



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:34 PM EDT

PDB ID : 3LDK / pdb_00003ldk
Title : Crystal Structure of A. japonicus CB05
Authors : Chuankhayan, P.; Chen, C.J.; Chaing, C.M.; Hsieh, C.Y.; Chen, C.D.; Hsieh, Y.C.
Deposited on : 2010-01-13
Resolution : 2.20 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

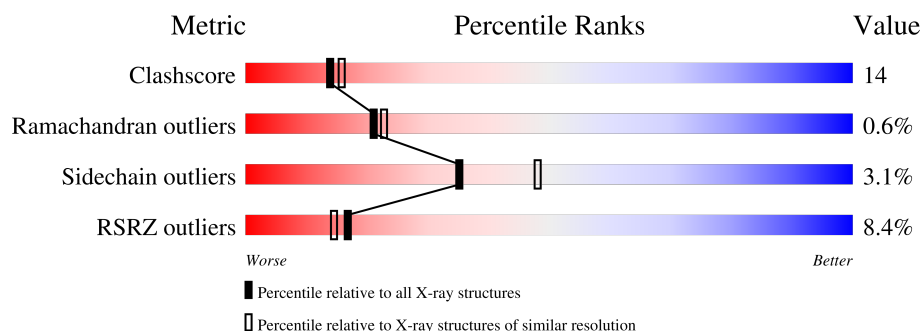
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	634	
2	B	2	

2 Entry composition [i](#)

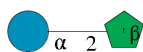
There are 3 unique types of molecules in this entry. The entry contains 5134 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			4883	3091	824	965	3			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total	O	0	0
			228	228		

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: Fructosyltransferase



• Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.35Å 110.97Å 66.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.6 (30.00-2.20) 88.6 (30.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.264 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5134	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: GLC, FRU

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	0.70	25/5014 (0.5%)	1.09	46/6858 (0.7%)

