



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:45 AM UTC

PDB ID : 1CGU / pdb_00001cgu
Title : CATALYTIC CENTER OF CYCLODEXTRIN GLYCOSYLTRANSFERASE
DERIVED FROM X-RAY STRUCTURE ANALYSIS COMBINED WITH
SITE-DIRECTED MUTAGENESIS
Authors : Klein, C.; Hollender, J.; Bender, H.; Schulz, G.E.
Deposited on : 1992-06-10
Resolution : 2.50 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

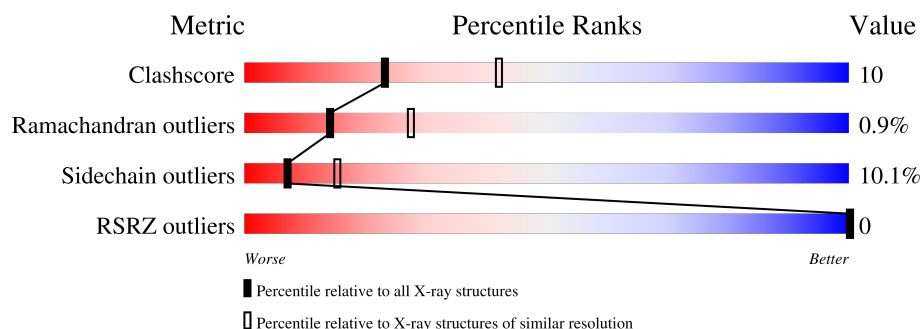
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	684	54% 35% 9%
2	B	2	50% 50%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5766 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 CYCLODEXTRIN GLYCOSYL-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	0	0	0
			5264	3322	891	1038	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ALA	ASP	conflict	UNP P30920

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

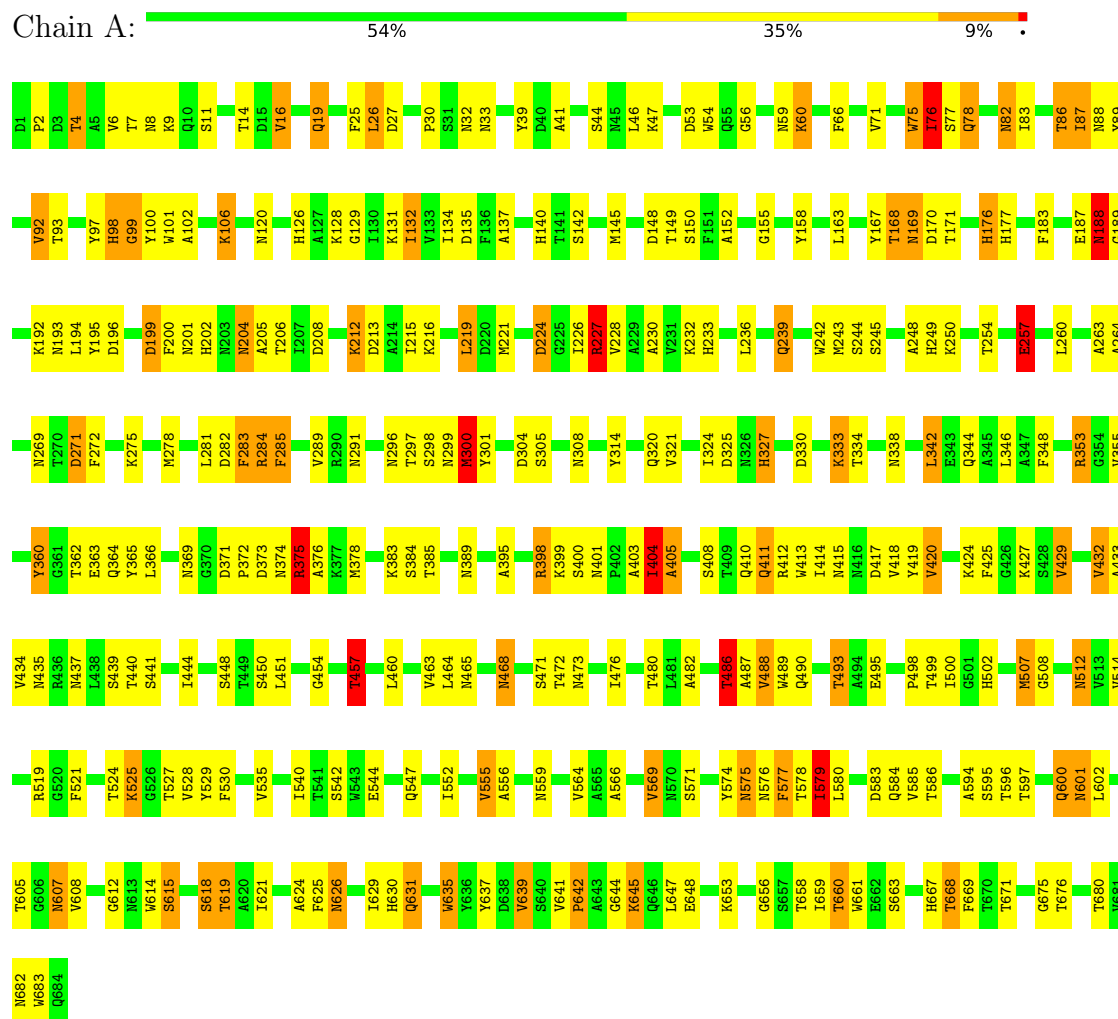
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	478	Total	O	0	0
			478	478		

