



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:36 AM UTC

PDB ID : 1V3L / pdb_00001v3l
Title : Crystal structure of F283L mutant cyclodextrin glycosyltransferase complexed with a pseudo-tetraose derived from acarbose
Authors : Kanai, R.; Haga, K.; Akiba, T.; Yamane, K.; Harata, K.
Deposited on : 2003-11-03
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

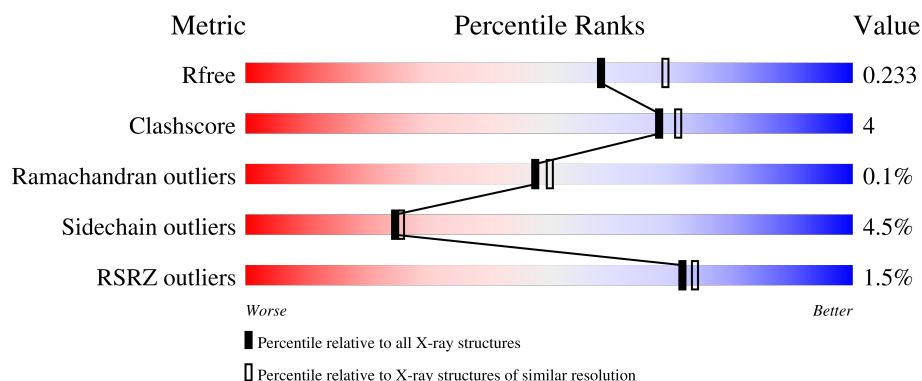
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2% 79% 17% .
1	B	686	% 79% 18% .
2	C	2	50% 50%
3	D	2	100%

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	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11214 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

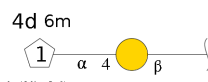
- Molecule 1 is a protein called Cyclomaltodextrin glucanotransferase.

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

There are 6 discrepancies between the modelled and reference sequences:

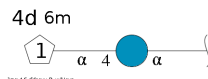
Chain	Residue	Modelled	Actual	Comment	Reference
A	283	LEU	PHE	engineered mutation	UNP P05618
A	452	PRO	ARG	SEE REMARK 999	UNP P05618
A	454	GLY	ALA	SEE REMARK 999	UNP P05618
B	283	LEU	PHE	engineered mutation	UNP P05618
B	452	PRO	ARG	SEE REMARK 999	UNP P05618
B	454	GLY	ALA	SEE REMARK 999	UNP P05618

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



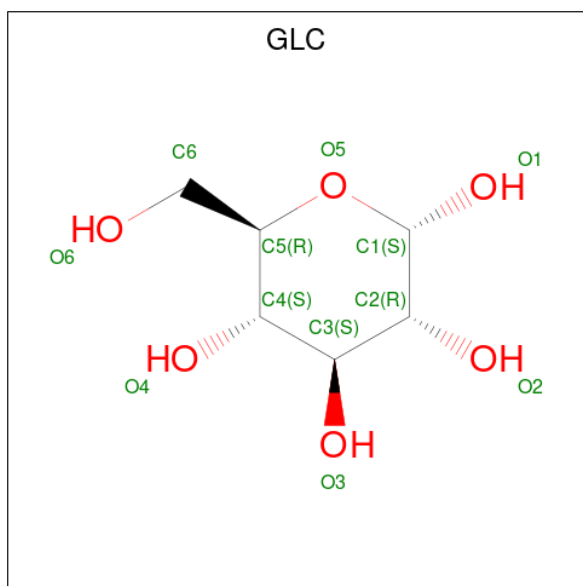
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 3 is an oligosaccharide called 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-alpha-D-glucopyranose.



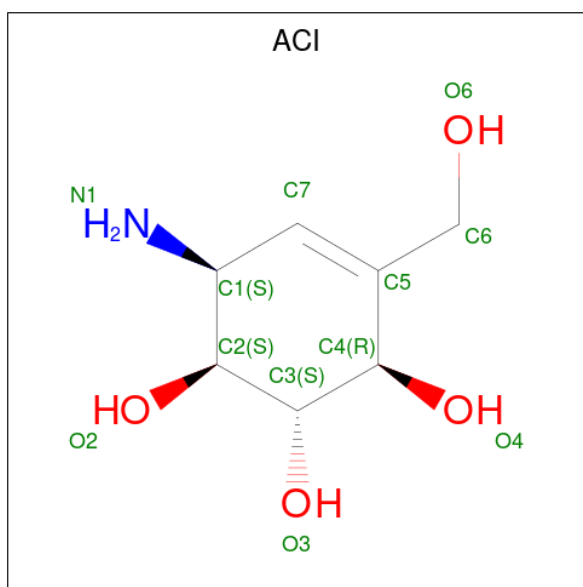
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			21	12	9			

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			12	7	1	4		
5	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

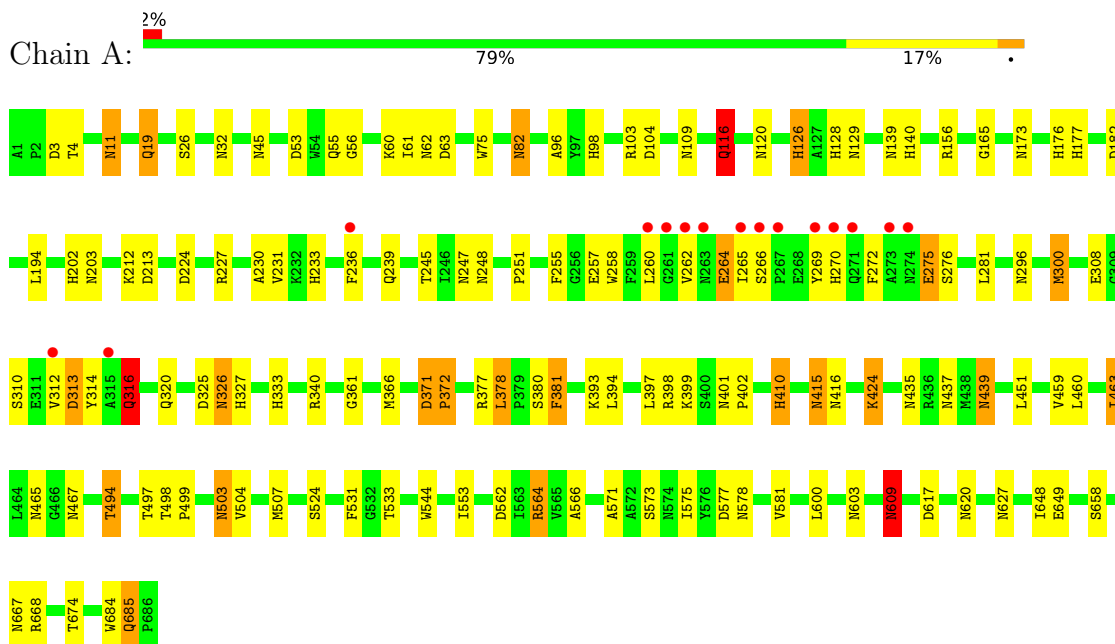
- Molecule 7 is water.

