



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:12 PM UTC

PDB ID : 1UKS / pdb_00001uks
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

<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

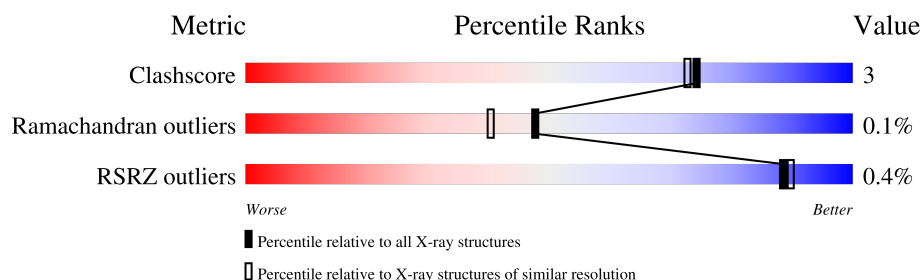
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	686	
1	B	686	
2	C	2	
2	D	2	

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	GAL	C	1	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	D	1	X	-	-	-
3	GLC	A	701	-	-	-	X
4	ACI	B	706	-	-	-	X

2 Entry composition

There are 6 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.

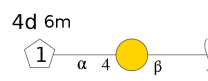
- Molecule 1 is a protein called Cyclomaltodextrin glucanotransferase.

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:

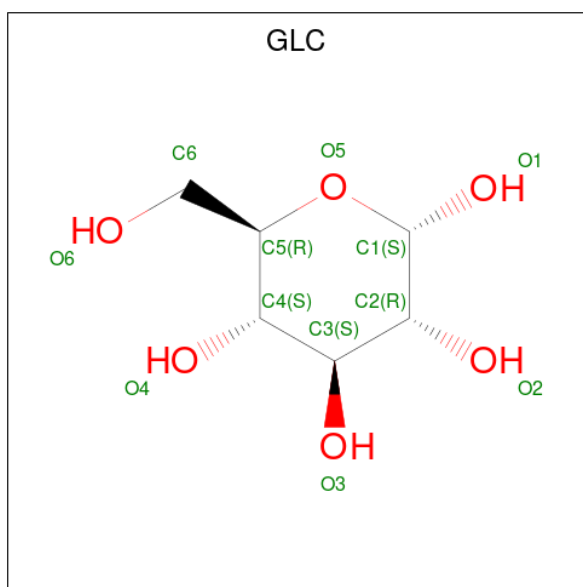
Chain	Residue	Modelled	Actual	Comment	Reference
A	183	LEU	PHE	engineered mutation	UNP P05618
A	259	LEU	PHE	engineered mutation	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	183	LEU	PHE	engineered mutation	UNP P05618
B	259	LEU	PHE	engineered mutation	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	UNP P05618

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-beta-D-galactopyranose.



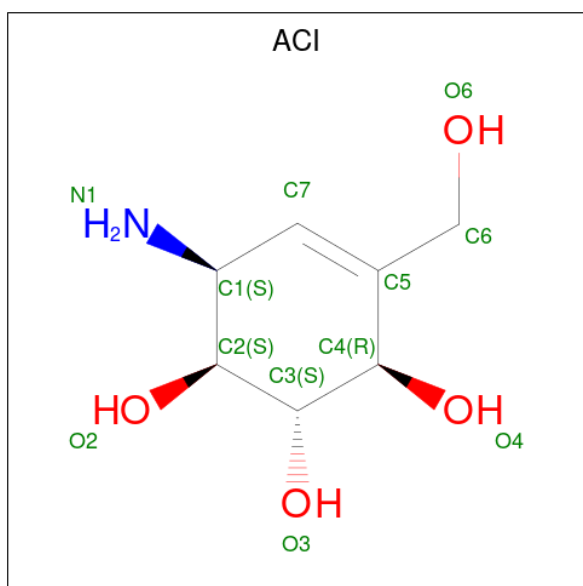
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			21	12	9			
2	D	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



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

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



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

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

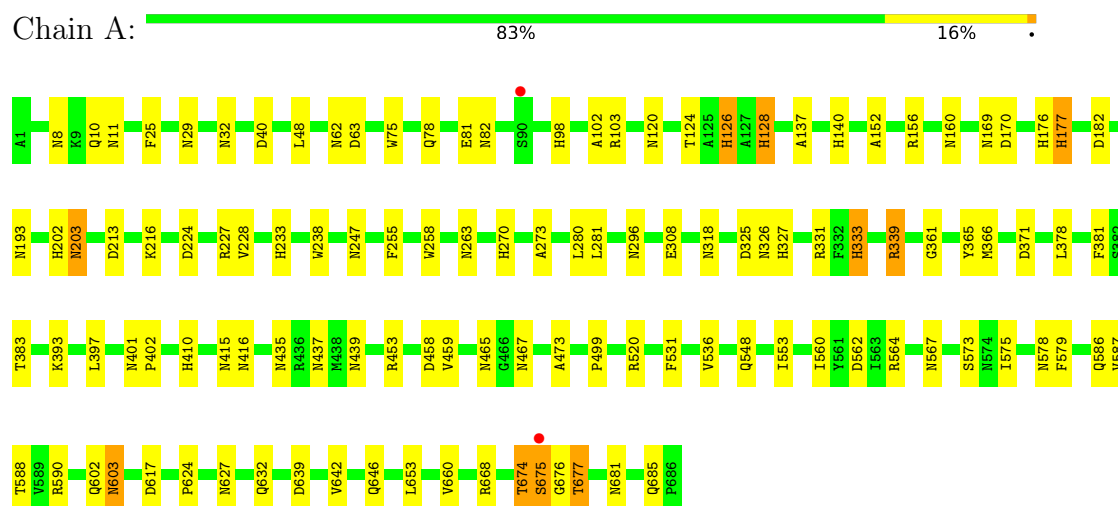
- Molecule 6 is water.