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	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PHE	C-N	11.11	1.47	1.33
1	A	216	ALA	C-N	10.77	1.47	1.33
1	A	545	ASN	C-N	10.54	1.47	1.33
1	A	166	ARG	C-N	-7.95	1.23	1.33
1	A	167	ARG	C-N	7.87	1.44	1.33
1	A	580	ILE	C-N	7.82	1.44	1.33
1	A	163	ASP	C-N	7.69	1.44	1.33
1	A	61	PRO	C-N	-7.59	1.24	1.33
1	A	284	ALA	C-N	7.56	1.43	1.33
1	A	102	GLY	C-N	7.46	1.44	1.33
1	A	76	GLY	C-N	-7.43	1.24	1.33
1	A	455	ASN	C-N	6.84	1.43	1.33
1	A	454	ASP	C-N	-6.79	1.24	1.33
1	A	476	LEU	C-N	-6.68	1.25	1.33
1	A	285	GLY	C-N	6.55	1.43	1.33
1	A	93	ALA	C-N	6.41	1.42	1.33
1	A	164	GLY	C-N	-6.36	1.25	1.33
1	A	581	GLU	C-N	6.01	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	SER	C-N	5.77	1.41	1.33
1	A	161	ALA	C-N	-5.76	1.26	1.33
1	A	101	ASN	C-N	-5.74	1.24	1.33
1	A	215	THR	C-N	5.73	1.41	1.33
1	A	456	GLN	CA-C	5.70	1.60	1.52
1	A	162	ARG	C-N	5.41	1.41	1.33
1	A	645	GLY	C-N	5.03	1.40	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	ASP	N-CA-C	-14.13	96.00	113.38
1	A	26	THR	N-CA-C	-8.42	102.78	113.72
1	A	477	ALA	O-C-N	-7.35	114.50	122.07
1	A	61	PRO	N-CA-C	-7.11	99.80	111.68
1	A	190	ARG	N-CA-C	7.05	117.90	108.38
1	A	345	SER	O-C-N	7.01	132.23	121.23
1	A	345	SER	CA-C-N	-6.98	111.62	122.37
1	A	345	SER	C-N-CA	-6.98	111.62	122.37
1	A	122	VAL	N-CA-C	6.66	118.06	108.48
1	A	608	ARG	O-C-N	-6.50	114.17	121.84
1	A	321	GLY	N-CA-C	-6.39	102.82	112.60
1	A	357	SER	N-CA-C	-6.30	106.19	114.31
1	A	556	SER	N-CA-C	6.29	118.67	108.41
1	A	164	GLY	CA-C-N	6.26	133.20	120.80
1	A	164	GLY	C-N-CA	6.26	133.20	120.80
1	A	188	ALA	O-C-N	6.04	130.36	123.48
1	A	275	SER	N-CA-C	-5.99	100.58	109.86
1	A	240	HIS	O-C-N	-5.95	114.92	123.07
1	A	345	SER	CB-CA-C	-5.91	109.74	116.54
1	A	123	ILE	N-CA-C	-5.83	101.25	107.77
1	A	309	GLY	N-CA-C	5.81	118.16	111.36
1	A	376	LEU	CA-C-N	5.79	125.74	119.78
1	A	376	LEU	C-N-CA	5.79	125.74	119.78
1	A	101	ASN	CA-C-N	-5.75	114.47	122.86
1	A	101	ASN	C-N-CA	-5.75	114.47	122.86
1	A	362	LEU	N-CA-C	-5.71	105.04	112.23
1	A	299	LEU	N-CA-C	5.71	119.36	110.17
1	A	42	PHE	N-CA-C	5.68	118.21	111.33
1	A	93	ALA	N-CA-C	-5.65	106.43	113.55
1	A	346	GLU	O-C-N	-5.64	115.37	122.19
1	A	596	VAL	CA-C-N	-5.62	114.04	122.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	VAL	C-N-CA	-5.62	114.04	122.24
1	A	244	PRO	CA-C-N	-5.40	111.23	121.54
1	A	244	PRO	C-N-CA	-5.40	111.23	121.54
1	A	345	SER	N-CA-C	5.34	116.42	108.31
1	A	370	ALA	N-CA-C	5.30	118.71	111.39
1	A	285	GLY	O-C-N	5.27	128.08	122.60
1	A	618	TRP	N-CA-C	5.25	119.66	112.68
1	A	227	LYS	N-CA-C	5.17	119.08	112.87
1	A	157	SER	N-CA-C	5.15	117.71	110.14
1	A	236	SER	N-CA-C	5.14	118.44	110.17
1	A	46	ARG	N-CA-C	5.13	116.88	109.48
1	A	346	GLU	N-CA-C	-5.12	105.72	112.94
1	A	177	ILE	N-CA-C	-5.08	98.78	109.34
1	A	627	PHE	N-CA-C	-5.07	102.98	110.48
1	A	244	PRO	O-C-N	5.00	129.06	122.86

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	ASP	Mainchain
1	A	455	ASN	Mainchain,Peptide
1	A	477	ALA	Mainchain

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	4883	0	4610	137	0
2	B	23	0	21	1	0
3	A	228	0	0	2	0
All	All	5134	0	4631	137	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 14.