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: CYCLODEXTRIN GLYCOSYL-TRANSFERASE



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.10Å 105.00Å 113.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 61.8 (10.00-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available) 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 30.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5766	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: CA, GLC

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	1.24	22/5395 (0.4%)	2.15	221/7362 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	HIS	CD2-NE2	-8.82	1.28	1.37
1	A	177	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	630	HIS	CG-ND1	-6.76	1.30	1.38
1	A	233	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	83	ILE	CA-CB	6.63	1.63	1.54
1	A	98	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	126	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	140	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	630	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	629	ILE	CA-CB	6.31	1.61	1.54
1	A	249	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	667	HIS	CD2-NE2	-6.23	1.31	1.37
1	A	176	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	314	TYR	CA-CB	-5.83	1.45	1.53
1	A	71	VAL	CA-CB	5.76	1.60	1.54
1	A	19	GLN	CA-CB	-5.57	1.45	1.53
1	A	176	HIS	CG-ND1	-5.54	1.32	1.38
1	A	202	HIS	CD2-NE2	-5.42	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	HIS	CG-ND1	-5.16	1.32	1.38
1	A	75	TRP	NE1-CE2	-5.11	1.31	1.37
1	A	327	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	502	HIS	CG-ND1	-5.05	1.32	1.38

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ARG	CB-CG-CD	-12.89	81.65	111.30
1	A	213	ASP	CA-CB-CG	12.05	124.65	112.60
1	A	597	THR	CA-CB-OG1	-10.15	94.37	109.60
1	A	417	ASP	CA-CB-CG	10.10	122.70	112.60
1	A	27	ASP	CA-CB-CG	9.96	122.56	112.60
1	A	656	GLY	O-C-N	9.86	127.37	121.85
1	A	245	SER	CA-CB-OG	9.81	130.72	111.10
1	A	385	THR	N-CA-C	9.64	122.96	110.53
1	A	656	GLY	N-CA-C	-9.23	101.81	110.21
1	A	82	ASN	OD1-CG-ND2	-9.13	113.47	122.60
1	A	576	ASN	OD1-CG-ND2	-8.99	113.61	122.60
1	A	659	ILE	N-CA-C	-8.58	97.54	109.21
1	A	92	VAL	N-CA-CB	-8.53	101.23	111.21
1	A	269	ASN	CB-CG-ND2	8.49	129.13	116.40
1	A	196	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	78	GLN	OE1-CD-NE2	-8.37	114.23	122.60
1	A	641	VAL	N-CA-CB	-8.22	99.70	111.21
1	A	32	ASN	OD1-CG-ND2	-8.15	114.45	122.60
1	A	320	GLN	CG-CD-NE2	8.15	128.63	116.40
1	A	86	THR	N-CA-CB	-7.81	97.71	110.43
1	A	188	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	415	ASN	CA-CB-CG	7.74	120.34	112.60
1	A	296	ASN	OD1-CG-ND2	-7.71	114.89	122.60
1	A	451	LEU	N-CA-C	-7.68	100.41	109.93
1	A	682	ASN	CA-CB-CG	-7.68	104.92	112.60
1	A	486	THR	CA-C-O	7.65	129.46	120.43
1	A	493	THR	CA-CB-OG1	-7.62	98.17	109.60
1	A	355	VAL	CA-C-N	7.55	128.66	120.13
1	A	355	VAL	C-N-CA	7.55	128.66	120.13
1	A	661	TRP	N-CA-C	7.52	120.23	110.53
1	A	202	HIS	CA-CB-CG	-7.50	106.30	113.80
1	A	53	ASP	N-CA-C	7.47	118.47	108.38
1	A	86	THR	CB-CA-C	7.47	122.07	109.75
1	A	257	GLU	O-C-N	7.46	132.07	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	A	585	VAL	O-C-N	-7.35	114.89	123.05
1	A	271	ASP	CA-CB-CG	7.30	119.91	112.60
1	A	269	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	597	THR	CA-CB-CG2	7.21	122.76	110.50
1	A	383	LYS	N-CA-C	-7.14	101.81	111.87
1	A	667	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	A	320	GLN	OE1-CD-NE2	-7.11	115.49	122.60
1	A	212	LYS	N-CA-C	-7.11	103.46	111.14
1	A	605	THR	CA-CB-OG1	-7.09	98.96	109.60
1	A	78	GLN	CG-CD-NE2	7.09	127.03	116.40
1	A	362	THR	N-CA-C	-7.02	103.97	112.54
1	A	88	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	A	444	ILE	N-CA-C	-6.99	97.66	107.80
1	A	219	LEU	N-CA-C	-6.98	103.67	111.28
1	A	297	THR	N-CA-C	-6.97	102.75	112.45
1	A	376	ALA	N-CA-C	6.97	119.52	110.53