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

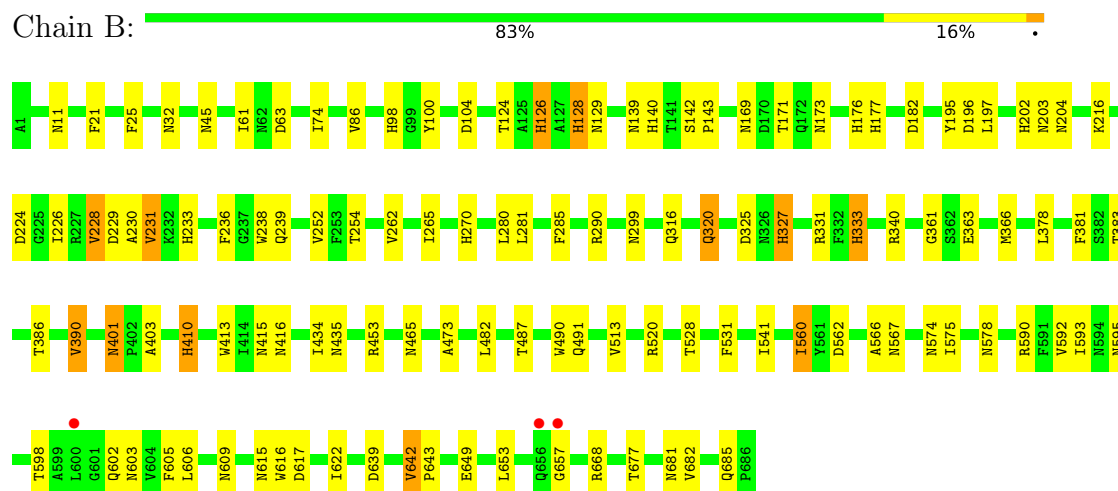
3 Residue-property plots

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: Cyclomaltodextrin glucanotransferase



• Molecule 1: Cyclomaltodextrin glucanotransferase



• Molecule 2: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-beta-D-galactopyranose



GAL1
GLD2

- Molecule 2: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-beta-D-galactopyranose

Chain D:

100%

GAL1
GLD2

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 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	78.3 (10.00-1.90) 92.4 (10.00-1.90)	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 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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, GLD, GLC, CA, GAL

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	0.92	16/5438 (0.3%)	1.63	87/7419 (1.2%)
1	B	0.93	18/5438 (0.3%)	1.64	93/7419 (1.3%)
All	All	0.93	34/10876 (0.3%)	1.63	180/14838 (1.2%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	VAL	CA-CB	9.11	1.65	1.54
1	B	228	VAL	CA-CB	8.52	1.64	1.54
1	B	177	HIS	CD2-NE2	-7.46	1.29	1.37
1	A	233	HIS	CD2-NE2	-7.37	1.29	1.37
1	A	140	HIS	CD2-NE2	-7.23	1.29	1.37
1	A	128	HIS	CD2-NE2	-7.21	1.29	1.37
1	B	140	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	327	HIS	CD2-NE2	-7.01	1.30	1.37
1	B	513	VAL	CA-CB	6.95	1.63	1.54
1	A	202	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.88	1.30	1.37
1	B	128	HIS	CD2-NE2	-6.85	1.30	1.37
1	B	126	HIS	CD2-NE2	-6.79	1.30	1.37
1	B	333	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	390	VAL	CA-CB	6.63	1.62	1.54
1	B	176	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	536	VAL	CA-CB	6.44	1.62	1.54
1	A	177	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	233	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	98	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	202	HIS	CD2-NE2	-6.13	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	98	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	593	ILE	CA-CB	5.87	1.61	1.54
1	A	270	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	270	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	676	GLY	CA-C	5.51	1.58	1.51
1	A	410	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	128	HIS	CG-ND1	-5.29	1.32	1.38
1	B	560	ILE	CA-CB	5.26	1.61	1.54
1	B	177	HIS	CG-ND1	-5.00	1.32	1.38

