	A	684	TRP	CD1-CG-CD2	9.77	114.11	106.30
1	A	377	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	A	24	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	B	662	TRP	CD1-CG-CD2	9.55	113.94	106.30
1	A	662	TRP	CD1-CG-CD2	9.10	113.58	106.30
1	B	653	LEU	CA-CB-CG	8.81	135.56	115.30
1	A	684	TRP	CE2-CD2-CG	-8.52	100.48	107.30
1	B	684	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	A	413	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	B	238	TRP	CD1-CG-CD2	8.44	113.05	106.30
1	B	412	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	B	662	TRP	CE2-CD2-CG	-8.24	100.71	107.30
1	B	238	TRP	CE2-CD2-CG	-8.16	100.77	107.30
1	A	616	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	B	490	TRP	CD1-CG-CD2	8.12	112.79	106.30
1	B	258	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	B	413	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	B	564	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	544	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	B	684	TRP	CE2-CD2-CG	-7.72	101.12	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	564	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	544	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	A	413	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	B	238	TRP	CG-CD2-CE3	7.44	140.60	133.90
1	B	218	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	377	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	B	290	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	616	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	B	616	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	218	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	490	TRP	CD1-CG-CD2	7.27	112.12	106.30
1	A	590	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	544	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	B	258	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	A	378	LEU	CA-CB-CG	7.19	131.83	115.30
1	B	616	TRP	CD1-CG-CD2	7.17	112.04	106.30
1	B	413	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	A	662	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	218	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	B	544	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	238	TRP	CD1-CG-CD2	6.96	111.86	106.30
1	B	490	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	B	329	MET	CG-SD-CE	-6.93	89.11	100.20
1	B	54	TRP	CD1-CG-CD2	6.86	111.79	106.30
1	A	101	TRP	CD1-CG-CD2	6.85	111.78	106.30
1	B	227	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	238	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	B	54	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	490	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	75	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	636	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	B	375	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	684	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	B	156	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	258	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B	75	TRP	CD1-CG-CD2	6.66	111.63	106.30
1	B	564	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	B	636	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	103	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	530	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	B	47	ARG	NE-CZ-NH1	6.56	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	TRP	CE2-CD2-CG	-6.40	102.18	107.30
1	B	101	TRP	CD1-CG-CD2	6.38	111.40	106.30
1	A	340	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	258	TRP	CD1-CG-CD2	6.35	111.38	106.30
1	A	75	TRP	CD1-CG-CD2	6.34	111.37	106.30
1	B	238	TRP	CB-CG-CD1	-6.34	118.76	127.00
1	A	54	TRP	CE2-CD2-CG	-6.32	102.24	107.30
1	A	684	TRP	CB-CG-CD1	-6.32	118.79	127.00
1	A	101	TRP	CE2-CD2-CG	-6.31	102.25	107.30
1	A	75	TRP	CG-CD2-CE3	6.28	139.55	133.90
1	B	75	TRP	CE2-CD2-CG	-6.28	102.28	107.30
1	A	249	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	436	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	95	THR	N-CA-CB	-6.20	98.52	110.30
