



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:38 PM GMT

PDB ID : 1UKS
Title : Crystal structure of F183L/F259L mutant 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 : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

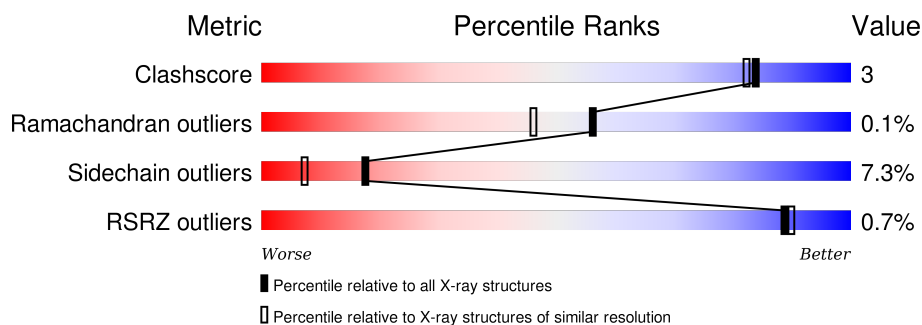
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. 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></div> <div>84%</div> <div>14%</div> <div></div> </div>
1	B	686	<div> <div></div> <div>83%</div> <div>14%</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	A	701	-	-	-	X
2	ACI	A	702	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLD	A	703	-	-	-	X
2	GAL	A	704	X	-	-	X
2	ACI	B	706	-	-	-	X
2	GLD	B	707	-	-	-	X
2	GAL	B	708	X	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11443 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 Cyclomalto-dextrin glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5306	3348	906	1036	16			
1	B	686	Total	C	N	O	S	0	0	0
			5306	3348	906	1036	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	LEU	PHE	ENGINEERED	UNP P05618
A	259	LEU	PHE	ENGINEERED	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	183	LEU	PHE	ENGINEERED	UNP P05618
B	259	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 a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

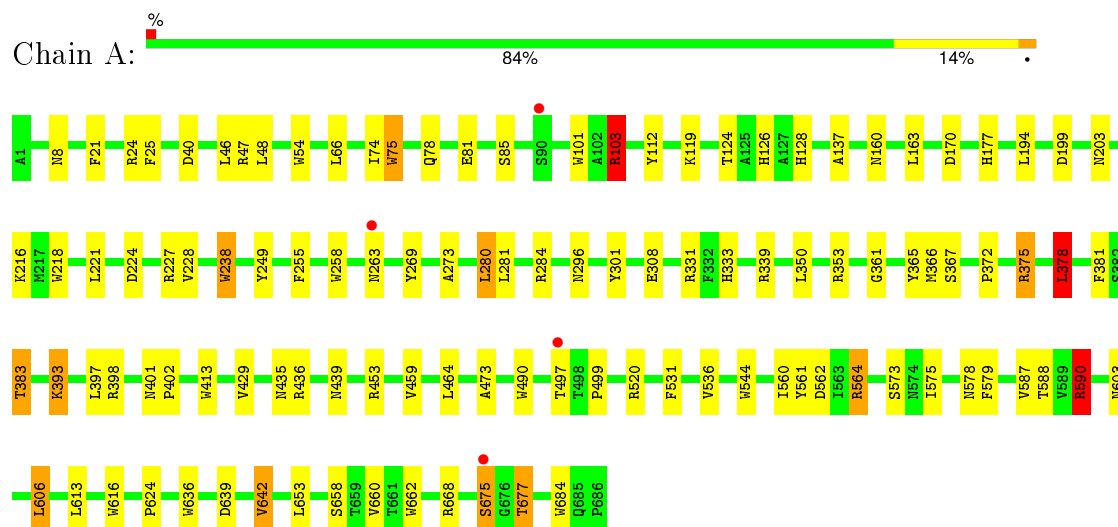
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	386	Total 386	O 386	0	0
4	B	353	Total 353	O 353	0	0