1	A	82	ASN	CA-CB-CG	6.96	119.56	112.60
1	A	304	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	547	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	502	HIS	CB-CG-CD2	-6.92	122.21	131.20
1	A	60	LYS	N-CA-C	6.90	118.80	111.28
1	A	33	ASN	N-CA-C	-6.77	100.97	110.31
1	A	400	SER	N-CA-C	6.75	120.39	111.75
1	A	325	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	499	THR	CB-CA-C	6.72	120.48	110.14
1	A	360	TYR	N-CA-C	6.64	119.61	110.24
1	A	199	ASP	N-CA-C	6.62	119.38	109.25
1	A	305	SER	CB-CA-C	-6.61	100.51	110.88
1	A	101	TRP	CG-CD2-CE3	6.60	140.50	133.90
1	A	374	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	54	TRP	CG-CD2-CE3	6.54	140.44	133.90
1	A	321	VAL	N-CA-C	6.54	117.26	107.51
1	A	683	TRP	CG-CD2-CE3	6.54	140.44	133.90
1	A	584	GLN	CG-CD-NE2	6.52	126.19	116.40
1	A	473	ASN	CA-CB-CG	-6.52	106.08	112.60
1	A	200	PHE	N-CA-C	6.48	119.62	110.23
1	A	488	VAL	N-CA-C	-6.48	99.40	108.27
1	A	334	THR	N-CA-C	-6.45	99.50	109.24
1	A	59	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	A	87	ILE	CB-CG1-CD1	-6.42	100.32	113.80
1	A	239	GLN	CA-CB-CG	-6.41	101.28	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	PRO	N-CA-C	6.39	120.87	111.03
1	A	346	LEU	O-C-N	6.35	128.94	122.09
1	A	353	ARG	NE-CZ-NH2	-6.34	113.49	119.20
1	A	639	VAL	N-CA-C	6.34	118.52	108.89
1	A	204	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	248	ALA	N-CA-C	6.32	119.84	111.75
1	A	283	PHE	CA-CB-CG	-6.28	107.52	113.80
1	A	128	LYS	CA-CB-CG	-6.26	101.57	114.10
1	A	177	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	2	PRO	N-CA-C	6.21	121.09	111.21
1	A	535	VAL	N-CA-C	-6.20	99.44	108.11
1	A	398	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	A	597	THR	N-CA-CB	-6.14	101.83	111.05
1	A	493	THR	CA-CB-CG2	6.13	120.91	110.50
1	A	364	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	A	205	ALA	N-CA-C	6.09	118.71	111.71
1	A	249	HIS	CA-C-N	-6.08	116.93	122.28
1	A	249	HIS	C-N-CA	-6.08	116.93	122.28
1	A	468	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	584	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	A	66	PHE	CA-C-O	6.04	126.82	120.42
1	A	441	SER	CA-CB-OG	6.02	123.15	111.10
1	A	528	VAL	N-CA-CB	-6.01	104.15	111.00
1	A	371	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	54	TRP	N-CA-C	5.95	118.53	111.33
1	A	168	THR	N-CA-C	-5.94	102.12	110.50
1	A	614	TRP	CG-CD2-CE3	5.94	139.84	133.90
1	A	200	PHE	CA-C-O	5.94	127.72	121.19
1	A	101	TRP	N-CA-C	-5.92	103.19	110.65
1	A	412	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	A	576	ASN	N-CA-C	5.89	119.48	111.17
1	A	92	VAL	N-CA-C	5.88	116.57	107.99
1	A	405	ALA	N-CA-C	5.87	118.63	111.82
1	A	308	ASN	N-CA-C	5.83	118.42	111.71
1	A	176	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	A	170	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	401	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	89	TYR	CB-CA-C	-5.78	101.54	110.78
1	A	227	ARG	CB-CG-CD	5.77	124.57	111.30
1	A	408	SER	N-CA-CB	-5.77	102.11	110.36
1	A	205	ALA	CA-C-O	-5.76	113.59	120.10
1	A	529	TYR	N-CA-C	5.75	118.03	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	VAL	O-C-N	-5.74	117.15	123.18
1	A	512	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	495	GLU	N-CA-C	-5.71	102.84	110.55
1	A	454	GLY	O-C-N	-5.71	118.44	123.92
1	A	375	ARG	N-CA-C	5.71	117.84	110.65
1	A	342	LEU	CA-C-N	5.69	128.18	120.38
1	A	342	LEU	C-N-CA	5.69	128.18	120.38
1	A	669	PHE	O-C-N	-5.67	116.96	123.42
1	A	16	VAL	N-CA-C	-5.66	99.35	107.78
1	A	305	SER	N-CA-CB	5.65	118.21	110.01
1	A	228	VAL	N-CA-C	5.63	116.87	109.21
1	A	204	ASN	CB-CG-ND2	5.63	124.85	116.40
1	A	320	GLN	N-CA-C	5.63	118.61	110.28
1	A	366	LEU	N-CA-C	5.63	118.39	110.23
1	A	41	ALA	O-C-N	5.63	127.87	122.07
1	A	384	SER	CA-C-O	-5.62	112.87	119.05
1	A	427	LYS	CG-CD-CE	5.62	124.22	111.30
1	A	8	ASN	N-CA-C	5.61	118.52	107.98
1	A	682	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	101	TRP	CE2-CD2-CG	-5.59	100.50	107.20