All (137) 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:454:ASP:HB2	1:A:456:GLN:CG	1.67	1.25
1:A:454:ASP:CB	1:A:456:GLN:HG2	1.84	1.08
1:A:45:TRP:HB3	1:A:599:ALA:HB2	1.40	1.02
1:A:45:TRP:HB3	1:A:599:ALA:CB	1.97	0.95
1:A:344:GLY:HA2	1:A:353:GLU:OE1	1.77	0.85
1:A:454:ASP:HB2	1:A:456:GLN:HG2	0.87	0.84
1:A:454:ASP:O	1:A:455:ASN:HB2	1.76	0.82
1:A:207:ASP:HB2	1:A:210:VAL:HB	1.64	0.80
1:A:216:ALA:HA	1:A:219:GLN:OE1	1.83	0.79
1:A:531:ALA:O	1:A:624:GLN:HB2	1.81	0.79
1:A:164:GLY:HA3	1:A:166:ARG:NH1	2.00	0.76
1:A:295:ASN:HD21	1:A:373:GLY:H	1.33	0.76
1:A:33:LEU:H	1:A:562:ASN:HD21	1.31	0.75
1:A:295:ASN:ND2	1:A:373:GLY:H	1.85	0.75
1:A:45:TRP:CB	1:A:599:ALA:HB2	2.18	0.72
1:A:450:VAL:HG13	1:A:458:ALA:HB1	1.70	0.72
1:A:332:HIS:HD2	1:A:369:TYR:CE1	2.08	0.71
1:A:496:PRO:HB2	1:A:624:GLN:HE22	1.55	0.71
1:A:251:GLN:OE1	1:A:256:ALA:HA	1.91	0.71
1:A:475:LEU:HD22	1:A:646:LEU:HD22	1.73	0.70
1:A:213:ASN:HD22	1:A:215:THR:HB	1.56	0.70
1:A:332:HIS:HB3	1:A:369:TYR:CE2	2.27	0.69
1:A:452:GLU:O	1:A:458:ALA:HA	1.93	0.69
1:A:213:ASN:ND2	1:A:216:ALA:H	1.90	0.68
1:A:379:SER:O	1:A:384:LYS:HE2	1.93	0.68
1:A:454:ASP:CB	1:A:456:GLN:CG	2.58	0.67
1:A:46:ARG:O	1:A:598:ASN:ND2	2.30	0.65
1:A:332:HIS:HB3	1:A:369:TYR:CD2	2.32	0.64
1:A:439:GLU:H	1:A:439:GLU:CD	2.06	0.63
1:A:435:VAL:HG21	1:A:460:LEU:HD13	1.79	0.63
1:A:538:ALA:HB3	1:A:551:ASP:HB3	1.80	0.62
1:A:523:LEU:C	1:A:523:LEU:HD23	2.24	0.62
1:A:29:PRO:HB3	1:A:618:TRP:CE2	2.34	0.61
1:A:85:ALA:HA	1:A:104:PHE:HA	1.83	0.60
1:A:45:TRP:CE2	1:A:616:ARG:HB3	2.37	0.60
1:A:513:GLU:OE1	1:A:638:ARG:HD2	2.02	0.59
1:A:208:GLU:O	1:A:212:ARG:HG2	2.02	0.58
1:A:332:HIS:CD2	1:A:369:TYR:CE1	2.92	0.58
1:A:450:VAL:CG1	1:A:458:ALA:HB1	2.34	0.57
1:A:57:GLN:HG3	1:A:80:ASP:HA	1.87	0.57
1:A:196:ARG:HD3	1:A:226:GLU:OE2	2.06	0.56
1:A:506:PHE:CZ	1:A:596:VAL:HG21	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:HB2	1:A:360:GLY:HA2	1.87	0.55
1:A:295:ASN:HB2	1:A:314:THR:OG1	2.05	0.55
1:A:312:PHE:CE1	1:A:338:ALA:HB2	2.42	0.55
1:A:580:ILE:HA	1:A:584:GLN:O	2.07	0.55
1:A:298:PHE:CE1	1:A:311:VAL:HG22	2.42	0.54
1:A:29:PRO:HB3	1:A:618:TRP:CD2	2.42	0.54
1:A:316:GLY:HA2	1:A:333:ASP:O	2.07	0.54
1:A:199:ARG:HH11	1:A:199:ARG:HG3	1.73	0.54
1:A:57:GLN:HB2	1:A:418:THR:HB	1.90	0.54
1:A:606:ASN:HD22	1:A:606:ASN:N	2.06	0.54
1:A:582:ASN:C	1:A:584:GLN:N	2.65	0.53
1:A:82:ASP:OD2	1:A:107:GLN:NE2	2.42	0.53
1:A:154:GLU:OE2	1:A:190:ARG:HD3	2.09	0.52
1:A:591:ASP:H	1:A:606:ASN:HD21	1.57	0.52
1:A:605:ALA:HB3	1:A:609:PHE:HB3	1.90	0.52
1:A:431:THR:HA	1:A:460:LEU:O	2.10	0.52
1:A:202:VAL:HG21	1:A:221:VAL:HG22	1.90	0.52
1:A:435:VAL:HB	1:A:458:ALA:O	2.10	0.52
1:A:318:GLU:OE2	2:B:1:GLC:O3	2.26	0.52
1:A:579:VAL:O	1:A:585:GLU:HA	2.10	0.52
1:A:591:ASP:H	1:A:606:ASN:ND2	2.08	0.52
1:A:30:PRO:HG2	1:A:33:LEU:HD23	1.92	0.51
1:A:99:SER:OG	1:A:103:SER:HA	2.10	0.51
1:A:162:ARG:O	1:A:163:ASP:HB3	2.10	0.51
1:A:128:ASN:O	1:A:130:THR:HG23	2.11	0.51
1:A:25:THR:HG21	1:A:44:LEU:HD13	1.92	0.50
1:A:438:ASN:OD1	1:A:440:LEU:HB2	2.11	0.50
1:A:198:ALA:O	1:A:202:VAL:HG23	2.12	0.50