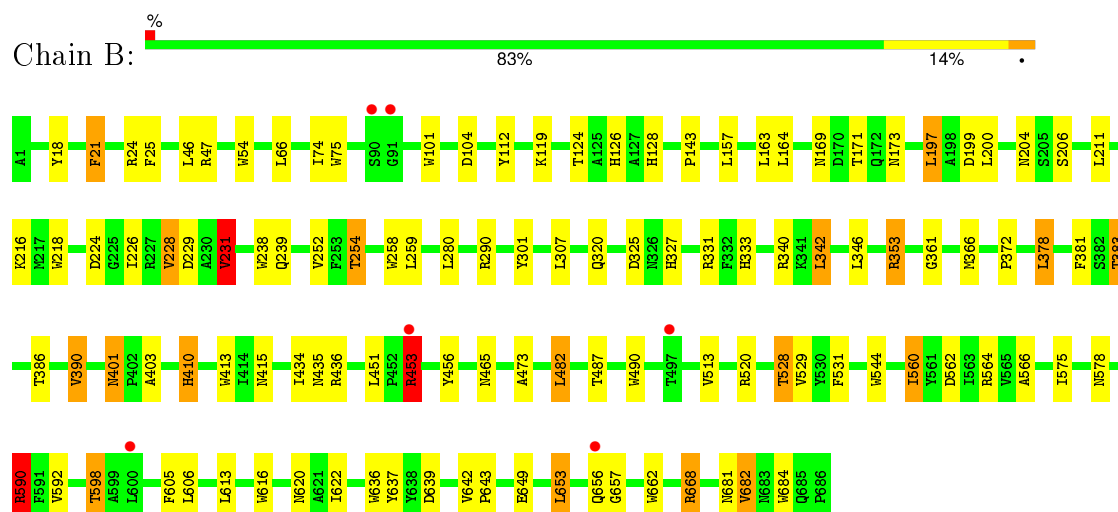
3 Residue-property plots [i](#)

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: Cyclomalto-dextrin glucanotransferase



• Molecule 1: Cyclomalto-dextrin glucanotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.85Å 74.53Å 78.94Å 85.19° 104.86° 101.04°	Depositor
Resolution (Å)	10.00 – 1.90 19.62 – 1.86	Depositor EDS
% Data completeness (in resolution range)	78.3 (10.00-1.90) 88.2 (19.62-1.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.86Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.162 , 0.215 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 103620 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11443	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.76	0/5438	1.43	67/7419 (0.9%)
1	B	0.76	0/5438	1.42	68/7419 (0.9%)
All	All	0.76	0/10876	1.43	135/14838 (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
2	A	1	0
2	B	1	0
All	All	2	0

