



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:59 AM UTC

PDB ID : 2OXB / pdb_00002oxb
Title : Crystal structure of a cell-wall invertase (E203Q) from Arabidopsis thaliana in complex with sucrose
Authors : Lammens, W.; Le Roy, K.; Van Laere, A.; Van den Ende, W.; Rabijns, A.
Deposited on : 2007-02-20
Resolution : 2.60 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

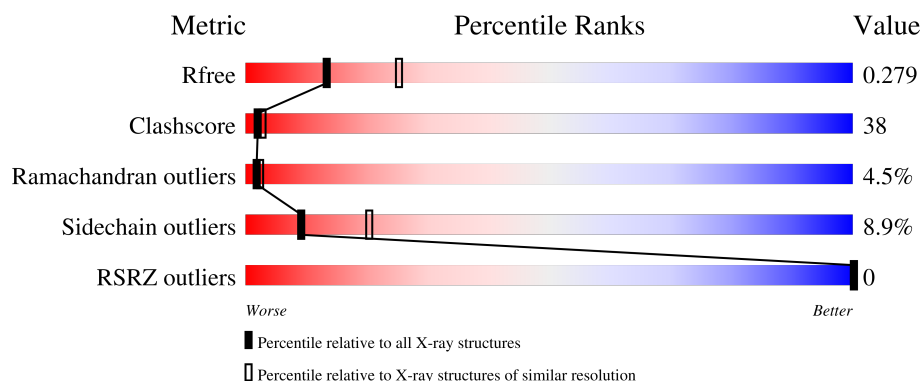
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

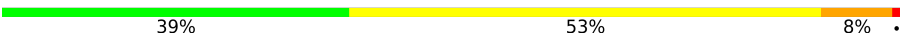
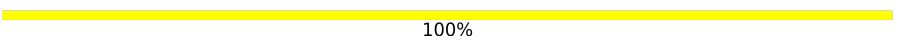
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	537	 39% 53% 8%
2	B	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4414 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.

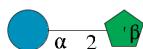
- Molecule 1 is a protein called Beta-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4315	2763	745	793	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	GLN	GLU	engineered mutation	UNP Q43866

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

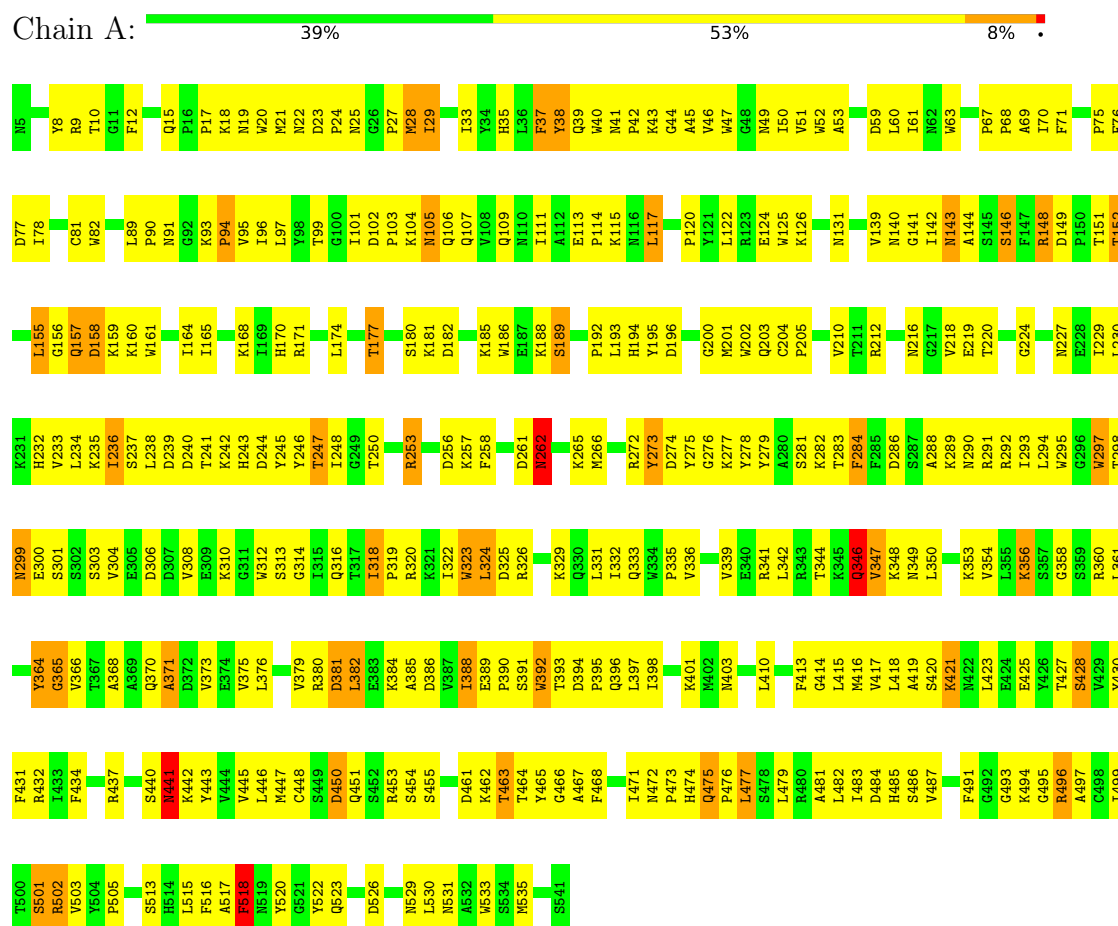
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		

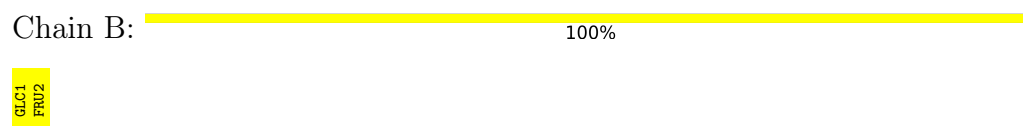
3 Residue-property plots