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	SER	CA-C-N	11.26	134.24	120.51
1	A	675	SER	C-N-CA	11.26	134.24	120.51
1	A	668	ARG	NE-CZ-NH1	-10.90	110.60	121.50
1	A	642	VAL	N-CA-CB	-10.53	100.38	111.64
1	B	415	ASN	CA-CB-CG	10.29	122.89	112.60
1	A	668	ARG	NE-CZ-NH2	9.99	128.19	119.20
1	A	642	VAL	CB-CA-C	9.77	118.90	109.33
1	B	325	ASP	CA-CB-CG	9.65	122.25	112.60
1	A	263	ASN	CA-CB-CG	9.40	122.00	112.60
1	B	642	VAL	N-CA-CB	-8.92	102.06	111.87
1	A	383	THR	N-CA-CB	-8.64	97.94	110.56
1	B	11	ASN	OD1-CG-ND2	-8.55	114.05	122.60
1	A	8	ASN	OD1-CG-ND2	-8.48	114.11	122.60
1	B	129	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	B	410	HIS	CB-CG-CD2	-8.18	120.57	131.20
1	A	435	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	A	169	ASN	CA-CB-CG	-8.04	104.56	112.60
1	B	383	THR	N-CA-CB	-7.99	98.67	110.49
1	A	325	ASP	CA-CB-CG	7.96	120.56	112.60
1	B	331	ARG	NE-CZ-NH2	-7.90	112.09	119.20
1	A	216	LYS	CB-CG-CD	-7.84	93.27	111.30
1	B	520	ARG	NE-CZ-NH2	7.83	126.25	119.20
1	B	231	VAL	N-CA-CB	-7.79	97.32	110.65
1	B	100	TYR	N-CA-C	7.74	122.40	113.19
1	A	193	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	A	63	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	598	THR	N-CA-CB	-7.47	98.56	111.55
1	B	98	HIS	CB-CG-CD2	-7.46	121.51	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	465	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	A	62	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	A	32	ASN	CA-CB-CG	7.26	119.86	112.60
1	B	262	VAL	N-CA-C	7.24	117.76	110.23
1	B	320	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	A	11	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	410	HIS	CA-CB-CG	7.12	120.92	113.80
1	B	173	ASN	CA-CB-CG	-7.09	105.51	112.60
1	B	642	VAL	CB-CA-C	7.08	117.53	109.89
1	A	10	GLN	OE1-CD-NE2	-7.00	115.60	122.60
1	B	228	VAL	CA-C-O	6.99	128.05	120.57
1	A	415	ASN	CA-CB-CG	6.99	119.59	112.60
1	B	63	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	676	GLY	O-C-N	-6.96	115.72	123.58
1	B	682	VAL	N-CA-CB	-6.93	97.80	112.00
1	B	415	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	327	HIS	CB-CG-CD2	-6.87	122.28	131.20
1	B	177	HIS	CB-CG-CD2	-6.85	122.29	131.20
1	A	674	THR	N-CA-C	-6.82	101.34	110.55
1	B	126	HIS	CB-CG-CD2	-6.75	122.43	131.20
1	B	567	ASN	CA-CB-CG	6.65	119.25	112.60
1	B	685	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	A	675	SER	N-CA-C	6.61	124.88	110.80
1	A	632	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	140	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	B	541	ILE	N-CA-C	-6.42	97.95	107.51
1	B	216	LYS	CB-CG-CD	-6.41	96.55	111.30
1	A	233	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	531	PHE	N-CA-C	-6.38	96.70	107.99
1	A	126	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	A	182	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	333	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	A	177	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	B	270	HIS	CA-CB-CG	-6.28	107.52	113.80
1	B	617	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	258	TRP	N-CA-C	-6.24	96.92	108.02
1	B	32	ASN	CA-CB-CG	6.23	118.83	112.60
1	A	8	ASN	CB-CG-ND2	6.23	125.74	116.40
1	B	416	ASN	N-CA-C	6.21	118.06	111.28
1	B	45	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	11	ASN	CB-CG-ND2	6.17	125.66	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	B	204	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	A	120	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	A	668	ARG	CG-CD-NE	-6.11	98.57	112.00
1	B	410	HIS	CB-CG-ND1	6.09	131.83	122.70
1	A	677	THR	N-CA-CB	-6.07	101.37	111.20
1	B	270	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	B	171	THR	N-CA-CB	-6.05	100.90	110.28
1	B	285	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	642	VAL	O-C-N	-6.01	117.90	121.69
1	B	139	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	318	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	B	685	GLN	CG-CD-NE2	5.99	125.39	116.40
1	B	415	ASN	CB-CG-ND2	5.98	125.37	116.40
1	B	128	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	416	ASN	N-CA-C	5.94	119.35	111.75
1	A	247	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	B	139	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	A	439	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	685	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	603	ASN	OD1-CG-ND2	-5.89	116.70	122.60
1	B	98	HIS	CB-CG-ND1	5.88	131.53	122.70
1	B	331	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	A	371	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	520	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	B	182	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	491	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	290	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	B	203	ASN	OD1-CG-ND2	-5.75	116.84	122.60
1	B	265	ILE	N-CA-C	-5.75	99.84	108.12
1	A	677	THR	O-C-N	-5.75	115.41	123.11
1	B	595	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	B	574	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	A	383	THR	CB-CA-C	5.70	120.19	110.56
1	B	327	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	102	ALA	N-CA-C	5.69	118.47	110.23
1	A	674	THR	CA-C-O	-5.65	115.14	121.81
1	A	160	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	62	ASN	N-CA-C	5.64	117.42	111.28
1	A	567	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	465	ASN	CB-CG-ND2	5.63	124.84	116.40
1	A	467	ASN	OD1-CG-ND2	-5.63	116.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	B	61	ILE	N-CA-C	-5.62	105.37	110.82
1	A	281	LEU	N-CA-C	-5.61	101.34	109.59
1	B	195	TYR	CB-CA-C	-5.59	110.14	116.63
1	A	326	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	553	ILE	CA-C-N	5.54	125.53	120.21
1	A	553	ILE	C-N-CA	5.54	125.53	120.21
1	A	586	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	A	202	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	383	THR	CB-CA-C	5.51	119.29	110.09
1	B	74	ILE	N-CA-CB	-5.50	101.82	111.39
1	B	252	VAL	N-CA-CB	-5.48	101.67	111.92
1	B	609	ASN	N-CA-C	5.47	119.05	112.93
1	A	11	ASN	CB-CG-ND2	5.45	124.58	116.40
1	A	331	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	A	646	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	B	682	VAL	CB-CA-C	5.40	120.19	110.48
1	A	331	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	339	ARG	CA-CB-CG	-5.39	103.33	114.10
1	B	603	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	393	LYS	CA-CB-CG	5.37	124.84	114.10
1	B	230	ALA	N-CA-C	5.35	118.78	111.39
1	A	140	HIS	CB-CG-ND1	5.33	130.70	122.70
1	A	602	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	A	213	ASP	CA-CB-CG	5.33	117.92	112.60
1	B	617	ASP	CA-C-N	5.33	124.96	119.05
1	B	617	ASP	C-N-CA	5.33	124.96	119.05
1	B	401	ASN	CB-CG-ND2	5.31	124.37	116.40
1	B	281	LEU	N-CA-C	-5.31	102.53	110.23
1	B	231	VAL	CB-CA-C	5.29	120.36	112.16
1	A	29	ASN	CA-C-N	5.29	124.79	119.19
1	A	29	ASN	C-N-CA	5.29	124.79	119.19
1	B	236	PHE	CA-CB-CG	5.28	119.08	113.80
1	B	616	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	A	152	ALA	CB-CA-C	-5.27	110.48	116.54
1	B	316	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	A	617	ASP	CA-C-N	5.24	125.55	119.47
1	A	617	ASP	C-N-CA	5.24	125.55	119.47
1	B	86	VAL	N-CA-C	-5.24	100.34	107.99
1	B	531	PHE	N-CA-C	-5.24	97.30	107.62
1	B	196	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	74	ILE	CB-CA-C	5.22	118.40	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	SER	CA-C-N	5.21	125.51	119.93
1	B	142	SER	C-N-CA	5.21	125.51	119.93
1	B	299	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	615	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	363	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	203	ASN	N-CA-C	-5.17	106.75	113.16
1	A	228	VAL	CA-C-O	5.16	126.10	120.57
1	A	674	THR	O-C-N	-5.16	116.97	122.85
1	B	413	TRP	CB-CG-CD1	-5.15	119.17	126.90
1	B	602	GLN	N-CA-C	-5.15	101.31	109.76
1	B	331	ARG	CA-CB-CG	-5.15	103.81	114.10
1	B	238	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	B	177	HIS	CB-CG-ND1	5.14	130.41	122.70
1	A	627	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	128	HIS	CB-CG-ND1	5.12	130.38	122.70
1	A	458	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	437	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	B	616	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	B	104	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	677	THR	N-CA-CB	-5.08	103.43	111.05
1	B	169	ASN	CA-C-O	5.04	127.55	121.65
1	B	490	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	A	156	ARG	N-CA-C	5.02	117.58	110.10
1	A	327	HIS	CB-CG-ND1	5.02	130.22	122.70
1	A	82	ASN	CB-CG-ND2	5.01	123.92	116.40
1	A	681	ASN	OD1-CG-ND2	-5.00	117.60	122.60