1:A:164:GLY:HA3	1:A:166:ARG:HH11	1.75	0.50
1:A:340:GLU:CD	1:A:340:GLU:N	2.70	0.49
1:A:451:GLY:N	1:A:459:THR:O	2.42	0.49
1:A:297:LEU:HD12	1:A:297:LEU:N	2.28	0.49
1:A:315:LEU:N	1:A:315:LEU:HD23	2.27	0.49
1:A:161:ALA:HB2	1:A:168:PHE:CZ	2.47	0.49
1:A:213:ASN:HD21	1:A:216:ALA:HB2	1.79	0.48
1:A:206:LEU:HB2	1:A:211:ALA:HB2	1.96	0.47
1:A:207:ASP:HB2	1:A:210:VAL:CB	2.40	0.47
1:A:332:HIS:C	1:A:369:TYR:CE2	2.92	0.47
1:A:298:PHE:HE1	1:A:311:VAL:HG22	1.80	0.47
1:A:244:PRO:O	1:A:245:ALA:HB2	2.15	0.47
1:A:215:THR:O	1:A:219:GLN:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASN:C	1:A:584:GLN:H	2.23	0.46
1:A:91:ASN:O	1:A:92:LEU:HB3	2.16	0.46
1:A:602:GLU:HG2	1:A:612:SER:OG	2.15	0.46
1:A:38:ASN:OD1	1:A:413:ALA:HB1	2.15	0.46
1:A:454:ASP:HB2	1:A:456:GLN:CD	2.34	0.46
1:A:33:LEU:H	1:A:562:ASN:ND2	2.06	0.46
1:A:364:TRP:CE3	1:A:572:GLY:HA2	2.52	0.45
1:A:585:GLU:HG2	1:A:586:GLN:N	2.31	0.45
1:A:597:ASP:O	1:A:598:ASN:CB	2.62	0.45
1:A:344:GLY:O	1:A:347:GLN:OE1	2.35	0.45
1:A:130:THR:OG1	1:A:160:VAL:HG13	2.16	0.45
1:A:296:VAL:C	1:A:297:LEU:HD12	2.42	0.45
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.32	0.44
1:A:202:VAL:HG21	1:A:221:VAL:CG2	2.48	0.44
1:A:364:TRP:HB2	1:A:611:LEU:HD13	1.99	0.44
1:A:180:HIS:HA	1:A:189:PHE:CZ	2.52	0.44
1:A:276:SER:CB	1:A:286:ARG:HA	2.48	0.44
1:A:488:THR:O	1:A:489:LEU:HD23	2.17	0.44
1:A:72:LEU:HD12	3:A:686:HOH:O	2.18	0.44
1:A:299:LEU:HG	1:A:428:LYS:HA	1.99	0.44
1:A:515:PRO:O	1:A:516:ALA:C	2.61	0.44
1:A:542:GLN:O	1:A:546:GLU:CA	2.65	0.43
1:A:397:VAL:HB	1:A:422:LEU:HD12	2.00	0.43
1:A:460:LEU:N	1:A:460:LEU:HD12	2.33	0.43
1:A:90:ALA:O	1:A:382:VAL:HA	2.18	0.43
1:A:312:PHE:CD1	1:A:338:ALA:HB2	2.53	0.43
1:A:160:VAL:HG23	1:A:171:LEU:HD21	2.01	0.43
1:A:334:MET:HG3	1:A:362:LEU:HB3	2.01	0.42
1:A:368:ALA:O	1:A:369:TYR:HB2	2.18	0.42
1:A:332:HIS:CB	1:A:369:TYR:CE2	3.00	0.42
1:A:272:ALA:O	1:A:273:THR:C	2.63	0.42
1:A:542:GLN:O	1:A:546:GLU:HA	2.18	0.42
1:A:32:ASN:CG	1:A:35:THR:HG23	2.45	0.42
1:A:197:SER:HB3	1:A:200:LEU:HD12	2.02	0.42
1:A:386:SER:OG	1:A:388:VAL:HG23	2.19	0.42
1:A:545:ASN:OD1	1:A:547:SER:HB2	2.20	0.42
1:A:598:ASN:HB3	1:A:599:ALA:H	1.62	0.42
1:A:384:LYS:HB2	3:A:797:HOH:O	2.20	0.41
1:A:487:ARG:HD3	1:A:489:LEU:HD21	2.02	0.41
1:A:454:ASP:CB	1:A:456:GLN:CD	2.92	0.41
1:A:597:ASP:O	1:A:598:ASN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:O	1:A:425:ARG:HG3	2.21	0.41
1:A:141:LEU:HD23	1:A:143:ILE:HG13	2.03	0.41
1:A:276:SER:HB2	1:A:286:ARG:HA	2.03	0.41
1:A:334:MET:HE2	1:A:362:LEU:HD23	2.03	0.41
1:A:467:ILE:O	1:A:468:ALA:C	2.64	0.41
1:A:57:GLN:HE21	1:A:80:ASP:H	1.68	0.41
1:A:332:HIS:HB3	1:A:369:TYR:CZ	2.56	0.41
1:A:519:ARG:HH11	1:A:519:ARG:HG2	1.86	0.40
1:A:250:ARG:O	1:A:251:GLN:C	2.65	0.40
1:A:435:VAL:HA	1:A:579:VAL:HG12	2.03	0.40
1:A:332:HIS:CA	1:A:369:TYR:CE2	3.04	0.40
1:A:437:ASP:OD2	1:A:453:SER:OG	2.39	0.40
1:A:621:ASN:H	1:A:621:ASN:HD22	1.70	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	632/634 (100%)	584 (92%)	44 (7%)	4 (1%)	21	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	598	ASN
1	A	455	ASN
1	A	214	GLU