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: Beta-fructofuranosidase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	106.45Å 106.45Å 50.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.51 – 2.60 19.51 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (19.51-2.60) 91.6 (19.51-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.268 0.215 , 0.279	Depositor DCC
R_{free} test set	951 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.187 for -h,-k,l 0.087 for h,-h-k,-l 0.090 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4414	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: FRU, GLC, NAG

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	0.53	0/4442	0.97	16/6034 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	N-CA-C	-7.09	103.48	111.14
1	A	288	ALA	N-CA-C	6.70	118.24	111.07
1	A	37	PHE	N-CA-C	-6.21	99.96	109.65
1	A	423	LEU	N-CA-C	5.94	119.84	112.24
1	A	371	ALA	N-CA-C	5.57	116.71	108.86
1	A	428	SER	N-CA-C	5.53	118.10	107.44
1	A	152	THR	N-CA-C	-5.44	103.35	110.53
1	A	364	TYR	N-CA-C	5.43	122.36	110.80
1	A	297	TRP	N-CA-C	5.34	118.13	111.24
1	A	67	PRO	CA-C-N	5.33	126.51	119.84
1	A	67	PRO	C-N-CA	5.33	126.51	119.84
1	A	157	GLN	N-CA-C	-5.21	106.94	113.15
1	A	279	TYR	N-CA-C	5.20	116.43	108.42
1	A	189	SER	CA-C-N	5.10	126.22	119.84
1	A	189	SER	C-N-CA	5.10	126.22	119.84
1	A	518	PHE	N-CA-C	5.06	116.98	109.69

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	4315	0	4219	331	0
2	B	23	0	21	0	0
3	A	42	0	39	3	0
4	A	34	0	0	3	0
All	All	4414	0	4279	332	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 38.

