WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1UKQ
Title : Crystal structure of cyclodextrin glucanotransferase complexed with a pseudo-maltotetraose derived from acarbose
Authors : Haga, K.; Kanai, R.; Sakamoto, O.; Harata, K.; Yamane, K.
Deposited on : 2003-09-01
Resolution : 2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
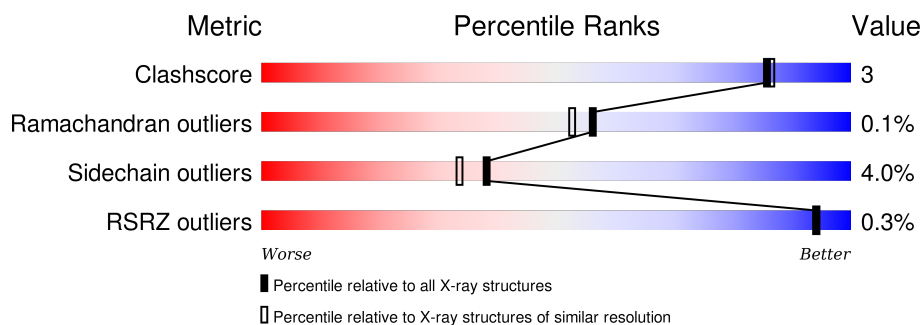Validation Pipeline (wwPDB-VP) : trunk26865

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 2.00 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		4.0%
RSRZ outliers		0.3%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 >=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 <=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	85% 13% •
1	B	686	86% 12% •

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	A	701	-	-	-	X
2	ACI	A	702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G6D	A	703	-	-	-	X
3	GLC	B	705	-	-	-	X
3	ACI	B	706	-	-	-	X
3	G6D	B	707	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11354 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 5312	C 3354	N 906	O 1036	S 16	0	0	0
1	B	686	Total 5312	C 3354	N 906	O 1036	S 16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total 44	C 25	N 1	O 18	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total 44	C 25	N 1	O 18	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	339	Total O 339 339	0	0
5	B	299	Total O 299 299	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 errors 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
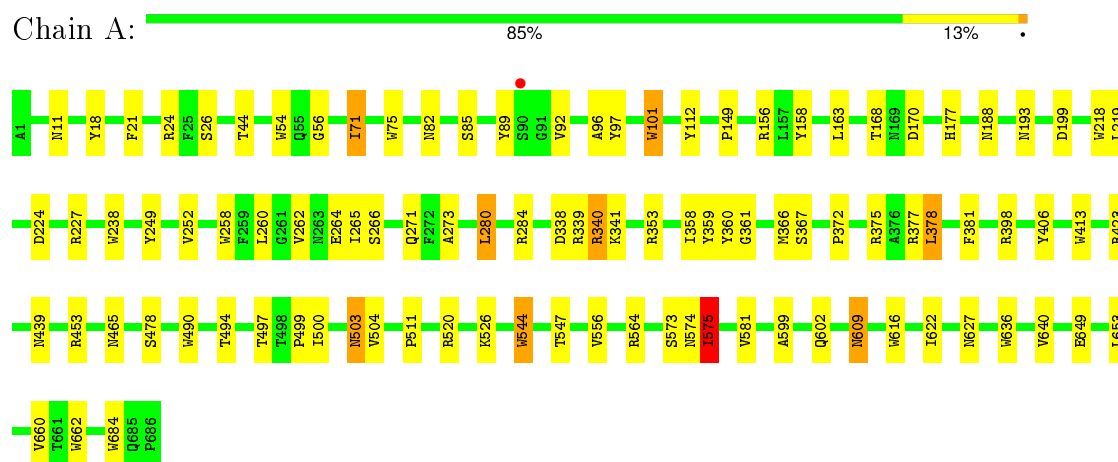
• Molecule 1: Cyclomaltodextrin glucanotransferase
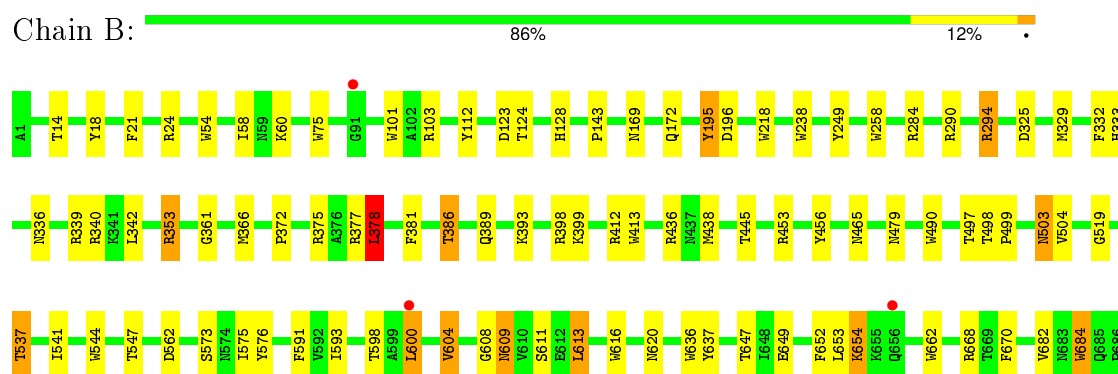
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.94Å 74.49Å 79.10Å 85.13° 105.02° 101.02°	Depositor
Resolution (Å)	10.00 – 2.00 48.54 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.0 (10.00-2.00) 94.9 (48.54-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.246 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 91145 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11354	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ACI, BGC, CA, G6D