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

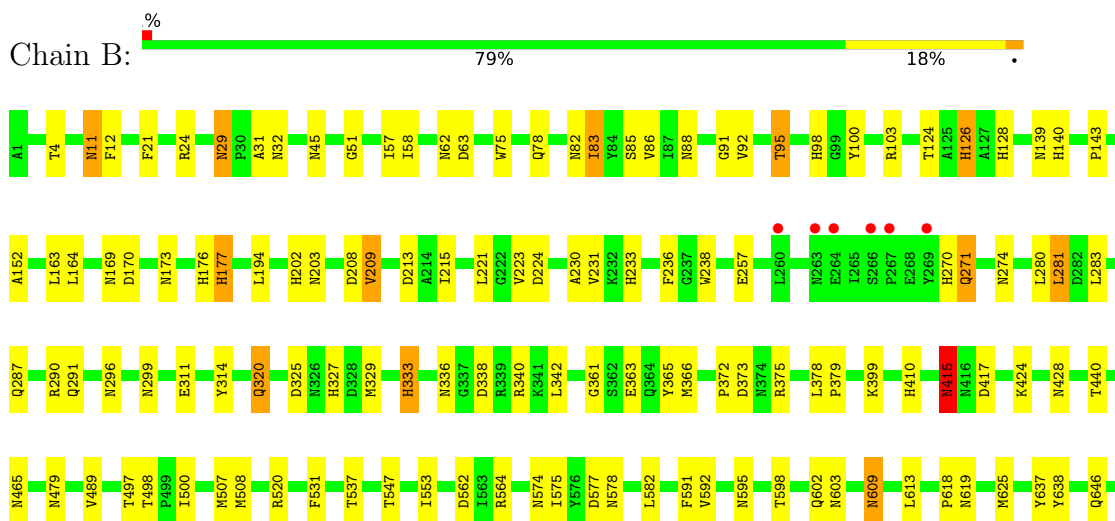
3 Residue-property plots

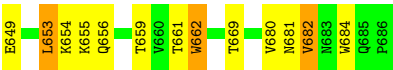
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

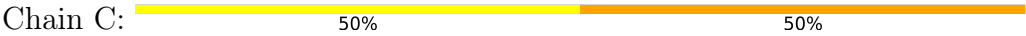


• Molecule 1: Cyclomaltodextrin glucanotransferase





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



- Molecule 3: 4,6-dideoxy-alpha-D-xylo-hexopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.97Å 73.71Å 80.08Å 85.47° 105.53° 101.43°	Depositor
Resolution (Å)	10.00 – 2.10 10.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	82.8 (10.00-2.10) 82.0 (10.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.09Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.169 , 0.232 0.169 , 0.233	Depositor DCC
R_{free} test set	4087 reflections (6.09%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11214	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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, GAL, GLC, GLD, 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	0.96	13/5442 (0.2%)	1.72	94/7424 (1.3%)
1	B	0.95	15/5442 (0.3%)	1.70	95/7424 (1.3%)
All	All	0.95	28/10884 (0.3%)	1.71	189/14848 (1.3%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	HIS	CD2-NE2	-7.47	1.29	1.37
1	A	128	HIS	CD2-NE2	-7.38	1.29	1.37
1	B	98	HIS	CD2-NE2	-7.33	1.29	1.37
1	B	126	HIS	CD2-NE2	-7.23	1.29	1.37
1	B	410	HIS	CD2-NE2	-7.11	1.30	1.37
1	B	176	HIS	CD2-NE2	-6.99	1.30	1.37
1	B	233	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	177	HIS	CD2-NE2	-6.87	1.30	1.37
1	B	333	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	176	HIS	CG-ND1	-6.71	1.30	1.38
1	A	327	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.67	1.30	1.37
1	B	327	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	233	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	202	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	333	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	140	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	270	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	128	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	270	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	209	VAL	CA-CB	5.85	1.61	1.54
1	B	177	HIS	CD2-NE2	-5.64	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	HIS	CG-ND1	-5.54	1.32	1.38
1	B	202	HIS	CD2-NE2	-5.45	1.31	1.37
1	B	83	ILE	CA-CB	5.24	1.59	1.54
1	A	177	HIS	CG-ND1	-5.12	1.32	1.38