All (332) 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:322:ILE:HG22	1:A:333:GLN:HG2	1.31	1.12
1:A:358:GLY:HA2	1:A:520:TYR:HA	1.38	1.04
1:A:168:LYS:HD2	1:A:201:MET:HB2	1.40	1.03
1:A:344:THR:HG22	1:A:346:GLN:H	1.26	1.00
1:A:210:VAL:HG21	1:A:324:LEU:HD23	1.43	0.99
1:A:148:ARG:NH1	1:A:201:MET:HE2	1.80	0.97
1:A:375:VAL:HG22	1:A:530:LEU:HD13	1.45	0.96
1:A:51:VAL:HG13	1:A:71:PHE:HB3	1.49	0.94
1:A:117:LEU:HD13	1:A:117:LEU:H	1.34	0.92
1:A:22:ASN:HB3	1:A:39:GLN:HB2	1.50	0.92
1:A:102:ASP:HB2	1:A:103:PRO:HD2	1.52	0.91
1:A:421:LYS:H	1:A:421:LYS:HD2	1.36	0.88
1:A:10:THR:H	1:A:15:GLN:HE22	1.23	0.86
1:A:235:LYS:HE3	1:A:281:SER:OG	1.76	0.84
1:A:93:LYS:HE3	1:A:114:PRO:HD2	1.59	0.84
1:A:151:THR:HG22	1:A:205:PRO:O	1.76	0.83
1:A:9:ARG:HH22	1:A:17:PRO:HA	1.44	0.82
1:A:99:THR:HG21	1:A:148:ARG:HB2	1.62	0.82
1:A:322:ILE:CG2	1:A:333:GLN:HG2	2.10	0.81
1:A:12:PHE:HB2	1:A:342:LEU:HD13	1.61	0.81
1:A:148:ARG:HH11	1:A:201:MET:HE2	1.42	0.80
1:A:82:TRP:HZ3	1:A:148:ARG:HE	1.31	0.79
1:A:89:LEU:HD23	1:A:93:LYS:HG3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLN:O	1:A:495:GLY:HA3	1.82	0.78
1:A:416:MET:HB2	1:A:516:PHE:HB2	1.64	0.78
1:A:115:LYS:HD2	1:A:124:GLU:HB3	1.66	0.78
1:A:301:SER:HB2	1:A:502:ARG:HB2	1.65	0.78
1:A:503:VAL:HG22	1:A:505:PRO:HD3	1.67	0.76
1:A:104:LYS:HE3	1:A:106:GLN:NE2	2.00	0.76
1:A:472:ASN:HD22	1:A:474:HIS:HB2	1.49	0.76
1:A:43:LYS:HD2	1:A:49:ASN:ND2	2.00	0.76
1:A:216:ASN:HB3	1:A:290:ASN:HD22	1.49	0.76
1:A:336:VAL:O	1:A:339:VAL:HG12	1.87	0.75
1:A:106:GLN:HB2	1:A:144:ALA:HB1	1.69	0.75
1:A:530:LEU:C	1:A:531:ASN:HD22	1.96	0.74
1:A:373:VAL:HB	1:A:481:ALA:HB3	1.70	0.73
1:A:389:GLU:HG3	1:A:390:PRO:HD2	1.70	0.73
1:A:51:VAL:CG1	1:A:71:PHE:HB3	2.18	0.72
1:A:148:ARG:HG2	1:A:149:ASP:CG	2.15	0.71
1:A:529:ASN:HD22	1:A:530:LEU:H	1.40	0.70
1:A:253:ARG:HB3	1:A:253:ARG:HH11	1.56	0.70
1:A:529:ASN:ND2	1:A:530:LEU:H	1.90	0.70
1:A:454:SER:HB3	1:A:503:VAL:HG23	1.74	0.69
1:A:203:GLN:HE22	1:A:239:ASP:HB3	1.58	0.69
1:A:298:THR:HG22	1:A:502:ARG:HE	1.59	0.68