1	A	82	ASN	CB-CG-ND2	5.54	124.72	116.40
1	A	683	TRP	CE2-CD2-CG	-5.54	100.55	107.20
1	A	47	LYS	CA-CB-CG	-5.54	103.02	114.10
1	A	465	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	579	ILE	CA-CB-CG1	-5.51	101.03	110.40
1	A	556	ALA	O-C-N	-5.48	116.07	122.81
1	A	30	PRO	CA-N-CD	-5.47	104.35	112.00
1	A	54	TRP	O-C-N	-5.46	116.33	122.12
1	A	667	HIS	N-CA-C	-5.46	102.40	110.48
1	A	242	TRP	CG-CD2-CE3	5.45	139.35	133.90
1	A	512	ASN	O-C-N	-5.44	116.44	122.86
1	A	285	PHE	CA-CB-CG	5.43	119.23	113.80
1	A	206	THR	CB-CA-C	-5.40	102.41	110.88
1	A	495	GLU	CA-C-N	5.39	129.78	121.53
1	A	495	GLU	C-N-CA	5.39	129.78	121.53
1	A	482	ALA	N-CA-C	5.38	117.03	110.41
1	A	137	ALA	O-C-N	-5.38	115.13	121.32
1	A	77	SER	CA-CB-OG	5.37	121.84	111.10
1	A	76	ILE	CA-C-N	5.36	128.85	120.75
1	A	76	ILE	C-N-CA	5.36	128.85	120.75
1	A	4	THR	N-CA-CB	-5.36	102.23	110.16
1	A	272	PHE	CA-C-O	-5.36	115.38	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	VAL	CB-CA-C	5.34	118.30	110.98
1	A	132	ILE	N-CA-C	5.32	116.63	108.71
1	A	577	PHE	N-CA-C	-5.31	101.04	109.96
1	A	284	ARG	CA-CB-CG	5.30	124.71	114.10
1	A	11	SER	CA-C-O	5.30	126.96	120.60
1	A	193	ASN	CB-CA-C	-5.30	101.64	109.90
1	A	521	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	667	HIS	CB-CG-ND1	5.30	130.65	122.70
1	A	457	THR	CA-CB-OG1	-5.29	101.67	109.60
1	A	264	ALA	CA-C-O	5.29	127.01	121.19
1	A	527	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	158	TYR	CA-C-O	5.26	126.11	120.38
1	A	75	TRP	CG-CD2-CE3	5.25	139.16	133.90
1	A	169	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	404	ILE	CA-CB-CG1	5.24	119.30	110.40
1	A	163	LEU	N-CA-C	5.23	116.69	109.15
1	A	93	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	224	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	635	TRP	CE2-CD2-CG	-5.23	100.92	107.20
1	A	39	TYR	N-CA-C	5.22	117.97	109.24
1	A	201	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	327	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	320	GLN	N-CA-CB	-5.21	102.31	109.97
1	A	559	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	282	ASP	CA-C-O	5.18	127.19	121.39
1	A	605	THR	CA-CB-CG2	5.17	119.30	110.50
1	A	204	ASN	CA-C-O	5.17	126.77	120.62
1	A	348	PHE	CA-C-O	-5.16	115.40	121.07
1	A	489	TRP	O-C-N	-5.16	117.07	123.36
1	A	499	THR	N-CA-CB	-5.15	102.38	110.77
1	A	27	ASP	N-CA-CB	-5.14	103.17	110.58
1	A	344	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	189	GLY	CA-C-N	5.14	128.74	122.63
1	A	189	GLY	C-N-CA	5.14	128.74	122.63
1	A	320	GLN	O-C-N	-5.14	116.62	122.89
1	A	177	HIS	N-CA-C	-5.13	99.88	110.80
1	A	450	SER	N-CA-CB	-5.12	103.78	111.25
1	A	330	ASP	O-C-N	5.12	128.74	122.96
1	A	378	MET	CA-C-N	5.11	126.22	119.84
1	A	378	MET	C-N-CA	5.11	126.22	119.84
1	A	363	GLU	CB-CG-CD	5.10	121.26	112.60
1	A	99	GLY	CA-C-O	-5.09	113.51	119.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ASN	CB-CG-ND2	5.09	124.03	116.40
1	A	420	VAL	N-CA-C	-5.09	100.24	107.77
1	A	575	ASN	N-CA-C	5.09	117.85	110.17
1	A	398	ARG	CA-CB-CG	-5.08	103.94	114.10
1	A	188	ASN	N-CA-CB	-5.07	101.97	110.39
1	A	473	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	530	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	230	ALA	N-CA-C	5.06	118.37	111.39
1	A	8	ASN	CB-CG-ND2	-5.05	108.82	116.40
1	A	301	TYR	O-C-N	-5.04	116.87	122.07
1	A	413	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	342	LEU	CA-CB-CG	5.03	133.91	116.30
1	A	600	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	A	411	GLN	CB-CG-CD	-5.02	104.07	112.60
1	A	614	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	A	434	VAL	CB-CA-C	-5.02	101.82	110.65
1	A	167	TYR	N-CA-C	5.01	116.55	111.14
1	A	680	THR	CA-C-O	5.01	125.55	120.24
1	A	97	TYR	N-CA-C	5.01	118.16	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5264	0	5009	106	0
2	B	22	0	19	1	0
3	A	2	0	0	0	0
4	A	478	0	0	17	1
All	All	5766	0	5028	106	1