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	ASN	CA-CB-CG	9.53	122.13	112.60
1	B	609	ASN	OD1-CG-ND2	-8.88	113.72	122.60
1	A	415	ASN	CA-CB-CG	8.64	121.24	112.60
1	A	116	GLN	CG-CD-NE2	8.46	129.09	116.40
1	B	415	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	B	100	TYR	N-CA-C	8.13	123.03	113.20
1	B	325	ASP	CA-CB-CG	8.08	120.68	112.60
1	A	98	HIS	CB-CG-CD2	-8.03	120.77	131.20
1	B	682	VAL	N-CA-CB	-8.02	101.30	112.52
1	A	313	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	437	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	B	203	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	A	32	ASN	CA-CB-CG	7.85	120.45	112.60
1	B	98	HIS	CB-CG-CD2	-7.73	121.16	131.20
1	A	19	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	B	327	HIS	CB-CG-CD2	-7.68	121.22	131.20
1	A	63	ASP	CA-CB-CG	7.59	120.19	112.60
1	A	116	GLN	OE1-CD-NE2	-7.53	115.07	122.60
1	B	95	THR	N-CA-CB	-7.49	98.52	111.55
1	B	415	ASN	CB-CG-ND2	7.47	127.61	116.40
1	A	129	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	A	126	HIS	CB-CG-CD2	-7.39	121.59	131.20
1	B	296	ASN	OD1-CG-ND2	-7.39	115.20	122.60
1	B	86	VAL	N-CA-C	-7.39	97.80	108.36
1	A	177	HIS	CB-CG-CD2	-7.35	121.65	131.20
1	B	29	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	A	398	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	A	98	HIS	CB-CG-ND1	7.05	133.27	122.70
1	B	11	ASN	OD1-CG-ND2	-7.04	115.56	122.60
1	B	21	PHE	N-CA-C	-7.02	96.20	108.20
1	B	410	HIS	CB-CG-CD2	-7.01	122.09	131.20
1	A	156	ARG	N-CA-C	6.98	120.35	110.23
1	B	320	GLN	OE1-CD-NE2	-6.97	115.63	122.60
1	B	338	ASP	CA-CB-CG	6.97	119.57	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	609	ASN	CB-CG-ND2	6.96	126.84	116.40
1	A	213	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	238	TRP	CG-CD2-CE3	6.70	140.60	133.90
1	A	424	LYS	CG-CD-CE	-6.65	96.01	111.30
1	A	377	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	A	165	GLY	CA-C-N	6.56	127.33	121.82
1	A	165	GLY	C-N-CA	6.56	127.33	121.82
1	A	609	ASN	N-CA-C	6.55	120.27	112.93
1	B	98	HIS	CB-CG-ND1	6.54	132.51	122.70
1	A	685	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	A	182	ASP	CA-CB-CG	6.53	119.13	112.60
1	B	609	ASN	N-CA-C	6.46	121.18	113.16
1	A	139	ASN	OD1-CG-ND2	-6.44	116.16	122.60
1	B	271	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	A	300	MET	N-CA-C	6.43	120.22	112.38
1	B	177	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	531	PHE	N-CA-C	-6.39	96.68	107.99
1	B	299	ASN	CA-CB-CG	6.30	118.90	112.60
1	B	103	ARG	N-CA-C	-6.27	106.26	114.04
1	B	78	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	A	11	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	296	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	336	ASN	CA-CB-CG	-6.19	106.41	112.60
1	A	320	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	248	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	296	ASN	CB-CG-ND2	6.16	125.64	116.40
1	B	29	ASN	CB-CG-ND2	6.14	125.61	116.40
1	A	3	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	489	VAL	N-CA-C	-6.07	99.38	108.12
1	A	325	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	609	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	55	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	684	TRP	CG-CD2-CE3	6.04	139.94	133.90
1	B	51	GLY	N-CA-C	6.01	121.63	114.48
1	A	177	HIS	CB-CG-ND1	6.01	131.71	122.70
1	B	63	ASP	CA-CB-CG	5.99	118.58	112.60
1	A	327	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	B	498	THR	CA-CB-OG1	-5.96	100.67	109.60
1	B	281	LEU	N-CA-C	-5.93	101.50	110.28
1	A	648	ILE	O-C-N	-5.92	116.82	122.98
1	A	314	TYR	N-CA-C	-5.91	99.76	109.40
1	A	371	ASP	CA-CB-CG	5.91	118.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	B	140	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	A	627	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	B	274	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	104	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	213	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	230	ALA	N-CA-C	5.83	119.44	111.39
1	B	236	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	270	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	A	424	LYS	N-CA-CB	-5.75	101.15	110.81
1	B	230	ALA	N-CA-C	5.75	119.56	111.52
1	B	75	TRP	N-CA-C	-5.74	99.05	108.41
1	A	203	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	53	ASP	N-CA-C	5.72	115.66	108.45
1	A	61	ILE	N-CA-C	-5.71	105.28	110.82
1	B	327	HIS	CB-CG-ND1	5.71	131.26	122.70
1	A	326	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	439	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	577	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	291	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	498	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	116	GLN	CA-CB-CG	-5.66	102.77	114.10
1	A	75	TRP	CG-CD2-CE3	5.65	139.55	133.90
1	A	308	GLU	CA-CB-CG	-5.63	102.84	114.10
1	A	276	SER	N-CA-C	5.62	117.40	111.28
1	B	553	ILE	CA-C-N	5.60	125.91	119.92
1	B	553	ILE	C-N-CA	5.60	125.91	119.92
1	A	684	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	A	255	PHE	CA-CB-CG	5.60	119.40	113.80
1	B	176	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	75	TRP	CA-CB-CG	5.57	124.17	113.60
1	A	128	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	428	ASN	N-CA-C	-5.55	100.63	109.96
1	A	316	GLN	CA-CB-CG	5.55	125.20	114.10
1	B	51	GLY	CA-C-N	5.55	125.25	119.92
1	B	51	GLY	C-N-CA	5.55	125.25	119.92
1	B	287	GLN	CA-CB-CG	5.55	125.20	114.10
1	B	646	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	603	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	553	ILE	CA-C-N	5.53	125.50	120.03
1	A	553	ILE	C-N-CA	5.53	125.50	120.03
1	B	497	THR	N-CA-CB	-5.53	102.02	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	62	ASN	N-CA-C	5.51	117.28	111.28
1	B	233	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	B	653	LEU	CA-CB-CG	5.50	135.56	116.30
1	B	646	GLN	CA-CB-CG	5.50	125.10	114.10
1	B	57	ILE	N-CA-C	-5.48	105.19	110.72
1	B	574	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	275	GLU	N-CA-C	5.46	119.94	113.12
1	B	680	VAL	N-CA-C	-5.46	99.89	107.80
1	B	479	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	202	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	B	577	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	238	TRP	CB-CG-CD1	-5.43	118.76	126.90
1	B	287	GLN	CB-CA-C	-5.42	102.14	110.81
1	A	394	LEU	N-CA-C	5.41	118.35	111.69
1	B	662	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	A	684	TRP	CB-CG-CD1	-5.41	118.79	126.90
1	B	271	GLN	CG-CD-NE2	5.40	124.51	116.40
1	A	239	GLN	CG-CD-NE2	5.40	124.50	116.40
1	A	381	PHE	CA-CB-CG	-5.40	108.40	113.80
1	B	314	TYR	N-CA-C	-5.40	100.44	109.24
1	B	373	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	109	ASN	N-CA-C	-5.36	101.49	109.42
1	B	238	TRP	CE2-CD2-CG	-5.36	100.77	107.20
1	B	329	MET	CG-SD-CE	-5.36	89.11	100.90
1	B	270	HIS	CB-CG-CD2	-5.35	124.25	131.20
1	B	363	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	290	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	B	32	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	503	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	667	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	233	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	A	581	VAL	N-CA-C	-5.29	101.91	108.89
1	B	208	ASP	CA-C-O	-5.28	115.27	120.82
1	A	544	TRP	CG-CD2-CE3	5.28	139.18	133.90
1	B	126	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	126	HIS	CB-CG-ND1	5.27	130.61	122.70
1	B	500	ILE	CA-CB-CG1	5.27	119.36	110.40
1	B	595	ASN	N-CA-C	5.25	118.96	112.24
1	A	617	ASP	CA-C-N	5.25	125.55	119.47
1	A	617	ASP	C-N-CA	5.25	125.55	119.47
1	B	500	ILE	CA-CB-CG2	-5.24	101.59	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	29	ASN	CA-C-N	5.23	125.03	119.28
1	B	29	ASN	C-N-CA	5.23	125.03	119.28
1	B	12	PHE	CA-CB-CG	5.22	119.02	113.80
1	B	140	HIS	CB-CG-ND1	5.19	130.49	122.70
1	A	310	SER	N-CA-C	5.18	117.01	111.36
1	B	564	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	620	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	B	152	ALA	CB-CA-C	-5.15	110.61	116.54
1	A	416	ASN	N-CA-C	5.14	118.32	111.75
1	B	619	ASN	CA-CB-CG	-5.13	107.47	112.60
1	B	92	VAL	N-CA-C	-5.13	100.26	107.75
1	B	139	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	467	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	B	78	GLN	CG-CD-NE2	5.08	124.02	116.40
1	B	440	THR	CA-C-N	5.08	125.01	119.78
1	B	440	THR	C-N-CA	5.08	125.01	119.78
1	B	531	PHE	N-CA-C	-5.08	97.61	107.62
1	B	684	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	A	316	GLN	CB-CG-CD	5.06	121.21	112.60
1	A	451	LEU	CA-C-N	5.05	125.03	120.03
1	A	451	LEU	C-N-CA	5.05	125.03	120.03
1	A	120	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	B	311	GLU	N-CA-C	5.05	117.52	111.71
1	A	564	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	312	VAL	N-CA-CB	-5.04	105.40	112.35
1	A	494	THR	OG1-CB-CG2	5.04	119.37	109.30
1	B	62	ASN	N-CA-C	5.04	117.66	111.82
1	A	45	ASN	N-CA-C	-5.00	99.64	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5309	0	5052	38	0
1	B	5309	0	5052	36	0
2	C	21	0	20	2	0
3	D	21	0	20	0	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
5	A	12	0	11	2	0
5	B	12	0	11	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	267	0	0	2	0
7	B	237	0	0	4	0
All	All	11214	0	10186	76	0