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	0.81	0/5446	1.47	73/7429 (1.0%)
1	B	0.80	0/5446	1.44	64/7429 (0.9%)
All	All	0.81	0/10892	1.46	137/14858 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	ARG	NE-CZ-NH2	-18.14	111.23	120.30
1	A	398	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	A	112	TYR	CB-CG-CD2	-12.22	113.67	121.00
1	B	662	TRP	CD1-CG-CD2	9.58	113.97	106.30
1	B	490	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	662	TRP	CD1-CG-CD2	9.05	113.54	106.30
1	A	75	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	B	375	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	112	TYR	CB-CG-CD1	8.35	126.01	121.00
1	A	54	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	A	284	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	B	684	TRP	CD1-CG-CD2	8.27	112.91	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	TRP	CD1-CG-CD2	8.26	112.90	106.30
1	B	636	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	B	413	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	B	436	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	436	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	284	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	662	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	218	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	339	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	A	218	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	A	101	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	A	636	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	B	413	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	B	490	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	B	616	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	490	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	B	112	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	A	413	TRP	CD1-CG-CD2	7.48	112.29	106.30
1	A	636	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	A	684	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	B	684	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	B	75	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	662	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	544	TRP	CD1-CG-CD2	7.32	112.16	106.30
1	A	413	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	B	456	TYR	CB-CG-CD1	-7.29	116.62	121.00
1	B	616	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	A	544	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	B	453	ARG	CB-CG-CD	-7.14	93.03	111.60
1	B	636	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	B	218	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	B	353	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	616	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	616	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	75	TRP	CE2-CD2-CG	-6.98	101.71	107.30
1	A	218	TRP	CG-CD2-CE3	6.92	140.13	133.90
1	A	238	TRP	CE2-CD2-CG	-6.91	101.78	107.30
1	A	490	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	A	271	GLN	CA-CB-CG	6.87	128.52	113.40
1	A	684	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	B	258	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	B	294	ARG	NE-CZ-NH1	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	TRP	CD1-CG-CD2	6.74	111.69	106.30
1	B	54	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B	218	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	A	238	TRP	CD1-CG-CD2	6.56	111.55	106.30
1	B	541	ILE	N-CA-C	-6.53	93.37	111.00
1	B	101	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	A	564	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	A	101	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	75	TRP	CG-CD1-NE1	-6.47	103.62	110.10
1	B	75	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	A	54	TRP	CE2-CD2-CG	-6.44	102.15	107.30
1	A	249	TYR	CB-CG-CD2	-6.44	117.14	121.00
1	A	340	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	238	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	B	258	TRP	CE2-CD2-CG	-6.31	102.25	107.30
1	A	375	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	375	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	54	TRP	CD1-CG-CD2	6.24	111.30	106.30
1	B	290	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	B	544	TRP	CD1-CG-CD2	6.07	111.15	106.30
1	A	92	VAL	CA-CB-CG1	-6.06	101.81	110.90
1	A	75	TRP	CG-CD2-CE3	6.06	139.35	133.90
1	A	575	ILE	CA-CB-CG1	-6.04	99.52	111.00
1	B	544	TRP	CE2-CD2-CG	-5.98	102.51	107.30
1	A	218	TRP	CB-CG-CD1	-5.97	119.23	127.00
1	A	156	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	377	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	B	294	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	604	VAL	CG1-CB-CG2	-5.82	101.60	110.90
1	B	103	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	662	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	B	325	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	24	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	258	TRP	CD1-CG-CD2	5.73	110.88	106.30
1	A	636	TRP	CG-CD2-CE3	5.73	139.06	133.90
1	A	238	TRP	CG-CD2-CE3	5.68	139.02	133.90
1	B	537	THR	N-CA-CB	-5.65	99.56	110.30
1	A	258	TRP	CE2-CD2-CG	-5.63	102.80	107.30
1	A	406	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	B	438	MET	CG-SD-CE	-5.57	91.29	100.20
1	A	359	TYR	CB-CG-CD2	-5.53	117.69	121.00
1	A	54	TRP	CG-CD1-NE1	-5.50	104.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	238	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	227	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	24	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	18	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	89	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	423	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	398	ARG	CG-CD-NE	-5.41	100.44	111.80
1	B	238	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	A	662	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	B	398	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	412	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	218	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	A	490	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	A	377	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	423	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	576	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	660	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	A	158	TYR	CB-CG-CD2	-5.33	117.81	121.00
1	A	101	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	284	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	339	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	453	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	101	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	B	249	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	B	490	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	A	544	TRP	CG-CD2-CE3	5.20	138.57	133.90
1	B	218	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	A	238	TRP	CB-CG-CD1	-5.17	120.28	127.00
1	B	668	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	265	ILE	N-CA-C	-5.12	97.17	111.00
1	A	339	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	684	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	B	378	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	B	329	MET	CG-SD-CE	-5.06	92.10	100.20
1	A	413	TRP	CB-CG-CD1	-5.05	120.44	127.00
1	A	360	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	375	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	156	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	103	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	238	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	258	TRP	N-CA-C	-5.02	97.46	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	TYR	Sidechain
1	B	195	TYR	Sidechain