1:A:437:ARG:CZ	1:A:437:ARG:HA	2.23	0.68
1:A:159:LYS:HZ2	1:A:182:ASP:HA	1.59	0.67
1:A:502:ARG:HB3	1:A:502:ARG:HH11	1.59	0.67
1:A:379:VAL:HG11	1:A:410:LEU:HD13	1.76	0.66
1:A:203:GLN:NE2	1:A:239:ASP:HB3	2.12	0.65
1:A:18:LYS:HE3	1:A:19:ASN:ND2	2.11	0.65
1:A:23:ASP:HB2	1:A:39:GLN:HG3	1.79	0.65
1:A:297:TRP:O	1:A:298:THR:HB	1.96	0.65
1:A:242:LYS:HG3	3:A:660:NAG:H82	1.79	0.65
1:A:344:THR:HG22	1:A:346:GLN:N	2.08	0.64
1:A:421:LYS:HD2	1:A:421:LYS:N	2.09	0.64
1:A:177:THR:HG23	1:A:189:SER:HB3	1.80	0.64
1:A:451:GLN:O	1:A:462:LYS:HG3	1.97	0.64
1:A:59:ASP:O	1:A:61:ILE:HG12	1.98	0.63
1:A:104:LYS:HE3	1:A:106:GLN:HE22	1.63	0.63
1:A:445:VAL:HG11	1:A:471:ILE:HD11	1.81	0.63
1:A:349:ASN:O	1:A:350:LEU:HG	1.99	0.62
1:A:416:MET:HA	1:A:427:THR:O	1.99	0.62
1:A:216:ASN:CB	1:A:290:ASN:HD22	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLN:O	1:A:535:MET:HB2	1.99	0.62
1:A:164:ILE:C	1:A:165:ILE:HD12	2.25	0.62
1:A:414:GLY:HA3	1:A:430:TYR:HA	1.79	0.62
1:A:262:ASN:N	1:A:262:ASN:HD22	1.96	0.61
1:A:180:SER:HB2	1:A:186:TRP:CE3	2.36	0.60
1:A:216:ASN:HB3	1:A:290:ASN:ND2	2.15	0.60
1:A:261:ASP:C	1:A:262:ASN:HD22	2.09	0.60
1:A:159:LYS:NZ	1:A:182:ASP:HA	2.16	0.60
1:A:289:LYS:HG3	1:A:291:ARG:NH1	2.17	0.60
1:A:421:LYS:H	1:A:421:LYS:CD	2.01	0.60
1:A:41:ASN:ND2	1:A:44:GLY:H	1.99	0.60
1:A:356:LYS:HZ2	1:A:356:LYS:HB2	1.66	0.60
1:A:237:SER:OG	1:A:244:ASP:OD2	2.20	0.60
1:A:503:VAL:HA	4:A:867:HOH:O	2.01	0.60
1:A:306:ASP:O	1:A:310:LYS:HG2	2.02	0.59
1:A:371:ALA:H	1:A:483:ILE:HB	1.66	0.59
1:A:10:THR:H	1:A:15:GLN:NE2	1.97	0.59
1:A:19:ASN:HB3	1:A:44:GLY:O	2.02	0.59
1:A:117:LEU:H	1:A:117:LEU:CD1	2.12	0.59
1:A:322:ILE:O	1:A:323:TRP:HB3	2.03	0.59
1:A:168:LYS:HD2	1:A:201:MET:CB	2.24	0.58
1:A:22:ASN:HB3	1:A:39:GLN:CB	2.29	0.58
1:A:210:VAL:CG2	1:A:324:LEU:HD23	2.27	0.58
1:A:51:VAL:HG12	1:A:52:TRP:N	2.17	0.58
1:A:294:LEU:HD13	1:A:322:ILE:HG21	1.85	0.58
1:A:310:LYS:HE3	1:A:312:TRP:O	2.03	0.58
1:A:454:SER:HB2	1:A:462:LYS:NZ	2.19	0.58
1:A:236:ILE:HD11	1:A:238:LEU:CD1	2.34	0.58