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

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:GLU:HG2	1:B:669:THR:HG22	1.69	0.73
5:A:702:ACI:C7	2:C:2:GLD:H63	2.23	0.68
1:A:260:LEU:HD13	1:A:265:ILE:HG13	1.76	0.67
1:B:378:LEU:HD12	1:B:379:PRO:HD2	1.76	0.67
1:A:397:LEU:HD11	1:A:459:VAL:HG11	1.79	0.63
1:B:340:ARG:HH12	1:B:465:ASN:HD22	1.45	0.62
1:B:361:GLY:HA3	1:B:366:MET:SD	2.39	0.62
1:A:116:GLN:HG3	7:A:1402:HOH:O	2.00	0.62
1:A:258:TRP:HB3	1:A:269:TYR:CD2	2.37	0.60
1:A:257:GLU:HB2	1:A:281:LEU:HD12	1.85	0.58
1:B:602:GLN:HG3	1:B:656:GLN:HB2	1.86	0.57
1:B:88:ASN:ND2	1:B:91:GLY:H	2.03	0.57
1:B:280:LEU:HB2	1:B:320:GLN:HE22	1.70	0.57
1:A:564:ARG:HD2	1:A:575:ILE:HD11	1.87	0.56
1:A:361:GLY:HA3	1:A:366:MET:SD	2.45	0.56
1:B:4:THR:HB	1:B:399:LYS:HD2	1.88	0.56
1:B:333:HIS:HD2	7:B:1387:HOH:O	1.90	0.55
1:A:562:ASP:HB3	1:A:575:ILE:HG23	1.90	0.53
1:B:625:MET:HG2	1:B:638:TYR:HB2	1.90	0.53
1:B:361:GLY:HA2	1:B:378:LEU:HD13	1.90	0.52
1:B:88:ASN:HD21	1:B:91:GLY:H	1.58	0.52
1:A:410:HIS:HE1	1:A:424:LYS:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:HB2	1:B:281:LEU:HD12	1.92	0.51
1:A:258:TRP:HB3	1:A:269:TYR:HD2	1.75	0.51
1:A:609:ASN:ND2	1:A:649:GLU:H	2.08	0.51
1:A:564:ARG:HD2	1:A:575:ILE:CD1	2.41	0.51
1:B:333:HIS:HE1	7:B:1224:HOH:O	1.92	0.51
1:B:83:ILE:HD12	1:B:85:SER:HB2	1.93	0.50
1:A:260:LEU:HB3	1:A:264:GLU:O	2.12	0.49
1:B:170:ASP:OD1	1:B:177:HIS:HE1	1.95	0.49
1:A:410:HIS:CE1	1:A:424:LYS:HB3	2.47	0.49
1:A:247:ASN:HA	1:A:251:PRO:HB3	1.94	0.49
1:B:24:ARG:HD2	1:B:375:ARG:O	2.13	0.49
1:B:126:HIS:HE1	1:B:224:ASP:OD1	1.94	0.49
1:B:520:ARG:HD3	1:B:547:THR:HG22	1.94	0.48
5:A:702:ACI:H7	2:C:2:GLD:H63	1.94	0.48
1:A:260:LEU:HD13	1:A:265:ILE:HA	1.96	0.47
1:B:591:PHE:O	1:B:637:TYR:HA	2.14	0.47
1:A:316:GLN:HG3	1:A:507:MET:HE2	1.96	0.47
1:A:4:THR:HB	1:A:399:LYS:HD2	1.96	0.47
1:A:668:ARG:NH1	1:A:685:GLN:HG3	2.29	0.46
1:A:266:SER:O	1:A:269:TYR:HB3	2.16	0.46
1:A:231:VAL:HB	1:A:272:PHE:CZ	2.51	0.46
1:A:499:PRO:HB2	1:A:573:SER:HB3	1.97	0.46
1:A:393:LYS:HE3	1:A:463:ILE:HD13	1.98	0.45
1:B:126:HIS:HD2	7:B:1342:HOH:O	1.99	0.45
1:B:598:THR:HB	1:B:602:GLN:HB3	1.97	0.45
1:B:603:ASN:O	1:B:654:LYS:HA	2.16	0.45
1:A:340:ARG:HH12	1:A:465:ASN:HD22	1.65	0.45
1:A:460:LEU:O	1:A:463:ILE:HB	2.16	0.45
1:B:340:ARG:HH12	1:B:465:ASN:ND2	2.15	0.45
1:A:26:SER:O	1:A:56:GLY:HA3	2.17	0.44
1:A:126:HIS:HE1	1:A:224:ASP:OD2	2.01	0.44
1:A:19:GLN:HE22	1:A:326:ASN:HB2	1.82	0.44
1:A:82:ASN:OD1	1:A:96:ALA:HB1	2.17	0.44
1:A:212:LYS:HB3	1:A:245:THR:HG21	2.00	0.43
1:B:231:VAL:HG22	1:B:257:GLU:O	2.18	0.43
1:B:29:ASN:HD21	1:B:31:ALA:HB3	1.84	0.43
1:A:401:ASN:HA	1:A:402:PRO:HD2	1.89	0.43
1:B:618:PRO:HG3	1:B:662:TRP:CZ2	2.54	0.42
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.74	0.42
1:A:566:ALA:HA	1:A:571:ALA:O	2.19	0.42
1:B:562:ASP:HB3	1:B:575:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HG23	1:B:124:THR:HG21	2.02	0.41
1:B:592:VAL:HB	1:B:681:ASN:HA	2.01	0.41
1:A:300:MET:HB2	1:A:415:ASN:O	2.20	0.41
1:A:371:ASP:HA	1:A:372:PRO:HA	1.81	0.41
1:B:508:MET:HE2	1:B:508:MET:HB3	1.92	0.41
1:A:11:ASN:ND2	7:A:1278:HOH:O	2.53	0.41
1:B:11:ASN:HB3	7:B:1330:HOH:O	2.19	0.41
1:B:415:ASN:HD22	1:B:417:ASP:H	1.69	0.41
1:B:655:LYS:HA	1:B:659:THR:O	2.20	0.41
1:B:215:ILE:HD12	1:B:215:ILE:HA	1.81	0.41
1:B:342:LEU:HD23	1:B:365:TYR:CD1	2.56	0.40
1:A:378:LEU:HD11	1:A:381:PHE:CZ	2.56	0.40
1:A:503:ASN:HD22	1:A:504:VAL:H	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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%)	19 (3%)	1 (0%)	48	50
1	B	684/686 (100%)	661 (97%)	23 (3%)	0	100	100
All	All	1368/1372 (100%)	1325 (97%)	42 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/564 (100%)	538 (95%)	26 (5%)	24	25
1	B	564/564 (100%)	539 (96%)	25 (4%)	25	26
All	All	1128/1128 (100%)	1077 (96%)	51 (4%)	24	25