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	5312	0	5050	29	0
1	B	5312	0	5050	28	0
2	A	44	0	40	1	0
3	B	44	0	40	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	339	0	0	3	0
5	B	299	0	0	0	0
All	All	11354	0	10180	59	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 3.

All (59) 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:18:TYR:HB2	1:A:71:ILE:HG12	1.67	0.76
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.45	0.64
1:A:149:PRO:HG3	1:A:168:THR:HG21	1.79	0.63
1:A:11:ASN:ND2	5:A:1441:HOH:O	2.31	0.62
1:A:599:ALA:H	1:A:602:GLN:HE21	1.47	0.60
1:B:389:GLN:O	1:B:393:LYS:HG2	2.06	0.55
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.90	0.54
1:A:273:ALA:HB2	1:A:280:LEU:HD22	1.92	0.52
1:B:593:ILE:HD11	1:B:684:TRP:HA	1.92	0.52
1:A:520:ARG:HG2	1:A:520:ARG:HH21	1.75	0.52
3:B:707:G6D:H1	3:B:708:GLC:O3	2.09	0.52
1:A:26:SER:O	1:A:56:GLY:HA3	2.09	0.51

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.59	0.51
1:A:609:ASN:ND2	1:A:649:GLU:H	2.09	0.51
1:A:82:ASN:ND2	1:A:101:TRP:H	2.09	0.50
1:B:445:THR:HG22	1:B:479:ASN:ND2	2.26	0.50
1:A:503:ASN:HD22	1:A:504:VAL:H	1.58	0.50
1:A:361:GLY:HA3	1:A:366:MET:SD	2.51	0.50
1:A:82:ASN:HD22	1:A:96:ALA:HB1	1.76	0.49
2:A:702:ACI:C7	2:A:703:G6D:HC63	2.42	0.49
1:A:71:ILE:HD11	1:A:358:ILE:HD12	1.95	0.48
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.49	0.48
1:B:593:ILE:HG21	1:B:604:VAL:HG11	1.96	0.48
1:A:338:ASP:HB3	1:A:341:LYS:HD3	1.96	0.47
1:B:608:GLY:HA3	1:B:613:LEU:HD23	1.96	0.47
1:A:260:LEU:HD22	1:A:264:GLU:HG2	1.96	0.47
1:B:598:THR:HG22	1:B:654:LYS:HD2	1.95	0.47
1:B:124:THR:O	1:B:128:HIS:HD2	1.98	0.47
1:B:386:THR:HA	1:B:389:GLN:HG3	1.97	0.47
1:B:609:ASN:ND2	1:B:649:GLU:H	2.13	0.46
1:B:499:PRO:HB2	1:B:573:SER:HB3	1.98	0.46
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.51	0.46
1:A:575:ILE:HD12	1:B:575:ILE:HD11	1.97	0.46
1:A:599:ALA:N	1:A:602:GLN:HE21	2.14	0.46
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.97	0.46
1:B:378:LEU:HD21	1:B:381:PHE:CE1	2.51	0.45
1:B:195:TYR:HE2	3:B:707:G6D:HC61	1.81	0.45
1:B:58:ILE:HG23	1:B:124:THR:HG21	2.00	0.44
1:B:562:ASP:HB3	1:B:575:ILE:HG23	1.99	0.43
1:A:520:ARG:HD3	1:A:547:THR:HG22	2.00	0.43
1:B:294:ARG:HB2	1:B:332:PHE:CZ	2.52	0.43
1:B:503:ASN:HD22	1:B:504:VAL:H	1.66	0.43
1:B:333:HIS:HB2	1:B:342:LEU:HD22	2.01	0.43
3:B:706:ACI:C7	3:B:707:G6D:C6A	2.97	0.43
1:B:361:GLY:HA3	1:B:366:MET:SD	2.59	0.43
1:B:519:GLY:O	1:B:547:THR:HA	2.19	0.42
1:A:193:ASN:HD22	1:A:199:ASP:HB2	1.84	0.42
1:A:556:VAL:HG23	1:A:581:VAL:HG11	2.01	0.42
1:B:14:THR:HB	1:B:399:LYS:HD3	2.02	0.41
1:A:149:PRO:HD2	5:A:1261:HOH:O	2.21	0.41
1:A:622:ILE:HG21	1:A:640:VAL:HG22	2.02	0.41
1:A:574:ASN:HA	5:A:1378:HOH:O	2.19	0.41
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:O	1:A:252:VAL:HB	2.21	0.41
1:B:591:PHE:O	1:B:637:TYR:HA	2.21	0.41
1:B:143:PRO:HB3	1:B:196:ASP:OD1	2.20	0.40
1:B:652:PHE:HE2	1:B:682:VAL:HG11	1.86	0.40
1:A:526:LYS:HA	1:A:544:TRP:CG	2.56	0.40
1:B:647:THR:HA	1:B:670:PHE:O	2.21	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	684/686 (100%)	664 (97%)	20 (3%)	0	100	100
1	B	684/686 (100%)	660 (96%)	23 (3%)	1 (0%)	56	53
All	All	1368/1372 (100%)	1324 (97%)	43 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU

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	564/564 (100%)	539 (96%)	25 (4%)	35	30
1	B	564/564 (100%)	544 (96%)	20 (4%)	43	40
All	All	1128/1128 (100%)	1083 (96%)	45 (4%)	38	33

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	44	THR
1	A	71	ILE
1	A	85	SER
1	A	163	LEU
1	A	188	ASN
1	A	219	LEU
1	A	262	VAL
1	A	266	SER
1	A	280	LEU
1	A	353	ARG
1	A	367	SER
1	A	372	PRO
1	A	378	LEU
1	A	439	ASN
1	A	478	SER
1	A	494	THR
1	A	497	THR
1	A	500	ILE
1	A	503	ASN
1	A	511	PRO
1	A	575	ILE
1	A	609	ASN
1	A	627	ASN
1	A	653	LEU
1	B	21	PHE
1	B	123	ASP
1	B	169	ASN
1	B	172	GLN
1	B	336	ASN
1	B	353	ARG
1	B	372	PRO
1	B	378	LEU
1	B	386	THR
1	B	497	THR