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 10.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:HG23	1:A:399:LYS:HD2	1.61	0.82
1:A:226:ILE:HB	1:A:254:THR:HG23	1.71	0.73
1:A:76:ILE:HD11	1:A:134:ILE:HG22	1.70	0.70
1:A:227:ARG:NH1	1:A:257:GLU:HG2	2.08	0.69
1:A:300:MET:HG3	1:A:419:TYR:HB2	1.75	0.68
1:A:291:ASN:HB3	1:A:298:SER:HB2	1.77	0.66
1:A:9:LYS:HD3	1:A:224:ASP:HA	1.78	0.65
1:A:653:LYS:HB2	1:A:660:THR:HG23	1.79	0.65
1:A:498:PRO:HB2	1:A:571:SER:HB3	1.80	0.64
1:A:414:ILE:HA	1:A:418:VAL:O	2.00	0.62
1:A:75:TRP:CZ2	1:A:227:ARG:HG3	2.34	0.61
1:A:460:LEU:HB3	1:A:463:VAL:HG22	1.83	0.60
1:A:410:GLN:HA	4:A:888:HOH:O	2.01	0.59
1:A:6:VAL:HA	1:A:131:LYS:HE2	1.85	0.59
1:A:596:THR:HB	1:A:600:GLN:HB3	1.84	0.58
1:A:92:VAL:HA	4:A:1210:HOH:O	2.03	0.57
1:A:580:LEU:HD23	4:A:731:HOH:O	2.06	0.56
1:A:586:THR:HB	1:A:676:THR:HG22	1.87	0.55
1:A:512:ASN:O	1:A:552:ILE:HG12	2.07	0.55
1:A:87:ILE:HG12	1:A:152:ALA:HB2	1.87	0.55
1:A:26:LEU:O	1:A:56:GLY:HA3	2.07	0.54
1:A:525:LYS:HD2	1:A:540:ILE:HB	1.89	0.54
1:A:263:ALA:O	1:A:284:ARG:HD3	2.07	0.53
1:A:432:VAL:HG22	1:A:488:VAL:HG22	1.90	0.53
1:A:25:PHE:HE2	1:A:60:LYS:HG3	1.74	0.53
1:A:463:VAL:HG23	1:A:464:LEU:HG	1.90	0.52
1:A:260:LEU:HB2	1:A:283:PHE:HB3	1.92	0.52
1:A:424:LYS:HG3	1:A:429:VAL:HG13	1.91	0.51
1:A:420:VAL:HG22	1:A:433:ALA:HA	1.94	0.50
1:A:612:GLY:HA2	1:A:619:THR:HB	1.94	0.50
1:A:648:GLU:HG3	1:A:668:THR:HG23	1.93	0.50
1:A:176:HIS:HB2	1:A:199:ASP:HB3	1.92	0.50
1:A:215:ILE:O	1:A:219:LEU:HG	2.12	0.49
1:A:285:PHE:CE1	1:A:289:VAL:HG21	2.47	0.49
1:A:78:GLN:HB3	1:A:99:GLY:O	2.13	0.49
1:A:25:PHE:CE2	1:A:60:LYS:HG3	2.47	0.48
1:A:98:HIS:HD2	1:A:100:TYR:H	1.60	0.48
1:A:612:GLY:O	1:A:615:SER:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:HB3	4:A:808:HOH:O	2.13	0.48
1:A:500:ILE:HD11	1:A:564:VAL:HG23	1.93	0.48
1:A:145:MET:HB2	1:A:148:ASP:HB3	1.96	0.48
1:A:464:LEU:HB3	1:A:486:THR:HG23	1.96	0.48
1:A:500:ILE:HG21	1:A:574:TYR:HB2	1.96	0.47
1:A:14:THR:HB	1:A:399:LYS:HD3	1.97	0.47
1:A:16:VAL:HG21	1:A:395:ALA:HB1	1.97	0.47
1:A:621:ILE:HG21	1:A:639:VAL:HG22	1.96	0.46
1:A:6:VAL:HG11	1:A:129:GLY:HA2	1.97	0.46
1:A:608:VAL:HA	4:A:1191:HOH:O	2.16	0.46
1:A:168:THR:HA	4:A:916:HOH:O	2.16	0.46
1:A:19:GLN:HB2	1:A:75:TRP:CE3	2.51	0.46
1:A:403:ALA:HA	1:A:425:PHE:HB2	1.96	0.46
1:A:232:LYS:NZ	4:A:757:HOH:O	2.48	0.46
1:A:607:ASN:HB2	4:A:1268:HOH:O	2.16	0.46
1:A:142:SER:OG	1:A:155:GLY:HA2	2.15	0.45
1:A:398:ARG:O	1:A:405:ALA:HB2	2.16	0.45
1:A:424:LYS:HZ2	1:A:429:VAL:HG22	1.79	0.45
1:A:435:ASN:OD1	1:A:437:ASN:HB3	2.15	0.45
1:A:637:TYR:HE2	4:A:767:HOH:O	1.99	0.45
1:A:243:MET:HE3	1:A:278:MET:HE2	1.98	0.45
1:A:507:MET:HG3	1:A:578:THR:HB	1.98	0.45
1:A:188:ASN:OD1	1:A:192:LYS:HD2	2.17	0.45
1:A:327:HIS:O	1:A:375:ARG:NH1	2.50	0.45
1:A:324:ILE:HD13	1:A:324:ILE:HG21	1.76	0.45
1:A:239:GLN:O	1:A:243:MET:HB2	2.17	0.45
1:A:131:LYS:HE3	4:A:762:HOH:O	2.17	0.45
1:A:457:THR:HA	1:A:468:ASN:OD1	2.17	0.45
1:A:626:ASN:O	1:A:631:GLN:HA	2.17	0.45
1:A:601:ASN:O	1:A:653:LYS:HA	2.17	0.44
1:A:132:ILE:HA	1:A:132:ILE:HD13	1.72	0.44
1:A:187:GLU:CD	1:A:625:PHE:HB3	2.42	0.44
1:A:216:LYS:HA	1:A:219:LEU:HD12	2.00	0.44
1:A:98:HIS:CD2	1:A:100:TYR:H	2.36	0.44
1:A:566:ALA:O	1:A:569:VAL:HG22	2.18	0.44
1:A:82:ASN:HA	1:A:102:ALA:HA	2.00	0.44
1:A:271:ASP:O	1:A:275:LYS:HG3	2.18	0.43
1:A:106:LYS:NZ	4:A:1263:HOH:O	2.50	0.43
1:A:369:ASN:O	1:A:373:ASP:HB2	2.18	0.43
1:A:602:LEU:HD12	1:A:602:LEU:HA	1.82	0.43
1:A:333:LYS:NZ	4:A:1178:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HG2	1:A:404:ILE:CG2	2.49	0.42
1:A:594:ALA:HB3	1:A:635:TRP:CD1	2.54	0.42
1:A:647:LEU:O	1:A:668:THR:HA	2.20	0.42
1:A:644:GLY:HA2	1:A:671:THR:O	2.20	0.42
1:A:257:GLU:OE2	2:B:1:GLC:C1	2.68	0.42
1:A:624:ALA:HA	1:A:637:TYR:CD1	2.54	0.42
1:A:389:ASN:OD1	1:A:463:VAL:HG11	2.20	0.42
1:A:76:ILE:HD11	1:A:134:ILE:CG2	2.44	0.42
1:A:471:SER:HA	1:A:476:ILE:HD13	2.02	0.42
1:A:621:ILE:HD13	1:A:639:VAL:HG11	2.02	0.42
1:A:645:LYS:NZ	4:A:1032:HOH:O	2.53	0.42
1:A:183:PHE:N	1:A:188:ASN:HD21	2.18	0.42
1:A:195:TYR:HA	4:A:835:HOH:O	2.20	0.41
1:A:555:VAL:CG2	1:A:579:ILE:HD12	2.50	0.41
1:A:208:ASP:O	1:A:212:LYS:HG3	2.20	0.41
1:A:507:MET:HE2	1:A:507:MET:HB3	1.94	0.41
1:A:519:ARG:HA	1:A:519:ARG:HD3	1.62	0.41
1:A:188:ASN:HB2	4:A:897:HOH:O	2.21	0.41
1:A:353:ARG:O	1:A:353:ARG:HD3	2.20	0.41
1:A:433:ALA:HB3	1:A:487:ALA:HB3	2.02	0.41
1:A:583:ASP:O	1:A:642:PRO:HA	2.21	0.41
1:A:618:SER:HA	4:A:945:HOH:O	2.20	0.41
1:A:514:VAL:HG13	1:A:552:ILE:HD11	2.02	0.40
1:A:514:VAL:HG11	1:A:577:PHE:CZ	2.55	0.40
1:A:257:GLU:HB3	1:A:281:LEU:HD12	2.03	0.40
1:A:508:GLY:HA3	1:A:512:ASN:HD22	1.86	0.40
1:A:675:GLY:HA3	4:A:1044:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1160:HOH:O	4:A:1235:HOH:O[3_645]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	682/684 (100%)	618 (91%)	58 (8%)	6 (1%)	14 27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	ASN
1	A	607	ASN
1	A	300	MET
1	A	365	TYR
1	A	7	THR
1	A	525	LYS