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	668	ARG	NE-CZ-NH1	-19.39	110.60	120.30
1	B	331	ARG	NE-CZ-NH2	-16.42	112.09	120.30
1	A	668	ARG	NE-CZ-NH2	15.78	128.19	120.30
1	B	331	ARG	NE-CZ-NH1	14.11	127.35	120.30
1	A	331	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	331	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	B	520	ARG	NE-CZ-NH2	11.89	126.25	120.30
1	B	590	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	A	375	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	590	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	375	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	A	590	ARG	NE-CZ-NH2	-9.69	115.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	A	662	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	B	490	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	A	284	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	B	238	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	A	284	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	590	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	B	290	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	B	662	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	B	616	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	B	684	TRP	CD1-CG-CD2	7.96	112.66	106.30
1	B	238	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	B	112	TYR	CB-CG-CD2	-7.81	116.32	121.00
1	B	413	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	B	616	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	490	TRP	CD1-CG-CD2	7.71	112.46	106.30
1	B	544	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	B	490	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	A	662	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	B	684	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	A	54	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	B	662	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	75	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	616	TRP	CD1-CG-CD2	7.52	112.31	106.30
1	A	413	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	B	353	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	436	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	413	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	249	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	54	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	218	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	490	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	398	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	684	TRP	CE2-CD2-CG	-7.26	101.50	107.30
1	A	218	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	544	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	A	684	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	B	636	TRP	CD1-CG-CD2	7.17	112.04	106.30
1	B	75	TRP	CD1-CG-CD2	7.16	112.03	106.30
1	A	238	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	B	258	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	A	103	ARG	NE-CZ-NH2	-7.12	116.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	TRP	CD1-CG-CD2	7.08	111.97	106.30
1	B	636	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B	218	TRP	CD1-CG-CD2	7.06	111.95	106.30
1	A	216	LYS	CB-CG-CD	-7.05	93.27	111.60
1	B	544	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	616	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	101	TRP	CD1-CG-CD2	6.94	111.86	106.30
1	A	636	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	B	101	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	A	238	TRP	CD1-CG-CD2	6.87	111.80	106.30
1	A	564	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	B	564	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	413	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	B	637	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	A	544	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	B	436	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	75	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	A	258	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	B	24	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	606	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	47	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	218	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	A	383	THR	N-CA-CB	-6.50	97.94	110.30
1	B	75	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	B	231	VAL	N-CA-CB	-6.45	97.32	111.50
1	A	101	TRP	CE2-CD2-CG	-6.43	102.15	107.30
1	A	112	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	A	103	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	668	ARG	CG-CD-NE	-6.30	98.57	111.80
1	A	47	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	682	VAL	N-CA-CB	-6.23	97.80	111.50
1	B	598	THR	N-CA-CB	-6.18	98.56	110.30
1	B	383	THR	N-CA-CB	-6.12	98.67	110.30
1	B	101	TRP	CE2-CD2-CG	-6.06	102.45	107.30
1	B	413	TRP	CB-CG-CD1	-6.02	119.17	127.00
1	A	301	TYR	CB-CG-CD2	-6.01	117.40	121.00
1	B	54	TRP	CE2-CD2-CG	-5.99	102.51	107.30
1	B	456	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	A	398	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	199	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	47	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	616	TRP	CG-CD2-CE3	5.86	139.17	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	TRP	CD1-CG-CD2	5.84	110.98	106.30
1	B	325	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	258	TRP	CE2-CD2-CG	-5.82	102.65	107.30
1	B	216	LYS	CB-CG-CD	-5.79	96.55	111.60
1	B	616	TRP	CB-CG-CD1	-5.75	119.52	127.00
1	B	238	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	A	675	SER	C-N-CA	5.69	134.24	122.30
1	A	662	TRP	CG-CD1-NE1	-5.67	104.44	110.10
1	B	453	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	54	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	A	24	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	684	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	A	561	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	436	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	290	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	413	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	A	378	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	B	18	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	B	668	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	B	258	TRP	CE2-CD2-CG	-5.33	103.03	107.30
1	B	238	TRP	CG-CD2-CE3	5.33	138.69	133.90
1	A	24	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	531	PHE	N-CA-C	-5.30	96.70	111.00
1	A	75	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	B	342	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	301	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	B	104	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	258	TRP	N-CA-C	-5.21	96.92	111.00
1	A	393	LYS	CA-CB-CG	5.20	124.84	113.40
1	A	675	SER	N-CA-C	5.14	124.88	111.00
1	B	75	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	B	531	PHE	N-CA-C	-5.07	97.30	111.00
1	A	218	TRP	CG-CD2-CE3	5.07	138.46	133.90
1	A	642	VAL	N-CA-CB	-5.06	100.38	111.50
1	A	269	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	194	LEU	CA-CB-CG	5.03	126.88	115.30
1	B	490	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	B	662	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	B	662	TRP	CG-CD2-CE3	5.01	138.41	133.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	704	GAL	C4
2	B	708	GAL	C4