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Mol	Chain	Res	Type
1	B	498	THR
1	B	503	ASN
1	B	537	THR
1	B	600	LEU
1	B	609	ASN
1	B	611	SER
1	B	613	LEU
1	B	620	ASN
1	B	653	LEU
1	B	654	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	82	ASN
1	A	94	ASN
1	A	126	HIS
1	A	177	HIS
1	A	188	ASN
1	A	193	ASN
1	A	333	HIS
1	A	465	ASN
1	A	503	ASN
1	A	548	GLN
1	A	602	GLN
1	A	609	ASN
1	A	627	ASN
1	B	55	GLN
1	B	59	ASN
1	B	120	ASN
1	B	128	HIS
1	B	129	ASN
1	B	140	HIS
1	B	173	ASN
1	B	439	ASN
1	B	465	ASN
1	B	479	ASN
1	B	503	ASN
1	B	609	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5　Carbohydrates ⓘ

8 carbohydrates 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	A	701	2	12,12,12	1.80	4 (33%)	17,17,17	2.18	5 (29%)
2	ACI	A	702	2	10,11,12	2.04	4 (40%)	8,15,17	1.81	3 (37%)
2	G6D	A	703	2	10,10,11	2.07	5 (50%)	13,14,16	2.12	4 (30%)
2	BGC	A	704	2	11,11,12	1.83	3 (27%)	15,15,17	1.71	5 (33%)
3	GLC	B	705	3	12,12,12	1.80	4 (33%)	17,17,17	1.74	4 (23%)
3	ACI	B	706	3	10,11,12	1.39	2 (20%)	8,15,17	1.41	2 (25%)
3	G6D	B	707	3	10,10,11	2.33	4 (40%)	13,14,16	2.04	3 (23%)
3	GLC	B	708	3	11,11,12	3.42	5 (45%)	15,15,17	2.14	5 (33%)