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	103	ARG
1	A	116	GLN
1	A	173	ASN
1	A	194	LEU
1	A	227	ARG
1	A	236	PHE
1	A	264	GLU
1	A	275	GLU
1	A	313	ASP
1	A	316	GLN
1	A	372	PRO
1	A	378	LEU
1	A	380	SER
1	A	410	HIS
1	A	439	ASN
1	A	463	ILE
1	A	494	THR
1	A	497	THR
1	A	524	SER
1	A	533	THR
1	A	578	ASN
1	A	600	LEU
1	A	609	ASN
1	A	658	SER
1	A	674	THR
1	B	82	ASN

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Mol	Chain	Res	Type
1	B	95	THR
1	B	143	PRO
1	B	163	LEU
1	B	164	LEU
1	B	169	ASN
1	B	173	ASN
1	B	194	LEU
1	B	209	VAL
1	B	221	LEU
1	B	223	VAL
1	B	271	GLN
1	B	283	LEU
1	B	372	PRO
1	B	415	ASN
1	B	424	LYS
1	B	507	MET
1	B	537	THR
1	B	578	ASN
1	B	582	LEU
1	B	609	ASN
1	B	613	LEU
1	B	653	LEU
1	B	661	THR
1	B	682	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	ASN
1	A	19	GLN
1	A	62	ASN
1	A	126	HIS
1	A	128	HIS
1	A	160	ASN
1	A	173	ASN
1	A	274	ASN
1	A	370	ASN
1	A	465	ASN
1	A	503	ASN
1	A	548	GLN
1	A	550	GLN

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Mol	Chain	Res	Type
1	A	594	ASN
1	A	603	ASN
1	A	609	ASN
1	A	620	ASN
1	A	646	GLN
1	A	685	GLN
1	B	11	ASN
1	B	29	ASN
1	B	88	ASN
1	B	93	ASN
1	B	126	HIS
1	B	129	ASN
1	B	177	HIS
1	B	188	ASN
1	B	203	ASN
1	B	263	ASN
1	B	316	GLN
1	B	320	GLN
1	B	333	HIS
1	B	364	GLN
1	B	410	HIS
1	B	415	ASN
1	B	465	ASN
1	B	548	GLN
1	B	550	GLN
1	B	609	ASN
1	B	628	GLN
1	B	681	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 ⓘ

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	1.65	1 (8%)	17,17,17	1.31	2 (11%)
2	GLD	C	2	2,5	9,9,10	2.74	4 (44%)	11,12,14	2.28	3 (27%)
3	GLC	D	1	3	12,12,12	1.95	3 (25%)	17,17,17	1.49	5 (29%)
3	GLD	D	2	3,5	9,9,10	2.19	3 (33%)	11,12,14	2.38	5 (45%)

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	2,5	-	-	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLD	D	2	3,5	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GLD	O5-C5	4.83	1.48	1.44
2	C	2	GLD	C4-C5	4.81	1.60	1.52
3	D	2	GLD	C3-C2	4.21	1.58	1.52
3	D	1	GLC	C1-C2	3.92	1.61	1.52
2	C	1	GAL	C4-C5	3.53	1.60	1.53
2	C	2	GLD	C4-C3	3.50	1.59	1.52
3	D	2	GLD	C4-C5	3.37	1.57	1.52
3	D	1	GLC	C3-C2	3.29	1.60	1.52
3	D	2	GLD	C1-C2	2.99	1.59	1.52
3	D	1	GLC	C4-C5	2.30	1.57	1.53
2	C	2	GLD	O5-C1	2.27	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	GLD	C1-O5-C5	5.08	119.25	111.80
2	C	2	GLD	O2-C2-C1	5.05	120.79	109.22
2	C	2	GLD	C1-O5-C5	3.45	116.87	111.80
3	D	1	GLC	C1-C2-C3	3.08	116.63	110.36
2	C	1	GAL	O5-C5-C4	2.81	114.77	109.70
3	D	2	GLD	C3-C4-C5	-2.79	106.78	111.21
3	D	2	GLD	O5-C1-C2	2.73	117.30	110.79
3	D	2	GLD	O3-C3-C2	2.64	115.99	110.20
3	D	2	GLD	O5-C5-C4	-2.55	106.92	109.39
2	C	2	GLD	O5-C1-C2	-2.38	105.10	110.79
3	D	1	GLC	C3-C4-C5	-2.34	106.00	110.23
3	D	1	GLC	O4-C4-C5	2.26	114.88	109.32
2	C	1	GAL	C4-C3-C2	2.20	114.69	110.83
3	D	1	GLC	O5-C1-C2	2.17	114.11	110.30
3	D	1	GLC	O2-C2-C3	-2.17	105.27	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GAL	C4