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	516/516 (100%)	500 (97%)	16 (3%)	35	48

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	57	GLN
1	A	137	SER
1	A	181	PRO
1	A	209	GLU
1	A	225	THR
1	A	228	ASN
1	A	268	TRP
1	A	297	LEU
1	A	299	LEU
1	A	345	SER
1	A	347	GLN
1	A	386	SER
1	A	427	LEU
1	A	606	ASN
1	A	624	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	57	GLN
1	A	101	ASN
1	A	156	GLN
1	A	173	GLN
1	A	213	ASN
1	A	260	GLN
1	A	295	ASN
1	A	327	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	HIS
1	A	403	GLN
1	A	430	GLN
1	A	511	GLN
1	A	554	GLN
1	A	562	ASN
1	A	606	ASN
1	A	621	ASN
1	A	624	GLN
1	A	639	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 ⓘ

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	1.39	2 (18%)	15,15,17	2.80	2 (13%)
2	FRU	B	2	2	11,12,12	0.81	0	10,18,18	0.87	1 (10%)

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	-	2/2/19/22	0/1/1/1
2	FRU	B	2	2	-	1/5/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	O5-C1	2.88	1.48	1.43
2	B	1	GLC	O5-C5	2.36	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O6-C6-C5	10.25	146.25	111.33
2	B	1	GLC	C6-C5-C4	-2.64	106.53	113.02
2	B	2	FRU	C6-C5-C4	-2.20	109.90	115.10

There are no chirality outliers.

All (3) torsion outliers are listed below:

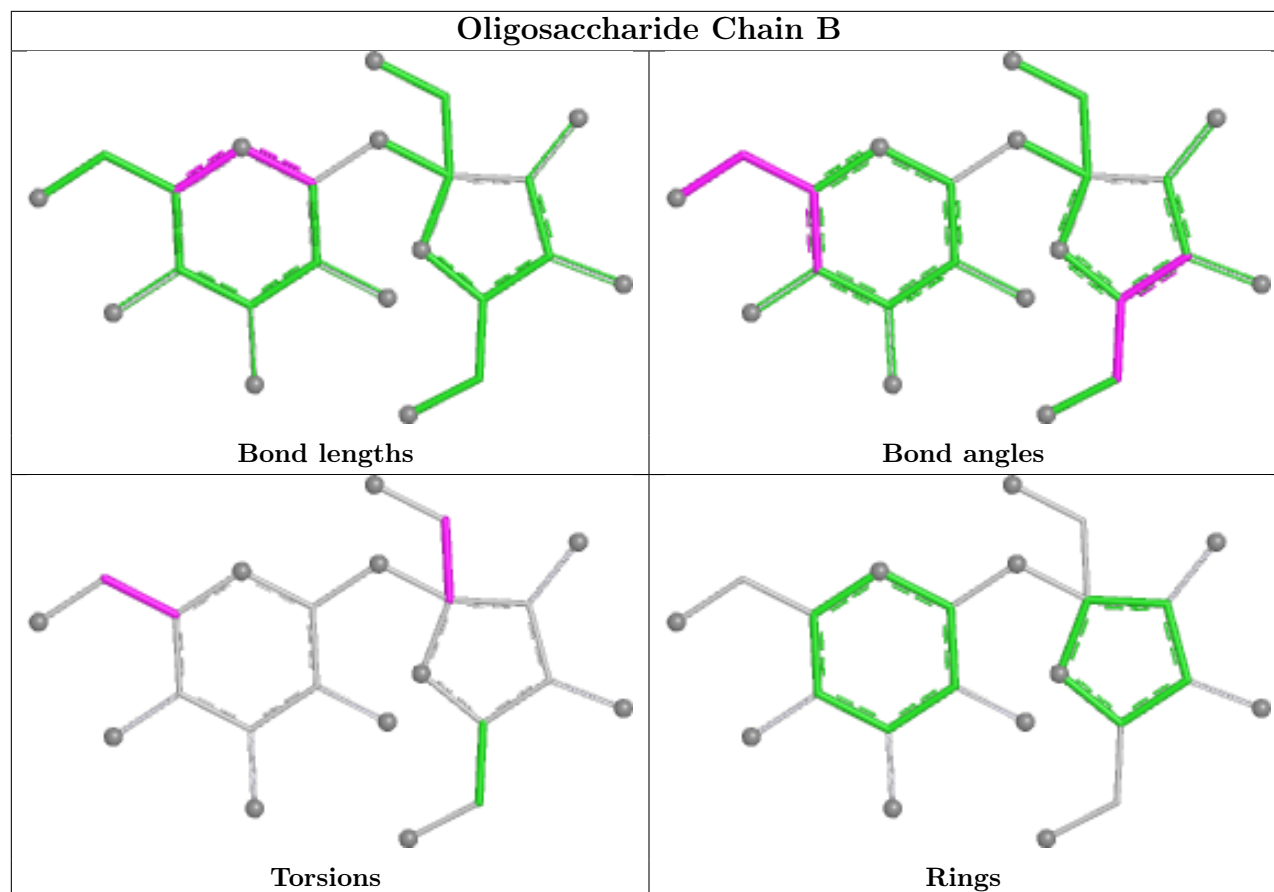
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	2	FRU	O1-C1-C2-C3

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](#)

There are no ligands in this entry.

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	634/634 (100%)	0.63	53 (8%)	17 14	22, 34, 68, 113	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	599	ALA	9.2
1	A	211	ALA	6.4
1	A	210	VAL	5.2
1	A	458	ALA	4.7
1	A	21	TYR	4.6
1	A	345	SER	4.4
1	A	598	ASN	4.3
1	A	347	GLN	3.7
1	A	456	GLN	3.7
1	A	206	LEU	3.5
1	A	454	ASP	3.5
1	A	343	VAL	3.4
1	A	214	GLU	3.3
1	A	457	THR	3.3
1	A	101	ASN	3.2
1	A	207	ASP	3.2
1	A	213	ASN	3.2
1	A	162	ARG	3.2
1	A	453	SER	3.1
1	A	349	GLY	3.1
1	A	20	SER	3.1
1	A	166	ARG	3.1
1	A	369	TYR	3.1
1	A	281	GLY	2.9
1	A	452	GLU	2.9
1	A	217	VAL	2.9
1	A	163	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	GLN	2.6
1	A	342	GLY	2.6
1	A	216	ALA	2.6
1	A	455	ASN	2.5
1	A	344	GLY	2.5
1	A	212	ARG	2.5
1	A	215	THR	2.5
1	A	440	LEU	2.5
1	A	348	GLU	2.4
1	A	441	VAL	2.4
1	A	451	GLY	2.4
1	A	209	GLU	2.3
1	A	346	GLU	2.3
1	A	438	ASN	2.3
1	A	31	THR	2.3
1	A	225	THR	2.3
1	A	444	GLU	2.3
1	A	218	GLN	2.2
1	A	652	GLU	2.2
1	A	322	LEU	2.2
1	A	450	VAL	2.2
1	A	621	ASN	2.1
1	A	584	GLN	2.1
1	A	208	GLU	2.1
1	A	459	THR	2.1
1	A	222	ASP	2.1