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	2	-	0/2/22/22	0/1/1/1
2	ACI	A	702	2	-	0/1/18/22	0/1/1/1
2	G6D	A	703	2	-	0/0/16/20	0/1/1/1
2	BGC	A	704	2	-	0/2/18/22	0/1/1/1
3	GLC	B	705	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACI	B	706	3	-	0/1/18/22	0/1/1/1
3	G6D	B	707	3	-	0/0/16/20	0/1/1/1
3	GLC	B	708	3	-	0/2/18/22	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GLC	C4-C5	2.06	1.57	1.53
3	B	705	GLC	C4-C5	2.07	1.57	1.53
3	B	706	ACI	C7-C5	2.08	1.41	1.33
2	A	704	BGC	C6-C5	2.11	1.56	1.50
2	A	701	GLC	O5-C1	2.14	1.47	1.43
3	B	707	G6D	O5-C1	2.19	1.47	1.43
2	A	703	G6D	C1-C2	2.26	1.57	1.52
2	A	702	ACI	C1-C7	2.35	1.55	1.49
2	A	702	ACI	C7-C5	2.39	1.42	1.33
2	A	703	G6D	O5-C1	2.47	1.47	1.43
3	B	707	G6D	O1-C1	2.47	1.48	1.39
2	A	703	G6D	C4A-C3A	2.52	1.56	1.52
2	A	703	G6D	C4A-C5A	2.58	1.56	1.51
3	B	705	GLC	O1-C1	2.59	1.48	1.39
2	A	701	GLC	C4-C3	2.77	1.59	1.52
3	B	706	ACI	C4-C5	2.78	1.56	1.50
2	A	704	BGC	C4-C5	2.78	1.60	1.52
3	B	707	G6D	C3A-C2	2.82	1.56	1.52
3	B	705	GLC	C3-C2	2.83	1.59	1.52
3	B	708	GLC	C6-C5	2.93	1.58	1.50
2	A	702	ACI	C6-C5	3.21	1.56	1.51
3	B	708	GLC	C4-C5	3.39	1.61	1.52
2	A	701	GLC	C1-C2	3.45	1.59	1.52
2	A	703	G6D	C3A-C2	3.64	1.57	1.52
3	B	708	GLC	C4-C3	3.64	1.58	1.52
2	A	702	ACI	C4-C5	3.78	1.58	1.50
3	B	705	GLC	C1-C2	4.00	1.60	1.52
2	A	704	BGC	C4-C3	4.08	1.59	1.52
3	B	708	GLC	C1-C2	4.82	1.62	1.52
3	B	707	G6D	C1-C2	5.36	1.63	1.52
3	B	708	GLC	C3-C2	8.03	1.63	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	G6D	O5-C1-C2	-3.67	103.94	109.80
2	A	701	GLC	C1-C2-C3	-3.34	105.47	110.43
2	A	704	BGC	O3-C3-C2	-2.96	104.17	110.12
2	A	703	G6D	C4A-C3A-C2	-2.94	106.56	110.56
2	A	701	GLC	C3-C4-C5	-2.90	105.14	110.20
3	B	707	G6D	O2-C2-C3A	-2.84	104.87	110.00
3	B	706	ACI	C2-C1-N1	-2.84	105.63	111.40
3	B	708	GLC	C3-C4-C5	-2.78	105.77	111.40
2	A	703	G6D	C1-C2-C3A	-2.75	106.34	110.43
3	B	705	GLC	O3-C3-C4	-2.32	105.12	110.34
3	B	705	GLC	O6-C6-C5	-2.21	104.04	111.33
2	A	704	BGC	O5-C1-C2	-2.18	106.32	109.80