1:A:276:GLY:HA2	1:A:465:TYR:CD1	2.39	0.58
1:A:33:ILE:HD12	1:A:120:PRO:HB2	1.85	0.58
1:A:218:VAL:HG11	1:A:230:LEU:HD21	1.86	0.58
1:A:275:TYR:O	1:A:465:TYR:HB3	2.04	0.57
1:A:274:ASP:HB3	1:A:278:TYR:HB2	1.86	0.57
1:A:165:ILE:HD12	1:A:165:ILE:N	2.18	0.57
1:A:93:LYS:HE2	1:A:95:VAL:CG1	2.34	0.57
1:A:93:LYS:HD2	1:A:94:PRO:N	2.20	0.57
1:A:99:THR:HG21	1:A:148:ARG:CB	2.33	0.57
1:A:25:ASN:HB3	1:A:52:TRP:CH2	2.40	0.56
1:A:465:TYR:HE2	1:A:501:SER:HB3	1.69	0.56
1:A:12:PHE:HB2	1:A:342:LEU:CD1	2.34	0.56
1:A:148:ARG:HG2	1:A:149:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASN:N	1:A:262:ASN:ND2	2.54	0.56
1:A:284:PHE:CE2	1:A:293:ILE:HB	2.41	0.56
1:A:164:ILE:HG22	1:A:177:THR:HB	1.88	0.56
1:A:93:LYS:HE2	1:A:95:VAL:HG13	1.87	0.56
1:A:289:LYS:HB2	1:A:291:ARG:HH11	1.71	0.56
1:A:180:SER:HB2	1:A:186:TRP:CD2	2.41	0.56
1:A:156:GLY:C	1:A:158:ASP:H	2.14	0.55
1:A:324:LEU:HD22	1:A:331:LEU:HD23	1.88	0.55
1:A:370:GLN:HA	1:A:483:ILE:O	2.06	0.55
1:A:24:PRO:HG3	1:A:316:GLN:OE1	2.05	0.55
1:A:12:PHE:CB	1:A:342:LEU:HD13	2.34	0.55
1:A:168:LYS:HB3	1:A:201:MET:HA	1.88	0.55
1:A:318:ILE:HD13	1:A:335:PRO:CB	2.37	0.55
1:A:70:ILE:HG22	1:A:81:CYS:SG	2.46	0.55
1:A:20:TRP:HB2	1:A:45:ALA:C	2.33	0.54
1:A:96:ILE:C	1:A:97:LEU:HD12	2.32	0.54
1:A:365:GLY:O	1:A:366:VAL:HG13	2.08	0.54
1:A:236:ILE:HD11	1:A:238:LEU:HD12	1.89	0.54
1:A:395:PRO:HG3	1:A:468:PHE:CE1	2.42	0.54
1:A:529:ASN:ND2	1:A:530:LEU:N	2.55	0.54
1:A:380:ARG:HG2	1:A:380:ARG:HH11	1.73	0.54
1:A:37:PHE:O	1:A:38:TYR:HB3	2.08	0.53
1:A:420:SER:HB2	1:A:425:GLU:HG2	1.90	0.53
1:A:395:PRO:HG3	1:A:468:PHE:CD1	2.43	0.53
1:A:479:LEU:HD12	1:A:491:PHE:O	2.08	0.53
1:A:382:LEU:HD21	1:A:473:PRO:HB2	1.91	0.53
1:A:235:LYS:HG3	1:A:273:TYR:CE2	2.44	0.53
1:A:502:ARG:HB3	1:A:502:ARG:NH1	2.24	0.53
1:A:102:ASP:HB2	1:A:103:PRO:CD	2.33	0.53
1:A:10:THR:OG1	1:A:15:GLN:NE2	2.41	0.52
1:A:300:GLU:OE1	1:A:313:SER:HA	2.09	0.52
1:A:52:TRP:CG	1:A:70:ILE:HB	2.45	0.52
1:A:386:ASP:HB2	1:A:434:PHE:CD1	2.45	0.52
1:A:382:LEU:HD22	1:A:443:TYR:CD1	2.45	0.51