1	A	54	TRP	CD1-CG-CD2	6.16	111.23	106.30
1	B	353	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	684	TRP	CG-CD1-NE1	-6.05	104.05	110.10
1	B	101	TRP	CE2-CD2-CG	-6.02	102.48	107.30
1	B	436	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	24	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	453	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	629	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	A	564	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	238	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	544	TRP	CG-CD2-CE3	5.87	139.18	133.90
1	B	520	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	290	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	B	24	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	636	TRP	CD1-CG-CD2	5.77	110.92	106.30
1	B	662	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	B	47	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	418	VAL	CG1-CB-CG2	-5.59	101.95	110.90
1	B	84	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	576	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	47	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	18	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	B	662	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	A	75	TRP	CA-CB-CG	5.51	124.17	113.70
1	A	662	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	B	21	PHE	N-CA-C	-5.48	96.20	111.00
1	B	413	TRP	CB-CG-CD1	-5.48	119.88	127.00
1	A	18	TYR	CB-CG-CD1	-5.45	117.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	24	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	438	MET	CG-SD-CE	-5.37	91.61	100.20
1	A	316	GLN	CA-CB-CG	5.37	125.20	113.40
1	B	287	GLN	CA-CB-CG	5.36	125.20	113.40
1	B	638	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	B	456	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	B	646	GLN	CA-CB-CG	5.32	125.10	113.40
1	A	238	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	A	531	PHE	N-CA-C	-5.30	96.68	111.00
1	A	424	LYS	CG-CD-CE	-5.30	96.01	111.90
1	A	424	LYS	N-CA-CB	-5.25	101.15	110.60
1	A	227	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	684	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	B	662	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	B	616	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	A	353	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	282	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	684	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	A	116	GLN	CG-CD-NE2	5.16	129.09	116.70
1	A	194	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	112	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	49	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	413	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	B	243	MET	CG-SD-CE	5.09	108.34	100.20
1	A	413	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	A	513	VAL	CG1-CB-CG2	-5.03	102.86	110.90
1	B	218	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	B	616	TRP	CB-CG-CD1	-5.01	120.48	127.00

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	5309	0	5052	37	0
1	B	5309	0	5052	35	0
2	A	11	0	10	0	0
2	B	23	0	21	0	0
3	A	12	0	11	2	0
3	B	12	0	11	0	0
4	A	9	0	9	2	0
4	B	9	0	9	0	0
5	A	12	0	11	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	267	0	0	2	0
7	B	237	0	0	4	0
All	All	11214	0	10186	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:GLU:HG2	1:B:669:THR:HG22	1.69	0.73
3:A:702:ACI:C7	4:A:703:GLD:H63	2.23	0.68
1:A:260:LEU:HD13	1:A:265:ILE:HG13	1.76	0.67
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.76	0.67
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.79	0.63
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.45	0.62
1:B:361:GLY:HA3	1:B:366:MET:SD	2.39	0.62
1:A:116:GLN:HG3	7:A:1402:HOH:O	2.00	0.62
1:A:258:TRP:HB3	1:A:269:TYR:CD2	2.37	0.60
1:A:257:GLU:HB2	1:A:281:LEU:HD12	1.85	0.58
1:B:602:GLN:HG3	1:B:656:GLN:HB2	1.86	0.57
1:B:88:ASN:ND2	1:B:91:GLY:H	2.03	0.57
1:B:280:LEU:HB2	1:B:320:GLN:HE22	1.70	0.57
1:A:564:ARG:HD2	1:A:575:ILE:HD11	1.87	0.56
1:A:361:GLY:HA3	1:A:366:MET:SD	2.45	0.56