2	A	704	BGC	C4-C3-C2	-2.17	107.61	110.56
2	A	702	ACI	C2-C1-N1	-2.07	107.19	111.40
2	A	704	BGC	O3-C3-C4	2.09	115.17	110.06
3	B	708	GLC	O1-C1-C2	2.13	114.91	109.21
3	B	706	ACI	O3-C3-C4	2.13	114.71	109.73
2	A	702	ACI	O6-C6-C5	2.27	116.58	111.75
2	A	702	ACI	C3-C4-C5	2.71	116.21	111.83
3	B	705	GLC	C1-C2-C3	3.01	114.91	110.43
2	A	701	GLC	C6-C5-C4	3.13	120.73	113.02
3	B	707	G6D	O1-C1-C2	3.23	117.87	109.21
3	B	705	GLC	O5-C1-C2	3.43	115.28	109.80
2	A	704	BGC	C4-C5-C6	3.56	118.93	112.38
3	B	708	GLC	C1-C2-C3	3.61	115.79	110.43
3	B	708	GLC	C1-O5-C5	3.77	120.41	113.47
2	A	701	GLC	C1-O5-C5	4.10	121.06	113.47
3	B	708	GLC	O5-C1-C2	4.17	116.46	109.80
2	A	703	G6D	O2-C2-C1	4.52	119.77	109.82
2	A	701	GLC	O5-C1-C2	4.59	117.12	109.80
3	B	707	G6D	O2-C2-C1	5.40	121.71	109.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	ACI	1	0
2	A	703	G6D	1	0
3	B	706	ACI	1	0
3	B	707	G6D	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	708	GLC	1	0

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	686/686 (100%)	-0.42	1 (0%)	95	95	5, 13, 25, 40	0
1	B	686/686 (100%)	-0.28	3 (0%)	93	93	7, 17, 33, 46	0
All	All	1372/1372 (100%)	-0.35	4 (0%)	94	94	5, 15, 30, 46	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	2.5
1	A	90	SER	2.4
1	B	656	GLN	2.1
1	B	91	GLY	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	GLC	A	701	12/12	0.60	0.61	23.77	15,23,27,30	0
3	GLC	B	705	12/12	0.49	0.80	22.71	19,26,30,31	0
2	ACI	A	702	11/12	0.62	0.54	22.28	20,24,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	G6D	A	703	10/11	0.56	0.55	20.67	20,25,31,31	0
3	G6D	B	707	10/11	0.53	0.70	20.55	19,23,29,32	0
3	ACI	B	706	11/12	0.61	0.51	20.44	18,23,28,30	0
2	BGC	A	704	11/12	0.66	0.46	-	17,23,26,28	0
3	GLC	B	708	11/12	0.48	0.53	-	20,26,29,32	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	CA	A	688	1/1	0.92	0.09	-0.10	17,17,17,17	0
4	CA	B	690	1/1	0.94	0.08	-1.12	18,18,18,18	0
4	CA	A	687	1/1	0.97	0.05	-2.18	9,9,9,9	0
4	CA	B	689	1/1	0.97	0.05	-2.80	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.