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	5306	0	5054	33	0
1	B	5306	0	5054	32	0
2	C	21	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	21	0	20	2	0
3	A	11	0	10	0	0
3	B	11	0	10	0	0
4	A	12	0	11	0	0
4	B	12	0	10	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	386	0	0	3	0
6	B	353	0	0	2	0
All	All	11443	0	10189	64	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 (64) 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	6: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
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	6: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LEU:HD21	2:D:2: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	4: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:40:ASP:HB2	1:A:48:LEU:HD12	1.97	0.46
1:A:273:ALA:HB2	1:A:280:LEU:HD22	1.98	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:A:674:THR:O	1:A:675:SER:C	2.60	0.45
1:B:229:ASP:OD1	2:D:1: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:A:124:THR:O	1:A:128:HIS:HD2	2.02	0.42
1:B:606:LEU:HB3	1:B:622:ILE:HB	2.01	0.42
1:A:25:PHE:HB3	6:A:1019:HOH:O	2.20	0.41
1:A:296:ASN:HB2	6:A:1479:HOH:O	2.21	0.41
1:B:401:ASN:ND2	1:B:403:ALA:H	2.17	0.41
1:A:378:LEU:HD21	1:A:381:PHE:CE1	2.56	0.41
1:A:81:GLU:OE2	1:A:103:ARG:HD2	2.21	0.41
1:A:520:ARG:HH21	1:A:520:ARG:HD2	1.74	0.41
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.55	0.41
1:A:401:ASN:HA	1:A:402:PRO:HD2	1.95	0.40
1:B:25:PHE:HB3	6:B:1040:HOH:O	2.22	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%)	48	40
All	All	1368/1372 (100%)	1331 (97%)	36 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	657	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