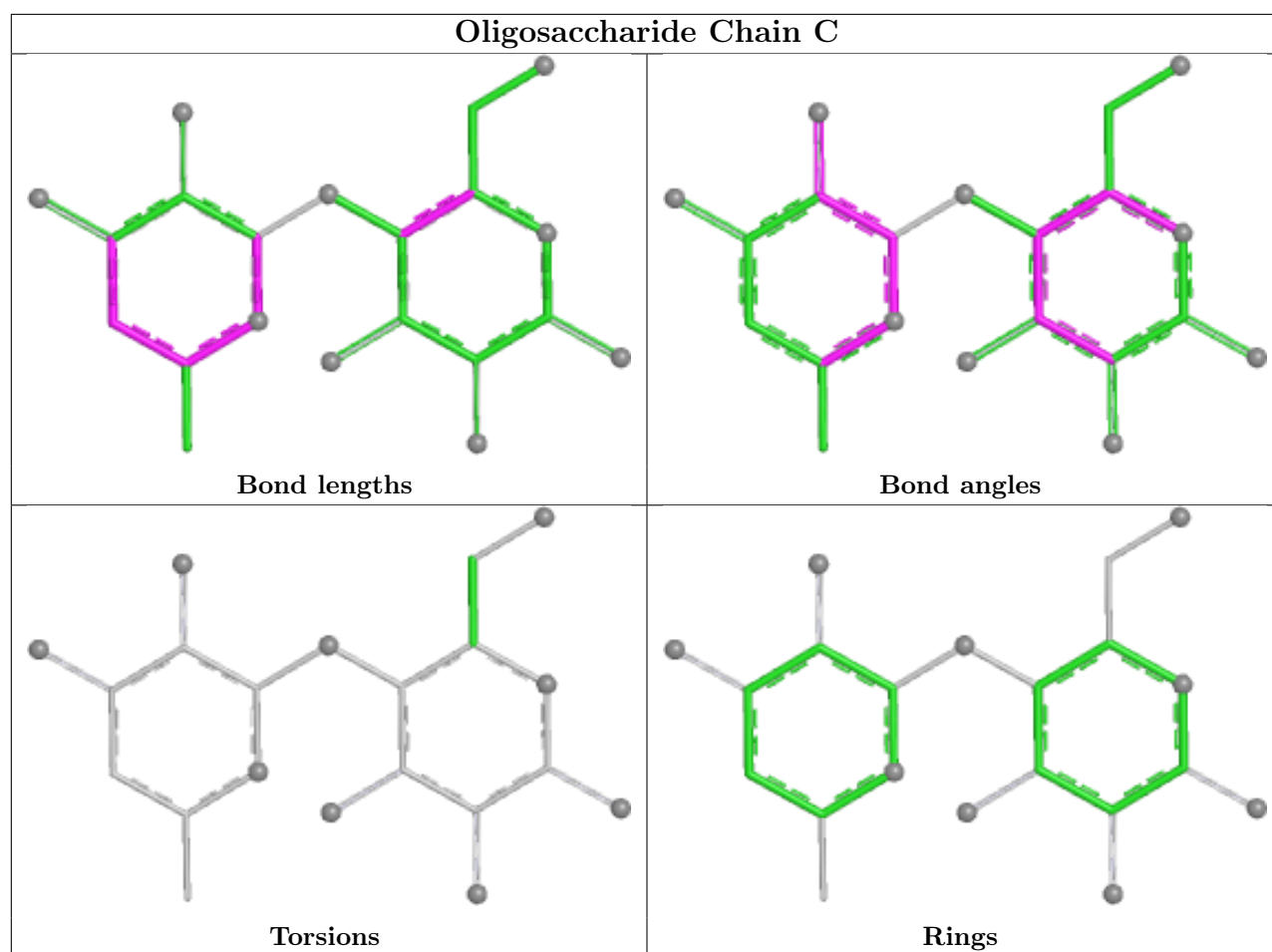
There are no torsion outliers.

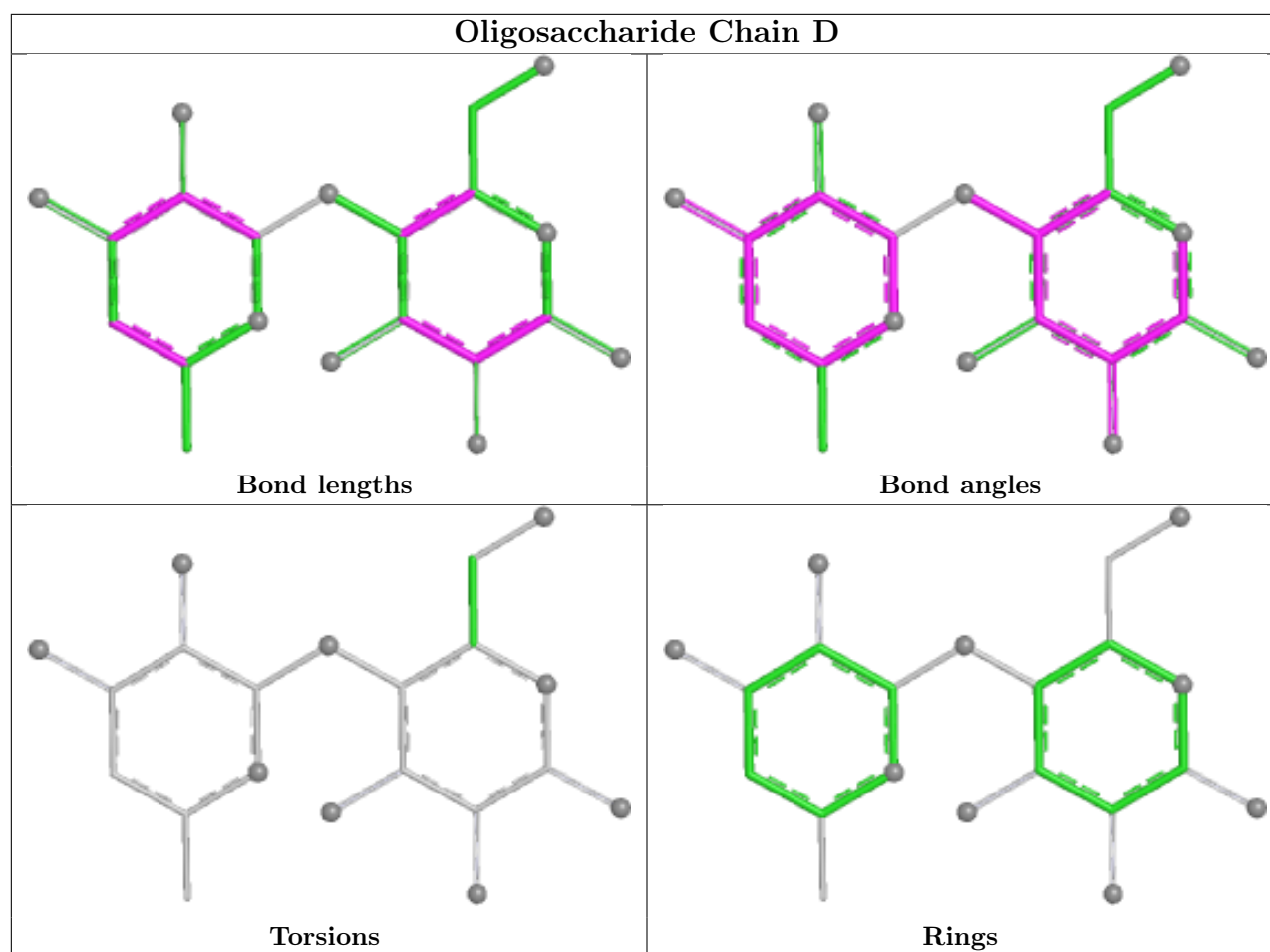
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLD	2	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	$\# Z > 2$
4	GLC	B	801	5	11,11,12	2.13	5 (45%)	15,15,17	1.72	4 (26%)
5	ACI	A	702	4,2	12,12,12	2.88	4 (33%)	11,17,17	1.72	3 (27%)
4	GLC	A	701	5	11,11,12	1.69	3 (27%)	15,15,17	2.02	6 (40%)
5	ACI	B	802	4,3	12,12,12	2.46	3 (25%)	11,17,17	1.89	2 (18%)