1:B:4:THR:HB	1:B:399:LYS:HD2	1.88	0.56
1:B:333:HIS:HD2	7:B:1387:HOH:O	1.90	0.55
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.90	0.53
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.90	0.53
1:B:361:GLY:HA2	1:B:378:LEU:HD13	1.90	0.52
1:B:88:ASN:HD21	1:B:91:GLY:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:HIS:HE1	1:A:424:LYS:HB3	1.74	0.51
1:B:257:GLU:HB2	1:B:281:LEU:HD12	1.92	0.51
1:A:258:TRP:HB3	1:A:269:TYR:HD2	1.75	0.51
1:A:609:ASN:ND2	1:A:649:GLU:H	2.08	0.51
1:A:564:ARG:HD2	1:A:575:ILE:CD1	2.41	0.51
1:B:333:HIS:HE1	7:B:1224:HOH:O	1.92	0.51
1:B:83:ILE:HD12	1:B:85:SER:HB2	1.93	0.50
1:A:260:LEU:HB3	1:A:264:GLU:O	2.12	0.49
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.95	0.49
1:A:410:HIS:CE1	1:A:424:LYS:HB3	2.47	0.49
1:A:247:ASN:HA	1:A:251:PRO:HB3	1.94	0.49
1:B:24:ARG:HD2	1:B:375:ARG:O	2.13	0.49
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.94	0.49
1:B:520:ARG:HD3	1:B:547:THR:HG22	1.94	0.48
3:A:702:ACI:H7	4:A:703:GLD:H63	1.94	0.48
1:A:260:LEU:HD13	1:A:265:ILE:HA	1.96	0.47
1:B:591:PHE:O	1:B:637:TYR:HA	2.14	0.47
1:A:4:THR:HB	1:A:399:LYS:HD2	1.96	0.47
1:A:668:ARG:NH1	1:A:685:GLN:HG3	2.29	0.46
1:A:266:SER:O	1:A:269:TYR:HB3	2.16	0.46
1:A:231:VAL:HB	1:A:272:PHE:CZ	2.51	0.46
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.97	0.46
1:A:393:LYS:HE3	1:A:463:ILE:HD13	1.98	0.45
1:B:126:HIS:HD2	7:B:1342:HOH:O	1.99	0.45
1:B:598:THR:HB	1:B:602:GLN:HB3	1.97	0.45
1:B:603:ASN:O	1:B:654:LYS:HA	2.16	0.45
1:A:460:LEU:O	1:A:463:ILE:HB	2.16	0.45
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.65	0.45
1:B:340:ARG:HH12	1:B:465:ASN:ND2	2.15	0.45
1:A:126:HIS:HE1	1:A:224:ASP:OD2	2.01	0.44
1:A:26:SER:O	1:A:56:GLY:HA3	2.17	0.44
1:A:19:GLN:HE22	1:A:326:ASN:HB2	1.82	0.44
1:A:82:ASN:OD1	1:A:96:ALA:HB1	2.17	0.44
1:A:212:LYS:HB3	1:A:245:THR:HG21	2.00	0.43
1:B:231:VAL:HG22	1:B:257:GLU:O	2.18	0.43
1:B:29:ASN:HD21	1:B:31:ALA:HB3	1.84	0.43
1:A:401:ASN:HA	1:A:402:PRO:HD2	1.89	0.43
1:B:618:PRO:HG3	1:B:662:TRP:CZ2	2.54	0.42
1:A:566:ALA:HA	1:A:571:ALA:O	2.19	0.42
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.74	0.42
1:B:562:ASP:HB3	1:B:575:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HG23	1:B:124:THR:HG21	2.02	0.41
1:B:592:VAL:HB	1:B:681:ASN:HA	2.01	0.41
1:A:300:MET:HB2	1:A:415:ASN:O	2.20	0.41
1:A:371:ASP:HA	1:A:372:PRO:HA	1.81	0.41
1:B:655:LYS:HA	1:B:659:THR:O	2.20	0.41
1:A:11:ASN:ND2	7:A:1278:HOH:O	2.53	0.41
1:B:11:ASN:HB3	7:B:1330:HOH:O	2.19	0.41
1:B:415:ASN:HD22	1:B:417:ASP:H	1.69	0.41
1:B:215:ILE:HA	1:B:215:ILE:HD12	1.81	0.41
1:B:342:LEU:HD23	1:B:365:TYR:CD1	2.56	0.40
1:A:378:LEU:HD11	1:A:381:PHE:CZ	2.56	0.40
1:A:503:ASN:HD22	1:A:504:VAL:H	1.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	684/686 (100%)	664 (97%)	19 (3%)	1 (0%)	53	55
1	B	684/686 (100%)	661 (97%)	23 (3%)	0	100	100
All	All	1368/1372 (100%)	1325 (97%)	42 (3%)	1 (0%)	53	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	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	564/564 (100%)	539 (96%)	25 (4%)	31	30
1	B	564/564 (100%)	533 (94%)	31 (6%)	24	21
All	All	1128/1128 (100%)	1072 (95%)	56 (5%)	27	24

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	103	ARG
1	A	116	GLN
1	A	173	ASN
1	A	194	LEU
1	A	236	PHE
1	A	264	GLU
1	A	313	ASP
1	A	316	GLN
1	A	353	ARG
1	A	372	PRO
1	A	378	LEU
1	A	380	SER
1	A	410	HIS
1	A	439	ASN
1	A	463	ILE
1	A	494	THR
1	A	497	THR
1	A	503	ASN
1	A	524	SER
1	A	578	ASN
1	A	600	LEU
1	A	609	ASN
1	A	653	LEU
1	A	658	SER
1	B	21	PHE
1	B	82	ASN

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Mol	Chain	Res	Type
1	B	95	THR
1	B	143	PRO
1	B	163	LEU
1	B	164	LEU
1	B	169	ASN
1	B	173	ASN
1	B	194	LEU
1	B	209	VAL
1	B	221	LEU
1	B	223	VAL
1	B	259	PHE
1	B	264	GLU
1	B	271	GLN
1	B	283	LEU
1	B	296	ASN
1	B	339	ARG
1	B	353	ARG
1	B	372	PRO
1	B	415	ASN
1	B	507	MET
1	B	537	THR
1	B	578	ASN
1	B	582	LEU
1	B	600	LEU
1	B	609	ASN
1	B	613	LEU
1	B	653	LEU
1	B	661	THR
1	B	682	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	19	GLN
1	A	55	GLN
1	A	59	ASN
1	A	62	ASN
1	A	94	ASN
1	A	126	HIS
1	A	128	HIS
1	A	465	ASN