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	5306	0	5054	32	0
1	B	5306	0	5054	32	0
2	A	44	0	41	0	0
2	B	44	0	40	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	386	0	0	3	0
4	B	353	0	0	2	0
All	All	11443	0	10189	63	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 (63) 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:528:THR:HG23	1:B:566:ALA:HB3	1.69	0.74
1:A:560:ILE:HD12	1:A:578:ASN:HA	1.71	0.72
1:A:203:ASN:O	1:A:677:THR:HG21	1.92	0.69
1:B:231:VAL:HG22	1:B:239:GLN:HE22	1.59	0.67
1:B:226:ILE:HB	1:B:254:THR:HB	1.77	0.66
1:A:653:LEU:HD12	1:A:660:VAL:HG13	1.78	0.65
1:B:333:HIS:HD2	4:B:1258:HOH:O	1.83	0.60
1:B:340:ARG:HH12	1:B:465:ASN:ND2	1.99	0.60
1:B:453:ARG:HH11	1:B:473:ALA:HB2	1.67	0.59
1:A:238:TRP:HD1	1:A:588:THR:HG21	1.68	0.59
1:A:78:GLN:NE2	1:A:137:ALA:H	2.03	0.57
1:A:361:GLY:HA3	1:A:366:MET:SD	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:VAL:HG22	1:B:643:PRO:HD2	1.89	0.55
1:A:170:ASP:OD1	1:A:177:HIS:HE1	1.90	0.54
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.91	0.54
1:A:378:LEU:HD21	1:A:381:PHE:CZ	2.43	0.54
1:B:124:THR:O	1:B:128:HIS:HD2	1.91	0.53
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.90	0.53
1:A:339:ARG:HG2	1:A:365:TYR:CD1	2.45	0.52
1:B:590:ARG:HD3	1:B:639:ASP:OD2	2.10	0.52
1:B:231:VAL:HG22	1:B:239:GLN:NE2	2.24	0.51
1:A:333:HIS:HD2	4:A:1153:HOH:O	1.93	0.51
1:B:560:ILE:HD12	1:B:578:ASN:HA	1.93	0.51
1:B:434:ILE:HG12	1:B:487:THR:HG23	1.92	0.51
1:B:197:LEU:HD21	2:B:707:GLD:H63	1.93	0.50
1:B:378:LEU:HD21	1:B:381:PHE:CZ	2.46	0.50
1:B:649:GLU:HA	1:B:668:ARG:O	2.11	0.50
1:A:126:HIS:HE1	1:A:224:ASP:OD2	1.95	0.49
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.93	0.49
1:B:143:PRO:HG3	2:B:706:ACI:O6	2.12	0.48
1:B:401:ASN:HD22	1:B:403:ALA:H	1.59	0.48
1:B:435:ASN:HB2	1:B:482:LEU:HD13	1.95	0.48
1:B:562:ASP:HB3	1:B:575:ILE:HG23	1.95	0.48
1:A:590:ARG:HD3	1:A:639:ASP:OD2	2.13	0.48
1:B:361:GLY:HA3	1:B:366:MET:SD	2.54	0.47
1:A:603:ASN:HB3	1:A:624:PRO:HB3	1.98	0.46
1:B:605:PHE:HB2	1:B:653:LEU:HG	1.97	0.46
1:A:273:ALA:HB2	1:A:280:LEU:HD22	1.98	0.46
1:A:40:ASP:HB2	1:A:48:LEU:HD12	1.97	0.46
1:A:587:VAL:CG1	1:A:675:SER:HA	2.46	0.45
1:B:228:VAL:HG22	1:B:231:VAL:HG23	1.97	0.45
1:B:229:ASP:OD1	2:B:708:GAL:H2	2.17	0.45
1:A:308:GLU:OE2	1:B:410:HIS:HE1	2.00	0.44
1:A:453:ARG:HH12	1:A:473:ALA:HB2	1.82	0.44
1:B:280:LEU:H	1:B:320:GLN:NE2	2.14	0.44
1:A:227:ARG:HG2	1:A:255:PHE:CE1	2.53	0.44
1:A:564:ARG:HD2	1:A:575:ILE:CD1	2.48	0.44
1:B:386:THR:O	1:B:390:VAL:HG13	2.17	0.44
1:A:562:ASP:HB3	1:A:575:ILE:HG23	2.00	0.43
1:B:592:VAL:HB	1:B:681:ASN:HA	2.00	0.43
1:B:21:PHE:CE1	1:B:327:HIS:HB3	2.55	0.42
1:B:606:LEU:HB3	1:B:622:ILE:HB	2.01	0.42
1:A:124:THR:O	1:A:128:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ASN:ND2	1:B:403:ALA:H	2.17	0.41
1:A:25:PHE:HB3	4:A:1019:HOH:O	2.20	0.41
1:A:296:ASN:HB2	4:A:1479:HOH:O	2.21	0.41
1:A:378:LEU:HD21	1:A:381:PHE:CE1	2.56	0.41
1:A:520:ARG:HD2	1:A:520:ARG:HH21	1.74	0.41
1:A:81:GLU:OE2	1:A:103:ARG:HD2	2.21	0.41
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.55	0.41
1:B:25:PHE:HB3	4:B:1040:HOH:O	2.22	0.40
1:A:401:ASN:HA	1:A:402:PRO:HD2	1.95	0.40
1:A:560:ILE:HA	1:A:579:PHE:O	2.22	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%)	667 (98%)	16 (2%)	1 (0%)	56	46
All	All	1368/1372 (100%)	1331 (97%)	36 (3%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	657	GLY