1:A:247:THR:HG21	1:A:266:MET:HG2	1.92	0.51
1:A:194:HIS:CG	1:A:195:TYR:H	2.27	0.51
1:A:354:VAL:HG12	1:A:526:ASP:OD1	2.10	0.51
1:A:194:HIS:CD2	1:A:195:TYR:H	2.28	0.51
1:A:381:ASP:OD1	1:A:384:LYS:HD3	2.11	0.51
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.26	0.50
1:A:235:LYS:HD3	1:A:235:LYS:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:CZ3	1:A:42:PRO:HB3	2.46	0.50
1:A:232:HIS:O	1:A:248:ILE:HA	2.11	0.50
1:A:146:SER:OG	1:A:168:LYS:HD3	2.11	0.50
1:A:216:ASN:HD22	1:A:216:ASN:N	2.09	0.50
1:A:310:LYS:HD2	1:A:312:TRP:CE2	2.46	0.50
1:A:193:LEU:HD21	1:A:258:PHE:HB2	1.92	0.50
1:A:216:ASN:HB3	1:A:290:ASN:O	2.11	0.50
1:A:347:VAL:O	1:A:347:VAL:HG13	2.12	0.50
1:A:300:GLU:OE1	1:A:314:GLY:N	2.38	0.50
1:A:413:PHE:HZ	1:A:477:LEU:HD11	1.76	0.50
1:A:467:ALA:HB3	1:A:499:ILE:HD11	1.93	0.50
1:A:170:HIS:O	1:A:171:ARG:HB2	2.12	0.49
1:A:416:MET:HE2	1:A:518:PHE:HB3	1.94	0.49
1:A:472:ASN:ND2	1:A:474:HIS:HB2	2.25	0.49
1:A:529:ASN:HD22	1:A:530:LEU:N	2.07	0.49
1:A:82:TRP:HB2	1:A:99:THR:O	2.12	0.49
1:A:219:GLU:HG2	1:A:220:THR:H	1.78	0.49
1:A:196:ASP:OD2	1:A:265:LYS:HE3	2.11	0.49
1:A:418:LEU:HD21	1:A:485:HIS:O	2.13	0.49
1:A:440:SER:O	1:A:442:LYS:N	2.45	0.49
1:A:294:LEU:N	1:A:320:ARG:O	2.42	0.49
1:A:413:PHE:O	1:A:413:PHE:CD1	2.66	0.49
1:A:60:LEU:HD11	1:A:293:ILE:HG12	1.95	0.48
1:A:382:LEU:CD1	1:A:474:HIS:HD2	2.25	0.48
1:A:159:LYS:HZ1	1:A:182:ASP:HB3	1.79	0.48
1:A:385:ALA:HB2	1:A:410:LEU:HD12	1.95	0.48
1:A:203:GLN:O	1:A:204:CYS:C	2.56	0.48
1:A:479:LEU:HA	1:A:491:PHE:O	2.12	0.48
1:A:139:VAL:HG13	1:A:140:ASN:N	2.29	0.48
1:A:394:ASP:O	1:A:398:ILE:HG12	2.13	0.48
1:A:454:SER:HB2	1:A:462:LYS:HZ3	1.77	0.48
1:A:20:TRP:HE1	1:A:22:ASN:HB2	1.79	0.48
1:A:247:THR:HG22	1:A:266:MET:HE3	1.96	0.48
1:A:440:SER:O	1:A:441:ASN:C	2.57	0.47
1:A:461:ASP:OD2	1:A:463:THR:HG23	2.14	0.47
1:A:28:MET:SD	1:A:35:HIS:HB2	2.54	0.47
1:A:10:THR:HG22	1:A:487:VAL:HG12	1.96	0.47
1:A:89:LEU:HB3	1:A:91:ASN:OD1	2.14	0.47
1:A:148:ARG:HG2	1:A:149:ASP:N	2.29	0.47
1:A:325:ASP:CG	1:A:326:ARG:N	2.72	0.47