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
4	GLC	B	801	5	-	0/2/19/22	0/1/1/1
5	ACI	A	702	4,2	-	1/2/22/22	0/1/1/1
4	GLC	A	701	5	-	0/2/19/22	0/1/1/1
5	ACI	B	802	4,3	-	0/2/22/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	ACI	C7-C5	7.05	1.42	1.32
5	A	702	ACI	C7-C5	5.85	1.41	1.32
5	A	702	ACI	C3-C4	5.07	1.60	1.53
5	A	702	ACI	C4-C5	4.73	1.55	1.51
4	B	801	GLC	C1-C2	3.99	1.61	1.52
5	B	802	ACI	C4-C5	3.40	1.54	1.51
4	A	701	GLC	C1-C2	3.27	1.60	1.52
4	B	801	GLC	C4-C5	3.18	1.59	1.53
4	B	801	GLC	C2-C3	2.88	1.56	1.52
4	A	701	GLC	C4-C5	2.81	1.59	1.53
4	B	801	GLC	O5-C5	2.46	1.48	1.43
5	B	802	ACI	C1-C7	2.36	1.55	1.50
5	A	702	ACI	O4-C4	2.29	1.46	1.42
4	B	801	GLC	C4-C3	2.24	1.58	1.52
4	A	701	GLC	C4-C3	2.10	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	ACI	C2-C1-N1	-4.55	102.15	111.40
4	A	701	GLC	C3-C4-C5	-3.44	103.99	110.23
5	A	702	ACI	C2-C3-C4	-3.20	105.15	110.22
4	B	801	GLC	C1-O5-C5	3.05	116.27	112.19
5	A	702	ACI	O3-C3-C4	2.94	115.47	109.64
4	B	801	GLC	O2-C2-C1	2.91	115.89	109.22
4	A	701	GLC	C1-C2-C3	2.91	113.89	109.64
4	B	801	GLC	C1-C2-C3	2.89	113.85	109.64
4	B	801	GLC	O2-C2-C3	-2.84	104.28	110.15
5	B	802	ACI	O4-C4-C3	-2.65	105.02	110.53
4	A	701	GLC	O2-C2-C3	-2.30	105.38	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	GLC	C2-C3-C4	-2.23	106.93	110.86
4	A	701	GLC	O5-C5-C4	-2.19	105.49	110.83
5	A	702	ACI	O4-C4-C5	-2.15	106.66	110.75
4	A	701	GLC	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	ACI	C7-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	ACI	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.73	15 (2%) 62 65	4, 14, 35, 88	0
1	B	686/686 (100%)	-0.64	6 (0%) 81 83	6, 17, 44, 84	0
All	All	1372/1372 (100%)	-0.68	21 (1%) 72 74	4, 15, 43, 88	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	PRO	5.6
1	A	265	ILE	5.4
1	A	266	SER	4.2
1	A	269	TYR	4.2
1	A	261	GLY	3.3
1	A	312	VAL	3.3
1	A	263	ASN	3.1
1	A	273	ALA	3.0
1	A	315	ALA	2.9
1	A	260	LEU	2.9
1	B	267	PRO	2.9
1	A	270	HIS	2.8
1	A	274	ASN	2.5
1	B	260	LEU	2.5
1	A	271	GLN	2.4
1	A	262	VAL	2.4
1	B	269	TYR	2.3
1	A	236	PHE	2.1
1	B	266	SER	2.1
1	B	263	ASN	2.1
1	B	264	GLU	2.0