4 monosaccharides 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	GAL	C	1	2	12,12,12	2.18	6 (50%)	17,17,17	2.47	5 (29%)
2	GLD	C	2	2,4	9,9,10	2.99	4 (44%)	11,12,14	2.21	4 (36%)
2	GAL	D	1	2	12,12,12	2.44	6 (50%)	17,17,17	2.45	7 (41%)
2	GLD	D	2	2,4	9,9,10	2.11	3 (33%)	11,12,14	2.00	4 (36%)

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	GAL	C	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLD	C	2	2,4	-	-	0/1/1/1
2	GAL	D	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLD	D	2	2,4	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLD	O5-C5	4.98	1.48	1.44
2	C	1	GAL	C3-C2	3.95	1.62	1.52
2	C	2	GLD	C4-C5	3.92	1.58	1.52
2	D	1	GAL	O5-C1	3.83	1.52	1.42
2	C	2	GLD	C3-C2	3.81	1.57	1.52
2	C	2	GLD	O5-C1	3.76	1.50	1.43
2	D	1	GAL	C4-C5	3.63	1.60	1.53
2	D	2	GLD	C1-C2	3.46	1.60	1.52
2	D	1	GAL	C1-C2	3.41	1.60	1.52
2	D	2	GLD	C4-C5	3.28	1.57	1.52
2	D	2	GLD	C4-C3	3.24	1.58	1.52
2	D	1	GAL	O1-C1	3.00	1.49	1.39
2	D	1	GAL	O5-C5	2.92	1.51	1.44
2	C	1	GAL	O5-C5	2.89	1.51	1.44
2	C	1	GAL	C4-C5	2.88	1.59	1.53
2	C	1	GAL	C4-C3	2.77	1.59	1.52
2	D	1	GAL	C6-C5	2.71	1.60	1.51
2	C	1	GAL	O4-C4	2.29	1.48	1.43
2	C	1	GAL	O5-C1	2.14	1.48	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GAL	O2-C2-C1	6.67	124.64	109.25
2	C	1	GAL	C1-C2-C3	-5.72	98.69	110.36
2	C	1	GAL	O2-C2-C3	4.97	122.10	110.38
2	C	2	GLD	C4-C3-C2	-4.36	105.00	110.38
2	C	1	GAL	O5-C1-C2	-3.89	103.45	110.30
2	D	1	GAL	C4-C3-C2	-3.85	104.07	110.83
2	C	2	GLD	C1-O5-C5	3.76	117.32	111.80
2	D	1	GAL	O4-C4-C5	3.43	117.77	109.32
2	D	2	GLD	C4-C3-C2	-3.40	106.18	110.38
2	C	2	GLD	O3-C3-C2	2.98	116.73	110.20
2	D	1	GAL	C1-O5-C5	2.80	119.08	113.65
2	C	1	GAL	C4-C3-C2	-2.78	105.96	110.83
2	C	1	GAL	O1-C1-O5	2.66	118.30	110.41
2	D	2	GLD	C6-C5-C4	-2.44	109.58	113.27
2	D	1	GAL	O4-C4-C3	-2.38	104.77	110.38
2	D	1	GAL	C1-C2-C3	-2.32	105.62	110.36
2	D	2	GLD	C3-C4-C5	2.30	114.85	111.21
2	D	2	GLD	O5-C5-C4	2.24	111.56	109.39
2	C	2	GLD	C3-C4-C5	-2.14	107.81	111.21
2	D	1	GAL	C3-C4-C5	-2.12	106.38	110.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GAL	C4
2	D	1	GAL	C4