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%)	528 (94%)	36 (6%)	22	10
1	B	564/564 (100%)	518 (92%)	46 (8%)	14	5
All	All	1128/1128 (100%)	1046 (93%)	82 (7%)	17	7

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	21	PHE
1	A	46	LEU
1	A	66	LEU
1	A	74	ILE
1	A	85	SER
1	A	103	ARG
1	A	119	LYS
1	A	160	ASN
1	A	163	LEU
1	A	199	ASP
1	A	221	LEU
1	A	228	VAL
1	A	263	ASN
1	A	280	LEU
1	A	281	LEU
1	A	350	LEU
1	A	353	ARG
1	A	367	SER
1	A	372	PRO
1	A	375	ARG
1	A	378	LEU
1	A	383	THR
1	A	393	LYS
1	A	429	VAL
1	A	435	ASN
1	A	439	ASN
1	A	464	LEU
1	A	497	THR
1	A	536	VAL
1	A	590	ARG
1	A	606	LEU
1	A	613	LEU

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Mol	Chain	Res	Type
1	A	642	VAL
1	A	658	SER
1	A	677	THR
1	B	21	PHE
1	B	46	LEU
1	B	66	LEU
1	B	74	ILE
1	B	119	LYS
1	B	157	LEU
1	B	163	LEU
1	B	164	LEU
1	B	169	ASN
1	B	171	THR
1	B	173	ASN
1	B	197	LEU
1	B	200	LEU
1	B	204	ASN
1	B	206	SER
1	B	211	LEU
1	B	228	VAL
1	B	231	VAL
1	B	252	VAL
1	B	254	THR
1	B	259	LEU
1	B	307	LEU
1	B	342	LEU
1	B	346	LEU
1	B	353	ARG
1	B	372	PRO
1	B	378	LEU
1	B	383	THR
1	B	390	VAL
1	B	401	ASN
1	B	410	HIS
1	B	415	ASN
1	B	451	LEU
1	B	453	ARG
1	B	482	LEU
1	B	513	VAL
1	B	528	THR
1	B	529	VAL
1	B	560	ILE

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Mol	Chain	Res	Type
1	B	590	ARG
1	B	598	THR
1	B	613	LEU
1	B	620	ASN
1	B	653	LEU
1	B	656	GLN
1	B	682	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	55	GLN
1	A	78	GLN
1	A	126	HIS
1	A	128	HIS
1	A	177	HIS
1	A	239	GLN
1	A	247	ASN
1	A	333	HIS
1	A	435	ASN
1	A	594	ASN
1	B	55	GLN
1	B	62	ASN
1	B	126	HIS
1	B	169	ASN
1	B	204	ASN
1	B	239	GLN
1	B	270	HIS
1	B	320	GLN
1	B	333	HIS
1	B	364	GLN
1	B	401	ASN
1	B	410	HIS
1	B	415	ASN
1	B	465	ASN
1	B	548	GLN
1	B	595	ASN
1	B	615	ASN
1	B	683	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	11,11,12	1.73	4 (36%)	14,15,17	2.03	4 (28%)
2	ACI	A	702	2	11,12,12	2.14	2 (18%)	9,17,17	2.04	3 (33%)
2	GLD	A	703	2	9,9,10	2.61	5 (55%)	10,12,14	1.79	3 (30%)
2	GAL	A	704	2	12,12,12	2.21	6 (50%)	17,17,17	2.84	6 (35%)
2	GLC	B	705	2	11,11,12	1.54	4 (36%)	14,15,17	1.51	4 (28%)
2	ACI	B	706	2	11,12,12	2.04	3 (27%)	9,17,17	1.71	2 (22%)
2	GLD	B	707	2	9,9,10	2.15	3 (33%)	10,12,14	1.83	4 (40%)
2	GAL	B	708	2	12,12,12	2.58	6 (50%)	17,17,17	2.51	7 (41%)