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

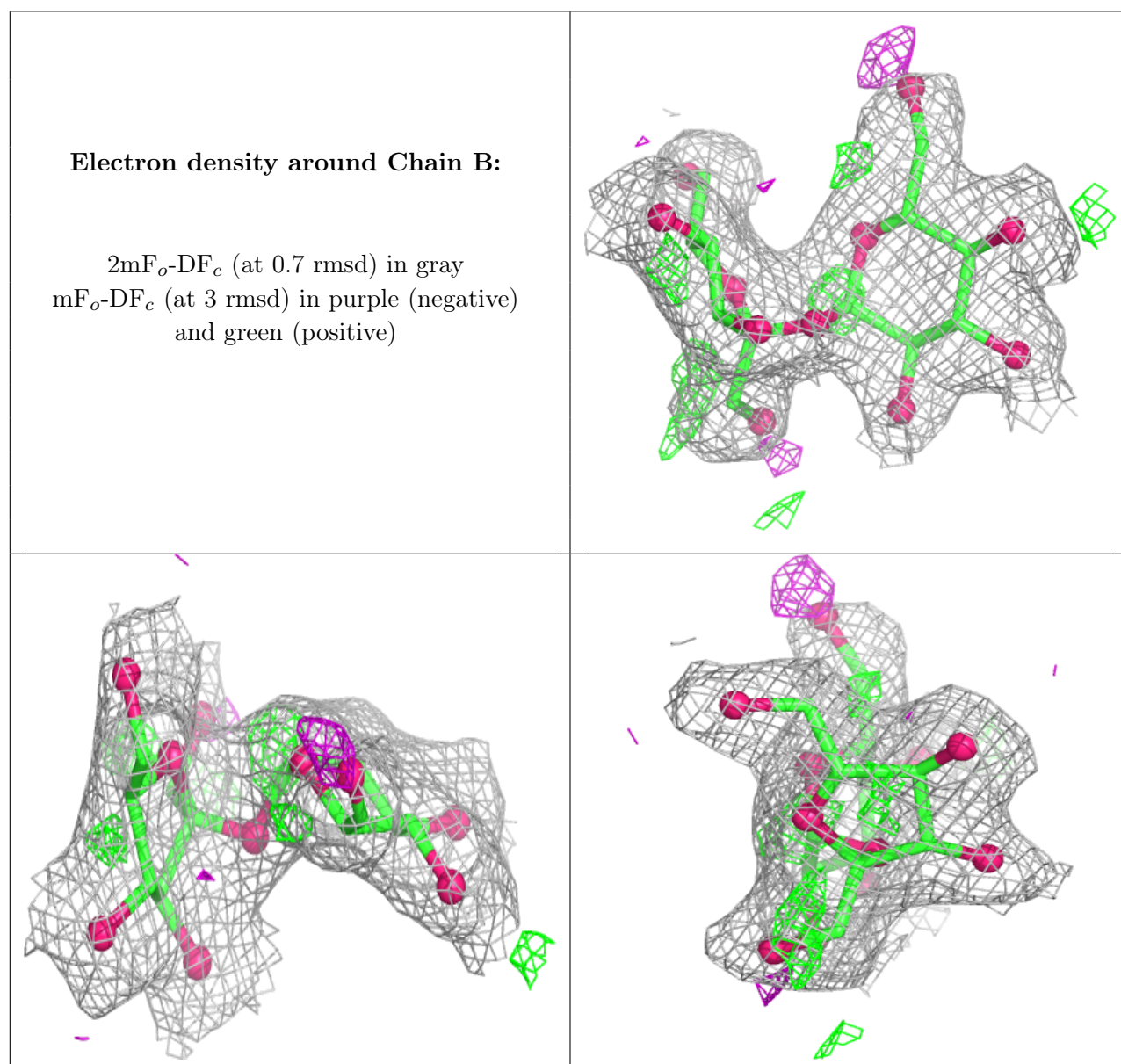
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	0.85	0.12	21,26,29,39	0
2	FRU	B	2	12/12	0.88	0.11	28,30,34,35	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.