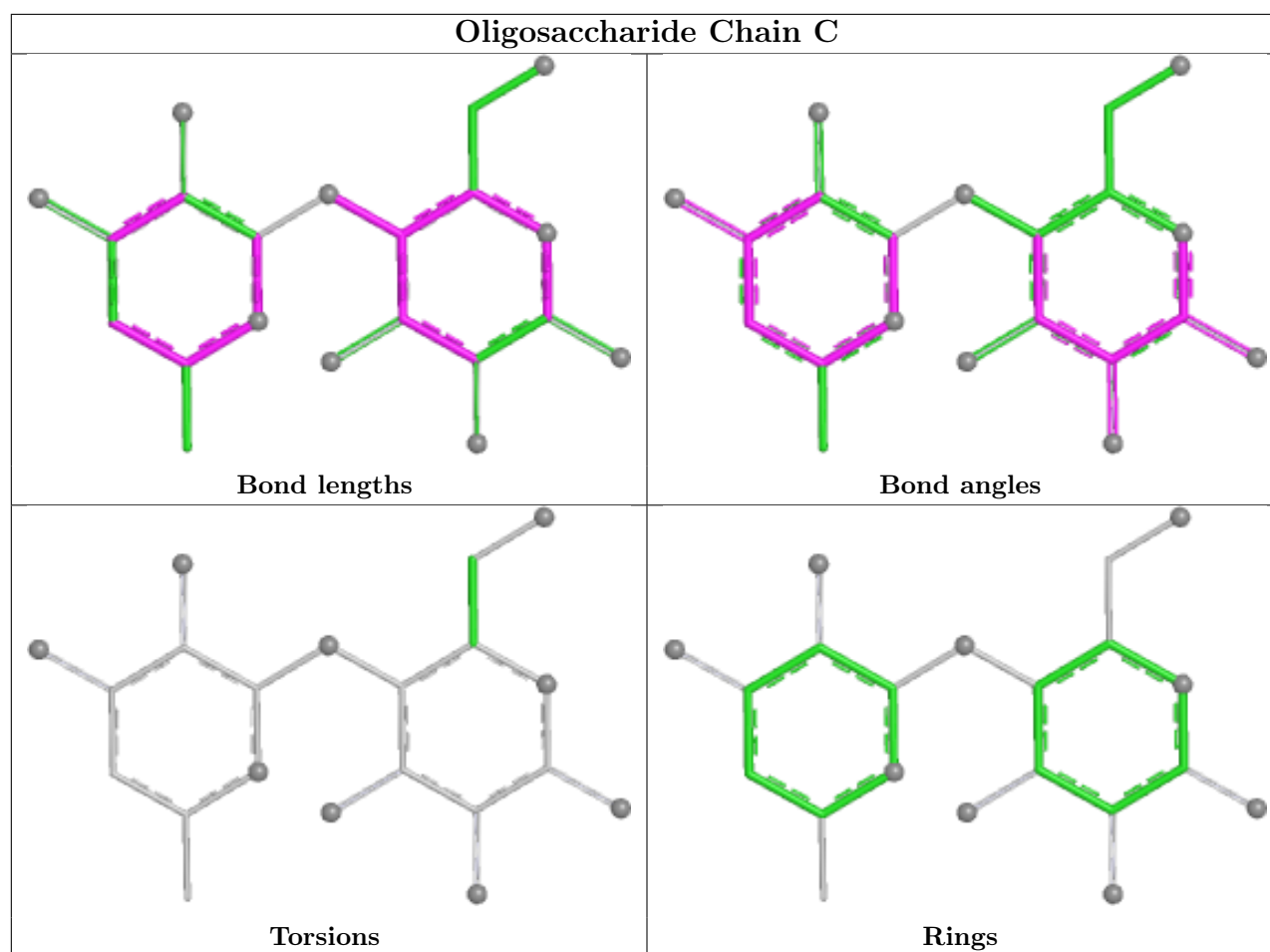
There are no torsion outliers.

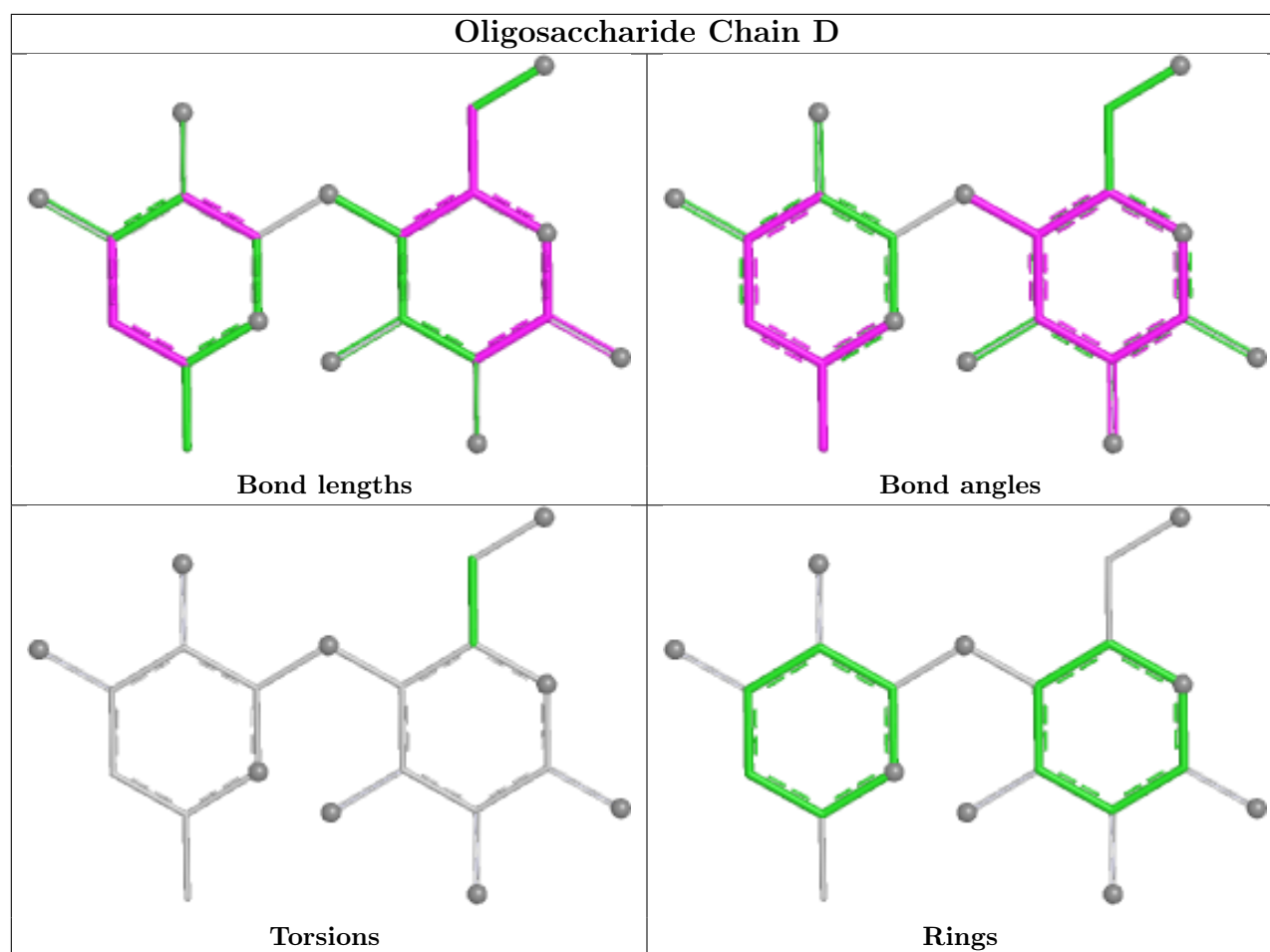
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GAL	1	0
2	D	2	GLD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	GLC	B	705	4	11,11,12	1.56	4 (36%)	15,15,17	1.47	4 (26%)
4	ACI	B	706	3,2	12,12,12	2.47	4 (33%)	11,17,17	1.44	3 (27%)
4	ACI	A	702	3,2	12,12,12	2.64	4 (33%)	11,17,17	1.92	4 (36%)
3	GLC	A	701	4	11,11,12	1.79	4 (36%)	15,15,17	1.76	3 (20%)