1:A:218:VAL:HG12	1:A:219:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:SER:CB	1:A:502:ARG:HB2	2.41	0.47
1:A:454:SER:N	1:A:462:LYS:HZ1	2.13	0.47
1:A:193:LEU:CD2	1:A:258:PHE:HB2	2.45	0.47
1:A:303:SER:O	1:A:306:ASP:HB2	2.14	0.47
1:A:310:LYS:HD2	1:A:312:TRP:CZ2	2.50	0.47
1:A:51:VAL:HG12	1:A:52:TRP:H	1.79	0.47
1:A:339:VAL:C	1:A:341:ARG:H	2.23	0.47
1:A:322:ILE:HG22	1:A:333:GLN:CG	2.22	0.47
1:A:465:TYR:CE2	1:A:501:SER:HB3	2.50	0.46
1:A:161:TRP:HB2	1:A:180:SER:HB3	1.96	0.46
1:A:37:PHE:HA	1:A:53:ALA:O	2.16	0.46
1:A:243:HIS:HB2	1:A:245:TYR:CE1	2.50	0.46
1:A:417:VAL:HA	1:A:515:LEU:HD12	1.98	0.46
1:A:432:ARG:CD	1:A:446:LEU:HD23	2.45	0.46
1:A:101:ILE:HG22	1:A:105:ASN:HA	1.98	0.46
1:A:368:ALA:HB3	1:A:513:SER:HB2	1.97	0.46
1:A:304:VAL:O	1:A:308:VAL:HG23	2.15	0.46
1:A:391:SER:O	1:A:393:THR:HG23	2.15	0.46
1:A:396:GLN:HA	1:A:466:GLY:HA3	1.97	0.46
1:A:159:LYS:NZ	1:A:182:ASP:HB3	2.30	0.46
1:A:286:ASP:HB2	1:A:293:ILE:HD13	1.97	0.46
1:A:113:GLU:O	1:A:126:LYS:N	2.46	0.45
1:A:193:LEU:O	1:A:257:LYS:HG3	2.16	0.45
1:A:318:ILE:HD13	1:A:335:PRO:HB3	1.97	0.45
1:A:450:ASP:HA	1:A:464:THR:HG23	1.98	0.45
1:A:155:LEU:O	1:A:160:LYS:O	2.34	0.45
1:A:432:ARG:HD2	1:A:446:LEU:HD23	1.98	0.45
1:A:380:ARG:HG2	1:A:380:ARG:NH1	2.31	0.45
1:A:413:PHE:CZ	1:A:477:LEU:HD11	2.50	0.45
1:A:20:TRP:H	1:A:45:ALA:HA	1.82	0.45
1:A:243:HIS:HE1	4:A:866:HOH:O	1.99	0.45
1:A:286:ASP:OD2	1:A:291:ARG:NH1	2.48	0.45
1:A:233:VAL:HG11	1:A:331:LEU:HD11	1.99	0.45
1:A:292:ARG:CD	1:A:322:ILE:HD11	2.46	0.45
1:A:291:ARG:CZ	1:A:293:ILE:HD11	2.46	0.45
1:A:49:ASN:O	1:A:51:VAL:HG23	2.17	0.45
1:A:235:LYS:HE3	1:A:281:SER:HG	1.75	0.45
1:A:241:THR:O	1:A:242:LYS:HB2	2.16	0.45
1:A:361:LEU:C	1:A:361:LEU:HD12	2.41	0.45
1:A:111:ILE:HG22	1:A:131:ASN:OD1	2.16	0.45
1:A:23:ASP:HA	1:A:24:PRO:HD3	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:HD2	1:A:94:PRO:HD2	1.99	0.45
1:A:318:ILE:HD13	1:A:335:PRO:HB2	1.99	0.45
1:A:349:ASN:CG	1:A:350:LEU:N	2.75	0.44
1:A:75:PRO:O	1:A:77:ASP:N	2.51	0.44
1:A:322:ILE:HA	1:A:332:ILE:O	2.17	0.44