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	-	0/2/19/22	0/1/1/1
2	ACI	A	702	2	-	0/2/22/22	0/1/1/1
2	GLD	A	703	2	-	0/0/13/16	0/1/1/1
2	GAL	A	704	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	B	705	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACI	B	706	2	-	0/2/22/22	0/1/1/1
2	GLD	B	707	2	-	0/0/13/16	0/1/1/1
2	GAL	B	708	2	1/1/5/5	0/2/22/22	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GLC	C6-C5	2.01	1.59	1.51
2	B	705	GLC	O5-C1	2.06	1.47	1.43
2	B	705	GLC	C2-C3	2.12	1.55	1.52
2	A	701	GLC	O5-C5	2.12	1.48	1.43
2	A	703	GLD	C4-C3	2.12	1.56	1.52
2	B	706	ACI	C3-C4	2.18	1.55	1.53
2	B	705	GLC	C4-C5	2.24	1.57	1.53
2	B	705	GLC	C1-C2	2.31	1.57	1.52
2	A	704	GAL	O4-C4	2.37	1.48	1.43
2	A	703	GLD	O5-C5	2.37	1.48	1.43
2	B	706	ACI	O4-C4	2.52	1.47	1.42
2	B	708	GAL	C6-C5	2.52	1.60	1.51
2	A	701	GLC	C1-C2	2.59	1.58	1.52
2	A	704	GAL	O5-C1	2.67	1.48	1.43
2	B	708	GAL	O1-C1	2.70	1.49	1.39
2	A	704	GAL	C4-C3	2.72	1.59	1.52
2	A	704	GAL	O5-C5	2.83	1.51	1.44
2	B	708	GAL	O5-C5	2.87	1.51	1.44
2	A	704	GAL	C4-C5	2.87	1.59	1.53
2	B	707	GLD	C4-C5	3.02	1.57	1.51
2	A	701	GLC	O5-C1	3.11	1.48	1.43
2	A	702	ACI	O4-C4	3.31	1.48	1.42
2	B	707	GLD	C1-C2	3.46	1.60	1.52
2	A	703	GLD	C4-C5	3.60	1.58	1.51
2	B	708	GAL	C4-C5	3.62	1.60	1.53
2	A	703	GLD	O5-C1	3.76	1.50	1.43
2	B	707	GLD	C4-C3	3.78	1.58	1.52
2	B	708	GAL	C1-C2	3.81	1.60	1.52
2	A	704	GAL	C3-C2	3.89	1.62	1.52
2	A	703	GLD	C3-C2	4.01	1.57	1.52
2	B	708	GAL	O5-C1	4.86	1.52	1.43
2	A	702	ACI	C7-C5	5.13	1.40	1.32
2	B	706	ACI	C7-C5	5.23	1.40	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	GAL	C1-C2-C3	-7.89	98.69	110.43
2	B	706	ACI	C2-C3-C4	-3.99	105.87	110.73
2	A	704	GAL	O5-C1-C2	-3.98	103.45	109.80
2	A	703	GLD	C4-C3-C2	-3.95	105.00	110.23
2	B	708	GAL	C4-C3-C2	-3.60	104.07	110.79
2	B	708	GAL	C1-C2-C3	-3.23	105.62	110.43
2	A	702	ACI	O6-C6-C5	-3.21	104.37	112.12
2	B	707	GLD	C4-C3-C2	-3.06	106.18	110.23
2	A	704	GAL	C4-C3-C2	-2.59	105.96	110.79
2	B	705	GLC	C3-C4-C5	-2.54	105.77	110.20
2	B	708	GAL	O4-C4-C3	-2.47	104.77	110.34
2	A	702	ACI	O4-C4-C5	-2.40	105.20	110.36
2	B	707	GLD	C6-C5-C4	-2.28	109.58	113.38
2	B	708	GAL	C3-C4-C5	-2.19	106.38	110.20
2	A	701	GLC	C2-C3-C4	-2.15	107.39	111.04
2	B	706	ACI	C2-C1-N1	-2.04	107.25	111.40
2	A	701	GLC	C6-C5-C4	-2.03	108.01	113.02
2	A	703	GLD	C1-O5-C5	2.01	117.32	113.19
2	A	704	GAL	O4-C4-C3	2.07	114.99	110.34
2	B	707	GLD	O5-C1-C2	2.14	114.32	110.86
2	B	707	GLD	O2-C2-C1	2.18	113.58	109.21
2	B	705	GLC	O4-C4-C5	2.43	115.67	109.24
2	B	705	GLC	O2-C2-C1	2.47	114.15	109.21
2	B	705	GLC	C1-O5-C5	2.56	115.49	112.25
2	A	703	GLD	O3-C3-C2	2.88	116.73	110.27
2	A	704	GAL	O1-C1-O5	2.94	118.30	110.25
2	B	708	GAL	C1-O5-C5	3.03	119.08	113.47
2	A	702	ACI	C2-C3-C4	3.14	114.55	110.73
2	B	708	GAL	O4-C4-C5	3.22	117.77	109.24
2	A	701	GLC	O5-C1-C2	3.41	116.40	110.86
2	A	701	GLC	C1-O5-C5	5.11	118.73	112.25
2	A	704	GAL	O2-C2-C3	5.22	122.10	110.34
2	B	708	GAL	O2-C2-C1	6.73	124.64	109.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	704	GAL	C4
2	B	708	GAL	C4