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
3	GLC	B	705	4	-	2/2/19/22	0/1/1/1
4	ACI	B	706	3,2	-	0/2/22/22	0/1/1/1
4	ACI	A	702	3,2	-	0/2/22/22	0/1/1/1
3	GLC	A	701	4	-	2/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	ACI	C7-C5	5.57	1.40	1.32
4	A	702	ACI	C7-C5	5.46	1.40	1.32
4	A	702	ACI	C4-C5	5.14	1.55	1.51
4	B	706	ACI	C4-C5	3.87	1.54	1.51
4	B	706	ACI	C2-C1	3.38	1.57	1.52
4	A	702	ACI	O4-C4	3.25	1.48	1.42
3	A	701	GLC	O5-C1	3.11	1.48	1.43
4	A	702	ACI	C2-C1	2.64	1.56	1.52
3	A	701	GLC	C1-C2	2.59	1.58	1.52
4	B	706	ACI	O4-C4	2.47	1.47	1.42
3	A	701	GLC	O5-C5	2.40	1.48	1.43
3	B	705	GLC	C1-C2	2.30	1.57	1.52
3	B	705	GLC	O5-C5	2.25	1.47	1.43
3	B	705	GLC	C4-C5	2.25	1.57	1.53
3	A	701	GLC	C6-C5	2.18	1.59	1.51
3	B	705	GLC	O5-C1	2.07	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	GLC	C1-O5-C5	4.88	118.73	112.19
4	A	702	ACI	O4-C4-C5	-2.91	105.20	110.75
4	B	706	ACI	C2-C3-C4	-2.75	105.87	110.22
4	A	702	ACI	C2-C3-C4	2.74	114.55	110.22
4	A	702	ACI	O6-C6-C5	-2.66	104.37	112.74
4	A	702	ACI	C3-C4-C5	2.58	115.72	111.67
3	B	705	GLC	O4-C4-C5	2.58	115.67	109.32
3	B	705	GLC	C1-O5-C5	2.47	115.49	112.19
3	B	705	GLC	C3-C4-C5	-2.46	105.77	110.23
3	A	701	GLC	O5-C1-C2	2.35	116.40	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	706	ACI	C3-C4-C5	-2.18	108.24	111.67
3	B	705	GLC	O2-C2-C1	2.15	114.15	109.22
3	A	701	GLC	C6-C5-C4	-2.04	108.01	113.02
4	B	706	ACI	C2-C1-N1	-2.04	107.25	111.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	705	GLC	O5-C5-C6-O6
3	B	705	GLC	C4-C5-C6-O6
3	A	701	GLC	O5-C5-C6-O6
3	A	701	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	ACI	1	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, 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%)	-0.60	2 (0%) 90 91	8, 15, 27, 49	0
1	B	686/686 (100%)	-0.47	3 (0%) 88 90	9, 17, 34, 54	0
All	All	1372/1372 (100%)	-0.54	5 (0%) 88 90	8, 16, 32, 54	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	SER	3.9
1	B	600	LEU	3.6
1	B	656	GLN	2.6
1	A	90	SER	2.2
1	B	657	GLY	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