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	565/565 (100%)	508 (90%)	57 (10%)	7 15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	44	SER
1	A	46	LEU
1	A	76	ILE
1	A	86	THR
1	A	106	LYS
1	A	120	ASN
1	A	135	ASP
1	A	149	THR
1	A	150	SER
1	A	169	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	171	THR
1	A	188	ASN
1	A	194	LEU
1	A	204	ASN
1	A	221	MET
1	A	227	ARG
1	A	236	LEU
1	A	244	SER
1	A	250	LYS
1	A	257	GLU
1	A	300	MET
1	A	333	LYS
1	A	338	ASN
1	A	342	LEU
1	A	372	PRO
1	A	375	ARG
1	A	404	ILE
1	A	411	GLN
1	A	429	VAL
1	A	439	SER
1	A	440	THR
1	A	448	SER
1	A	457	THR
1	A	472	THR
1	A	480	THR
1	A	486	THR
1	A	490	GLN
1	A	493	THR
1	A	507	MET
1	A	524	THR
1	A	542	SER
1	A	555	VAL
1	A	569	VAL
1	A	575	ASN
1	A	579	ILE
1	A	595	SER
1	A	601	ASN
1	A	615	SER
1	A	618	SER
1	A	619	THR
1	A	631	GLN
1	A	645	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	658	THR
1	A	660	THR
1	A	663	SER
1	A	668	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	98	HIS
1	A	178	ASN
1	A	203	ASN
1	A	204	ASN
1	A	570	ASN
1	A	592	ASN
1	A	631	GLN
1	A	646	GLN