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Mol	Chain	Res	Type
1	A	503	ASN
1	A	548	GLN
1	A	609	ASN
1	B	11	ASN
1	B	29	ASN
1	B	55	GLN
1	B	59	ASN
1	B	88	ASN
1	B	93	ASN
1	B	116	GLN
1	B	120	ASN
1	B	126	HIS
1	B	177	HIS
1	B	316	GLN
1	B	320	GLN
1	B	333	HIS
1	B	410	HIS
1	B	415	ASN
1	B	465	ASN
1	B	548	GLN
1	B	609	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 carbohydrates in this entry.

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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
2	GLC	A	701	3	11,11,12	1.70	3 (27%)	15,15,17	2.20	7 (46%)
3	ACI	A	702	2,4	10,12,12	2.60	3 (30%)	13,17,17	2.23	4 (30%)
4	GLD	A	703	3,5	9,9,10	2.38	4 (44%)	11,12,14	2.53	3 (27%)
5	GAL	A	704	4	12,12,12	1.64	1 (8%)	17,17,17	1.31	2 (11%)
2	GLC	B	801	3	11,11,12	2.14	5 (45%)	15,15,17	1.86	4 (26%)
3	ACI	B	802	2,4	10,12,12	2.38	2 (20%)	13,17,17	2.27	3 (23%)
4	GLD	B	803	3,2	9,9,10	2.24	3 (33%)	11,12,14	2.64	5 (45%)
2	GLC	B	804	4	12,12,12	1.92	3 (25%)	17,17,17	1.49	5 (29%)

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	A	701	3	-	0/2/19/22	0/1/1/1
3	ACI	A	702	2,4	-	0/2/22/22	0/1/1/1
4	GLD	A	703	3,5	-	0/0/13/16	0/1/1/1
5	GAL	A	704	4	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	B	801	3	-	0/2/19/22	0/1/1/1
3	ACI	B	802	2,4	-	0/2/22/22	0/1/1/1
4	GLD	B	803	3,2	-	0/0/13/16	0/1/1/1
2	GLC	B	804	4	-	0/2/22/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GLC	C4-C3	2.12	1.57	1.52
3	A	702	ACI	O4-C4	2.16	1.46	1.42
3	B	802	ACI	C1-C7	2.23	1.55	1.49
2	B	801	GLC	C4-C3	2.26	1.58	1.52
2	B	804	GLC	C4-C5	2.28	1.57	1.53
2	B	801	GLC	O5-C5	2.31	1.48	1.43
4	A	703	GLD	O5-C1	2.34	1.47	1.43
4	A	703	GLD	O5-C5	2.59	1.48	1.43
2	A	701	GLC	C4-C5	2.80	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GLC	C2-C3	2.99	1.56	1.52
4	B	803	GLD	C1-C2	3.03	1.59	1.52
2	B	801	GLC	C4-C5	3.17	1.59	1.53
4	B	803	GLD	C4-C5	3.22	1.57	1.51
2	A	701	GLC	C1-C2	3.31	1.60	1.52
2	B	804	GLC	C3-C2	3.32	1.60	1.52
5	A	704	GAL	C4-C5	3.52	1.60	1.53
4	A	703	GLD	C4-C3	3.75	1.59	1.52
2	B	804	GLC	C1-C2	3.77	1.61	1.52
2	B	801	GLC	C1-C2	4.05	1.61	1.52
4	B	803	GLD	C3-C2	4.53	1.58	1.52
4	A	703	GLD	C4-C5	4.57	1.60	1.51
3	A	702	ACI	C3-C4	4.62	1.60	1.53
3	A	702	ACI	C7-C5	5.76	1.41	1.32
3	B	802	ACI	C7-C5	6.92	1.42	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	ACI	C2-C1-N1	-4.55	102.15	111.40
3	A	702	ACI	C6-C5-C7	-3.89	113.07	123.17
4	A	703	GLD	O5-C1-C2	-3.64	105.10	110.78
3	A	702	ACI	C2-C3-C4	-3.51	105.15	110.41
2	A	701	GLC	C3-C4-C5	-3.49	103.99	110.24
2	B	801	GLC	O2-C2-C3	-3.03	104.28	110.19
4	B	803	GLD	C3-C4-C5	-2.90	106.78	111.27
3	B	802	ACI	O4-C4-C3	-2.64	105.02	110.39
2	A	701	GLC	O2-C2-C3	-2.47	105.38	110.19