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

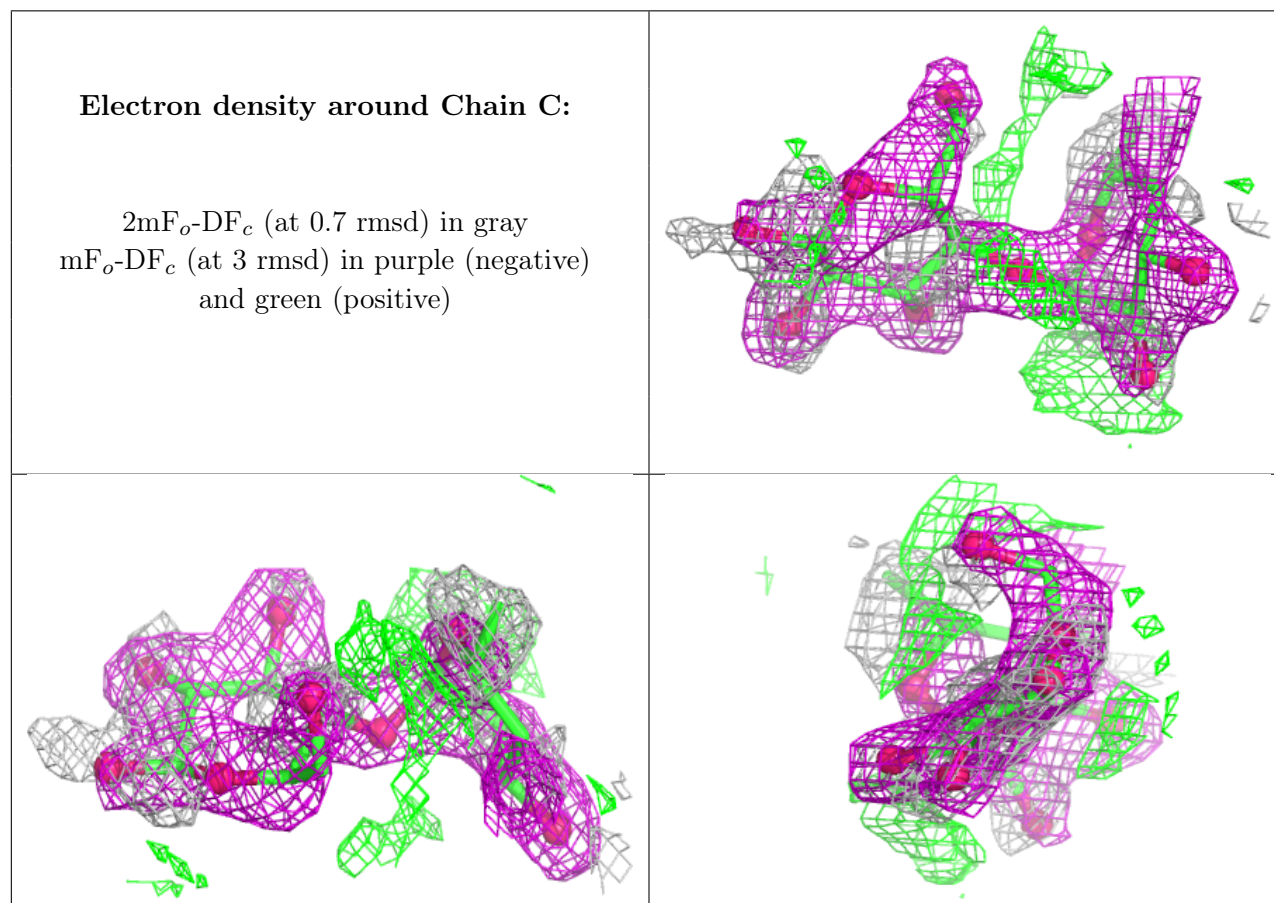
There are no non-standard protein/DNA/RNA residues in this entry.

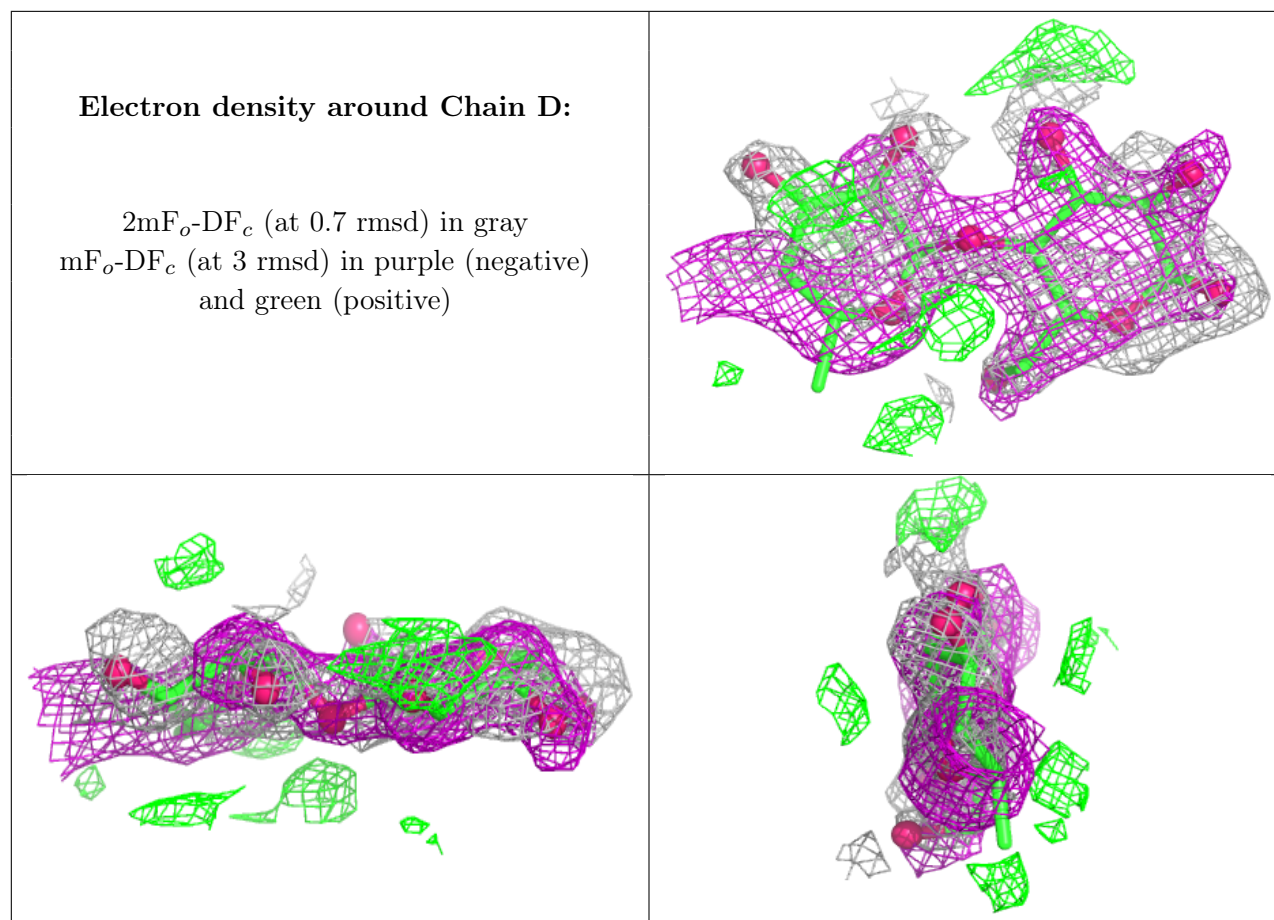
6.3 Carbohydrates [i](#)

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLD	C	2	9/10	0.54	0.13	15,26,34,35	0
3	GLD	D	2	9/10	0.63	0.14	17,23,35,36	0
2	GAL	C	1	12/12	0.69	0.11	16,25,35,37	0
3	GLC	D	1	12/12	0.70	0.10	15,24,29,36	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.





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(Å ²)	Q<0.9
5	ACI	A	702	12/12	0.52	0.29	8,25,32,33	0
4	GLC	B	801	11/12	0.60	0.29	18,23,32,37	0
5	ACI	B	802	12/12	0.64	0.27	15,20,32,41	0
4	GLC	A	701	11/12	0.77	0.23	7,19,29,37	0
6	CA	A	687	1/1	0.92	0.04	9,9,9,9	0
6	CA	A	688	1/1	0.92	0.10	21,21,21,21	0
6	CA	B	689	1/1	0.96	0.05	13,13,13,13	0
6	CA	B	690	1/1	0.96	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.