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 ⓘ

2 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	GLC	B	1	2	11,11,12	0.93	0	15,15,17	2.47	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	B	2	2	11,11,12	0.98	0	15,15,17	1.72	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
2	GLC	B	1	2	-	0/2/19/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O4-C4-C3	-5.17	98.20	110.38
2	B	2	GLC	C1-O5-C5	4.73	118.53	112.19
2	B	1	GLC	C1-C2-C3	-4.37	103.29	109.64
2	B	1	GLC	C1-O5-C5	4.36	118.03	112.19
2	B	1	GLC	O2-C2-C1	3.17	116.49	109.22
2	B	2	GLC	C3-C4-C5	-2.32	106.03	110.23
2	B	1	GLC	O4-C4-C5	2.26	114.89	109.32
2	B	1	GLC	O2-C2-C3	2.04	114.37	110.15
2	B	2	GLC	O4-C4-C5	2.03	114.32	109.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

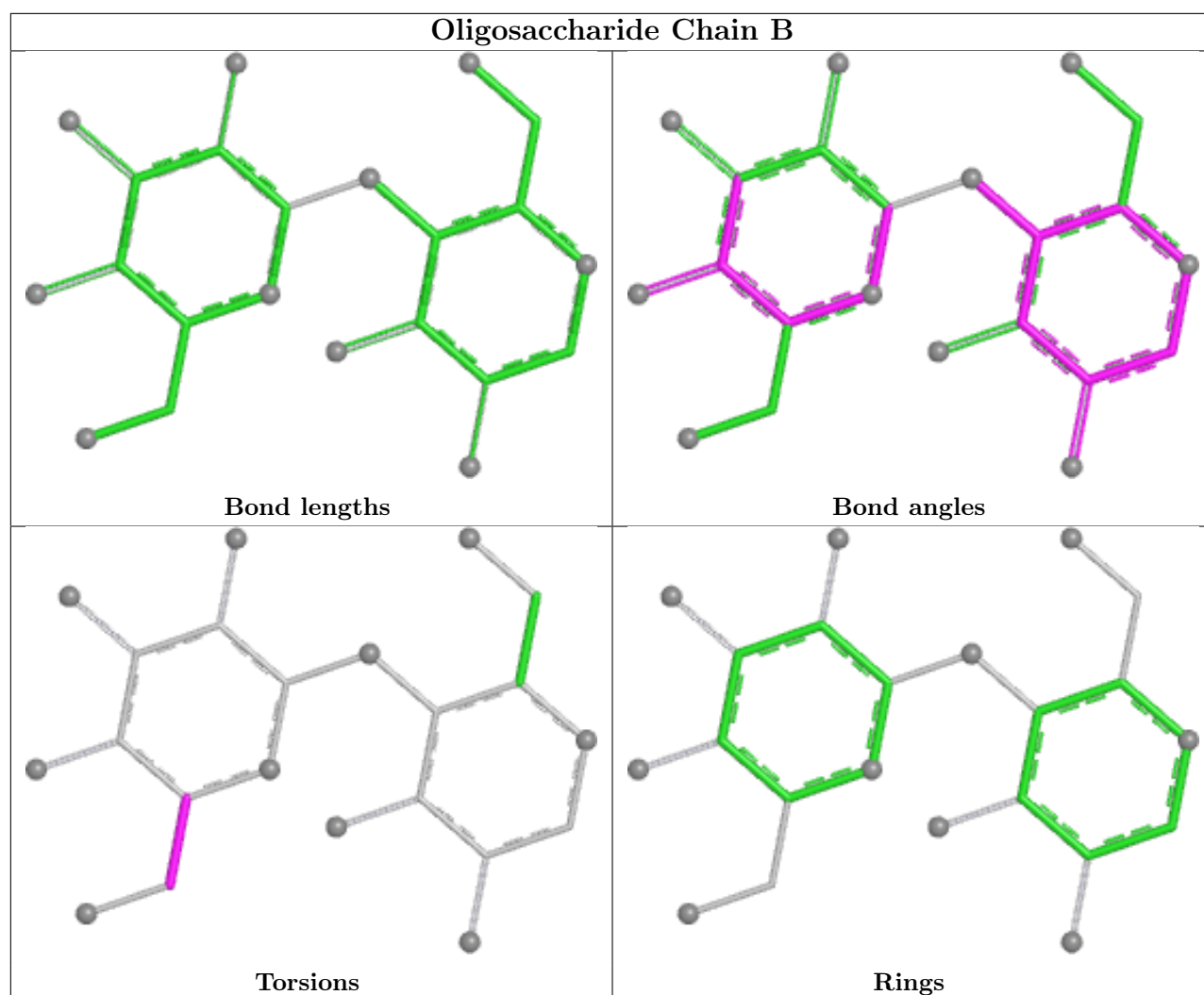
Mol	Chain	Res	Type	Atoms
2	B	2	GLC	O5-C5-C6-O6
2	B	2	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GLC	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 2 ligands modelled in this entry, 2 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	684/684 (100%)	-1.62	0 100 100	2, 11, 29, 40	0