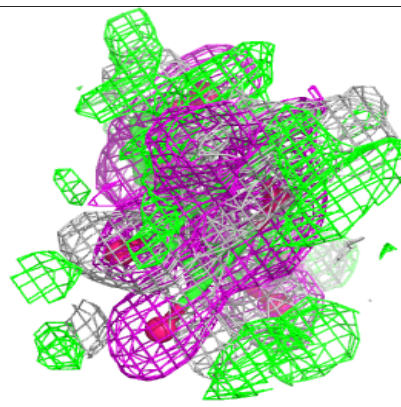
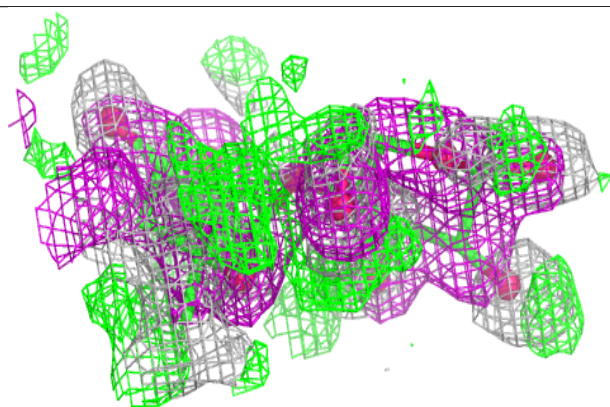
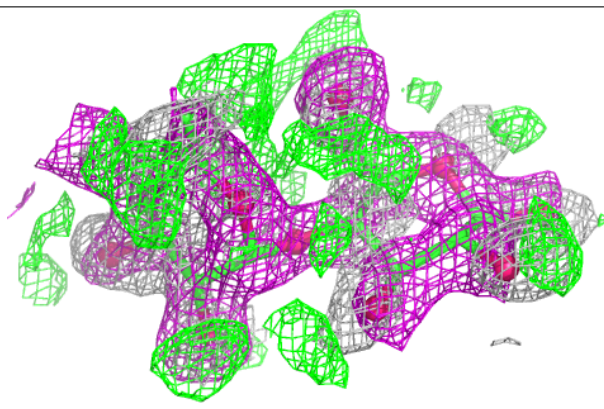
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	C	1	12/12	0.49	0.15	10,16,20,28	0
2	GLD	C	2	9/10	0.51	0.14	4,12,17,17	0
2	GAL	D	1	12/12	0.62	0.12	12,13,17,17	0
2	GLD	D	2	9/10	0.62	0.12	6,12,16,22	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

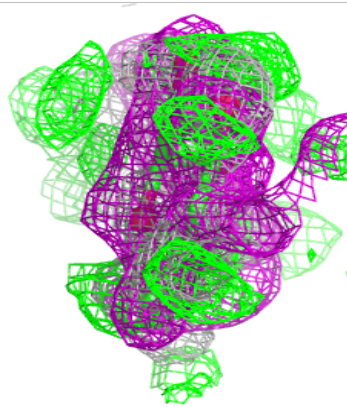
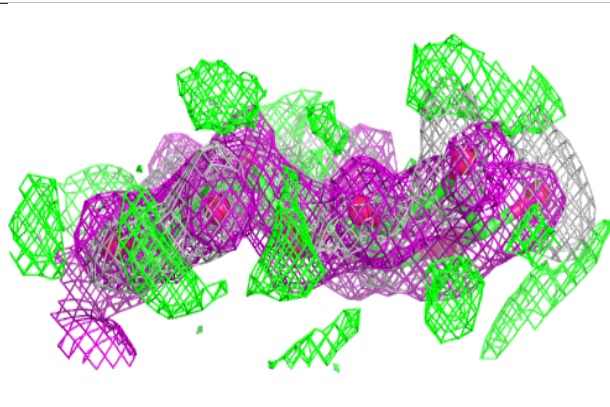
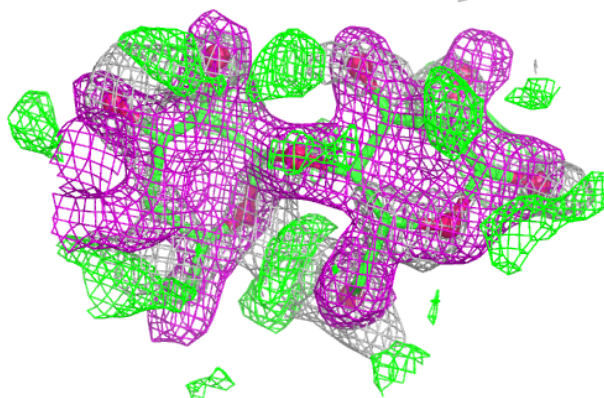
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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
4	ACI	B	706	12/12	0.42	0.43	9,14,22,23	0
4	ACI	A	702	12/12	0.43	0.37	11,14,17,20	0
3	GLC	A	701	11/12	0.60	0.43	10,13,16,22	0
3	GLC	B	705	11/12	0.73	0.34	12,16,20,21	0
5	CA	A	687	1/1	0.92	0.05	12,12,12,12	0
5	CA	A	688	1/1	0.93	0.11	36,36,36,36	0
5	CA	B	690	1/1	0.93	0.07	34,34,34,34	0
5	CA	B	689	1/1	0.97	0.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.