2	B	804	GLC	C3-C4-C5	-2.37	106.00	110.24
4	B	803	GLD	O5-C5-C4	-2.34	106.92	109.34
2	A	701	GLC	C2-C3-C4	-2.26	106.93	110.87
2	A	701	GLC	O5-C5-C4	-2.19	105.49	110.83
2	B	804	GLC	O2-C2-C3	-2.17	105.27	110.34
2	A	701	GLC	C1-O5-C5	2.00	114.94	112.19
2	B	804	GLC	O5-C1-C2	2.11	114.11	110.31
5	A	704	GAL	C4-C3-C2	2.20	114.69	110.83
2	B	804	GLC	O4-C4-C5	2.23	114.88	109.31
4	B	803	GLD	O3-C3-C2	2.64	115.99	110.20
5	A	704	GAL	O5-C5-C4	2.77	114.77	109.69
2	B	801	GLC	C1-O5-C5	2.97	116.27	112.19
2	A	701	GLC	O5-C1-C2	2.99	115.44	110.78
2	B	804	GLC	C1-C2-C3	3.14	116.63	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ACI	O3-C3-C4	3.26	115.47	109.56
2	B	801	GLC	C1-C2-C3	3.31	113.85	109.66
2	B	801	GLC	O2-C2-C1	3.33	115.89	109.17
2	A	701	GLC	C1-C2-C3	3.34	113.89	109.66
4	A	703	GLD	C1-O5-C5	3.65	116.87	111.63
3	A	702	ACI	C7-C1-N1	4.00	118.14	110.83
4	B	803	GLD	O5-C1-C2	4.18	117.30	110.78
3	B	802	ACI	C7-C1-N1	5.26	120.45	110.83
4	B	803	GLD	C1-O5-C5	5.31	119.25	111.63
4	A	703	GLD	O2-C2-C1	5.76	120.79	109.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	704	GAL	C4

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ACI	2	0
4	A	703	GLD	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

### 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	686/686 (100%)	-0.61	18 (2%) 56 62	4, 14, 35, 88	0
1	B	686/686 (100%)	-0.54	14 (2%) 65 69	6, 17, 44, 84	0
All	All	1372/1372 (100%)	-0.57	32 (2%) 60 65	4, 15, 43, 88	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	ILE	13.2
1	A	267	PRO	12.3
1	A	266	SER	9.5
1	A	263	ASN	6.6
1	A	269	TYR	6.1
1	A	271	GLN	5.5
1	A	260	LEU	5.5
1	B	267	PRO	5.5
1	A	270	HIS	5.1
1	A	261	GLY	4.9
1	A	262	VAL	4.7
1	B	265	ILE	4.5
1	A	312	VAL	4.3
1	B	263	ASN	4.3
1	A	315	ALA	3.8
1	A	264	GLU	3.4
1	B	260	LEU	3.4
1	B	262	VAL	3.2
1	B	269	TYR	3.1
1	A	274	ASN	2.9
1	B	264	GLU	2.8
1	A	273	ALA	2.6
1	B	261	GLY	2.4
1	B	315	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	272	PHE	2.3
1	A	314	TYR	2.3
1	A	90	SER	2.3
1	B	312	VAL	2.2
1	B	268	GLU	2.1
1	B	259	PHE	2.1
1	B	313	ASP	2.0
1	B	274	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
4	GLD	A	703	9/10	0.66	0.45	15,26,34,35	0
3	ACI	A	702	12/12	0.69	0.43	8,25,32,33	0
2	GLC	B	801	11/12	0.71	0.46	18,23,32,37	0
3	ACI	B	802	12/12	0.78	0.40	15,20,32,41	0
5	GAL	A	704	12/12	0.81	0.50	16,25,35,37	0
4	GLD	B	803	9/10	0.81	0.39	17,23,35,36	0
2	GLC	B	804	12/12	0.81	0.47	15,24,29,36	0
2	GLC	A	701	11/12	0.83	0.36	7,19,29,37	0
6	CA	A	688	1/1	0.93	0.12	21,21,21,21	0
6	CA	A	687	1/1	0.95	0.07	9,9,9,9	0
6	CA	B	690	1/1	0.96	0.06	26,26,26,26	0
6	CA	B	689	1/1	0.97	0.06	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.