There are no RSRZ outliers to report.

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

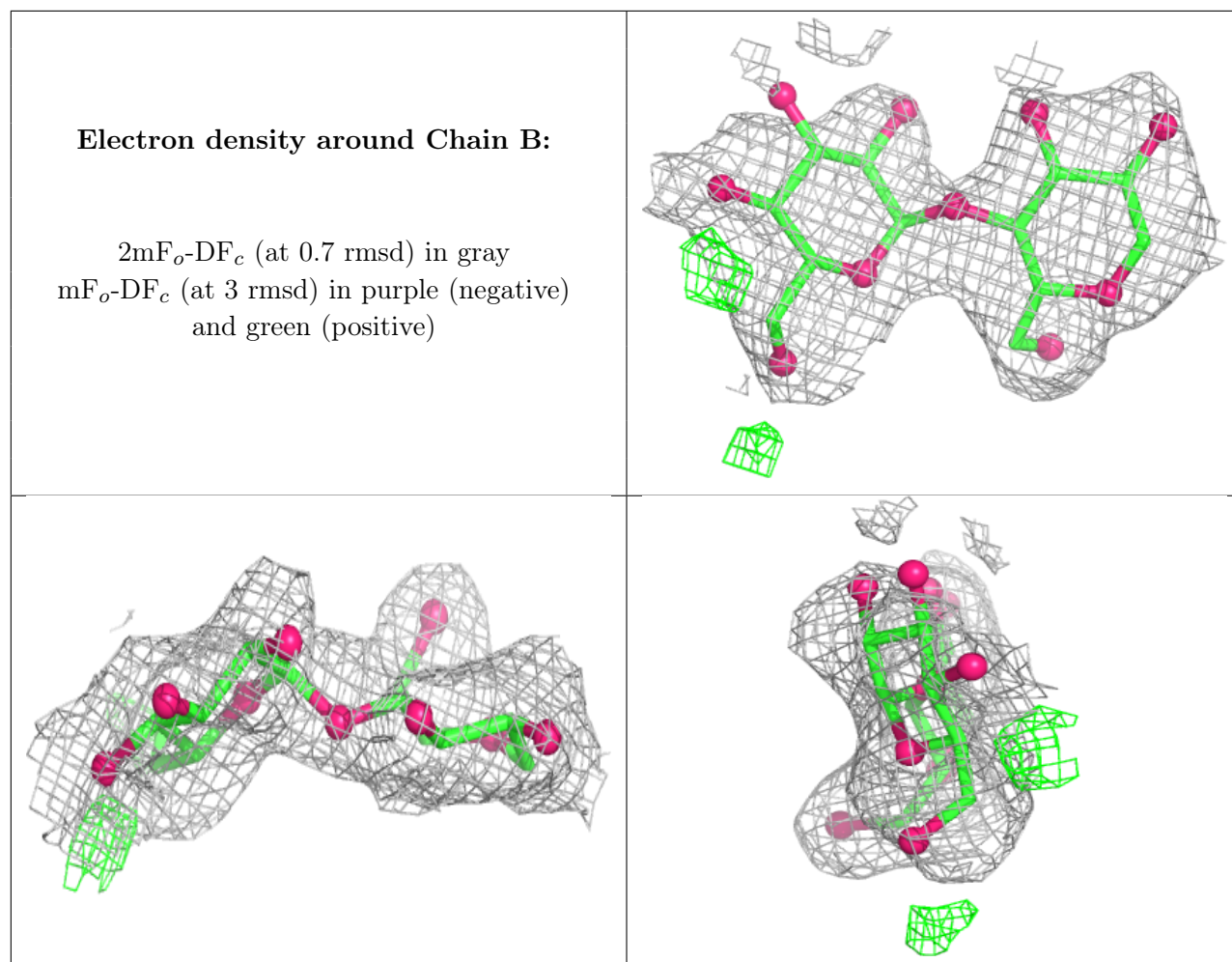
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	GLC	B	1	11/12	0.99	0.04	25,28,37,40	11
2	GLC	B	2	11/12	0.99	0.05	24,35,39,44	11

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($\text{\AA}^2$)	Q<0.9
3	CA	A	685	1/1	0.98	0.03	4,4,4,4	0
3	CA	A	686	1/1	1.00	0.04	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.