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	706	ACI	1	0
2	B	707	GLD	1	0
2	B	708	GAL	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 ⓘ

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, 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%)	-0.51	4 (0%)	90 91	8, 15, 27, 49	0
1	B	686/686 (100%)	-0.40	6 (0%)	85 87	9, 17, 34, 54	0
All	All	1372/1372 (100%)	-0.45	10 (0%)	89 90	8, 16, 32, 54	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	4.8
1	A	90	SER	3.7
1	A	675	SER	3.7
1	B	497	THR	3.0
1	A	497	THR	2.7
1	B	90	SER	2.7
1	B	91	GLY	2.6
1	B	656	GLN	2.5
1	B	453	ARG	2.4
1	A	263	ASN	2.1

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 ⓘ

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(\AA^2)	Q<0.9
2	GLC	A	701	11/12	0.71	0.68	33.15	10,13,16,22	0
2	ACI	B	706	12/12	0.50	0.73	26.29	9,14,22,23	0
2	ACI	A	702	12/12	0.52	0.59	24.24	11,14,17,20	0
2	GLD	B	707	9/10	0.65	0.68	22.44	6,12,16,22	0
2	GAL	B	708	12/12	0.69	0.66	17.98	12,13,17,17	0
2	GLD	A	703	9/10	0.61	0.56	16.16	4,12,17,17	0
2	GAL	A	704	12/12	0.49	0.51	14.39	10,16,20,28	0
2	GLC	B	705	11/12	0.78	0.53	-	12,16,20,21	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(\AA^2)	Q<0.9
3	CA	B	690	1/1	0.92	0.08	-0.30	34,34,34,34	0
3	CA	A	688	1/1	0.92	0.07	-0.36	36,36,36,36	0
3	CA	A	687	1/1	0.97	0.06	-1.38	12,12,12,12	0
3	CA	B	689	1/1	0.98	0.03	-3.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.