1:A:358:GLY:HA2	1:A:520:TYR:HD2	1.82	0.44
1:A:486:SER:HA	1:A:503:VAL:O	2.17	0.44
1:A:201:MET:HG3	1:A:202:TRP:N	2.33	0.44
1:A:27:PRO:HG2	1:A:284:PHE:HB3	2.00	0.44
1:A:89:LEU:C	1:A:91:ASN:H	2.25	0.44
1:A:192:PRO:O	1:A:193:LEU:C	2.61	0.44
1:A:371:ALA:HB1	1:A:533:TRP:O	2.18	0.44
1:A:430:TYR:CE1	1:A:448:CYS:HB2	2.53	0.44
1:A:437:ARG:HA	1:A:437:ARG:NE	2.32	0.44
1:A:18:LYS:HE3	1:A:19:ASN:HD21	1.82	0.44
1:A:320:ARG:HG3	1:A:320:ARG:HH11	1.82	0.44
1:A:61:ILE:HD12	1:A:339:VAL:HG23	2.00	0.44
1:A:93:LYS:HD2	1:A:94:PRO:CD	2.47	0.44
1:A:139:VAL:HG13	1:A:140:ASN:H	1.82	0.44
1:A:202:TRP:HA	1:A:236:ILE:HD13	2.00	0.44
1:A:246:TYR:C	1:A:247:THR:HG22	2.43	0.44
1:A:159:LYS:O	1:A:159:LYS:HG2	2.18	0.43
1:A:156:GLY:C	1:A:158:ASP:N	2.76	0.43
1:A:284:PHE:CD1	1:A:284:PHE:C	2.94	0.43
1:A:518:PHE:H	1:A:518:PHE:HD2	1.66	0.43
1:A:274:ASP:HB3	1:A:278:TYR:CB	2.48	0.43
1:A:392:TRP:HA	1:A:398:ILE:HD11	2.01	0.43
1:A:22:ASN:CG	1:A:23:ASP:H	2.26	0.43
1:A:212:ARG:HG3	1:A:229:ILE:HG22	2.01	0.43
1:A:493:GLY:O	1:A:494:LYS:HB2	2.19	0.43
1:A:236:ILE:HD12	1:A:236:ILE:C	2.44	0.43
1:A:360:ARG:HA	1:A:517:ALA:O	2.19	0.43
1:A:417:VAL:HG12	1:A:515:LEU:HD11	2.01	0.43
1:A:196:ASP:OD2	1:A:265:LYS:HB3	2.19	0.43
1:A:324:LEU:HD22	1:A:331:LEU:CD2	2.47	0.43
1:A:188:LYS:HD3	1:A:188:LYS:C	2.43	0.43
1:A:482:LEU:HD23	1:A:491:PHE:CE2	2.53	0.43
1:A:417:VAL:O	1:A:418:LEU:C	2.62	0.42
1:A:417:VAL:C	1:A:419:ALA:N	2.75	0.42
1:A:431:PHE:CE1	1:A:447:MET:HG3	2.54	0.42
1:A:22:ASN:ND2	1:A:23:ASP:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:HB2	1:A:70:ILE:H	1.84	0.42
1:A:25:ASN:HB3	1:A:52:TRP:CZ3	2.55	0.42
1:A:293:ILE:HG23	1:A:319:PRO:HB3	2.02	0.42
1:A:445:VAL:HG21	1:A:471:ILE:HG13	2.01	0.42
1:A:21:MET:HE3	1:A:316:GLN:HE21	1.84	0.42
1:A:46:VAL:O	1:A:47:TRP:C	2.62	0.42
1:A:495:GLY:O	1:A:497:ALA:N	2.53	0.42
1:A:37:PHE:O	1:A:38:TYR:CB	2.68	0.42
1:A:244:ASP:O	1:A:272:ARG:HA	2.20	0.42
1:A:373:VAL:HG11	1:A:415:LEU:HD13	2.01	0.42
1:A:234:LEU:HD23	1:A:266:MET:SD	2.60	0.42
1:A:236:ILE:O	1:A:236:ILE:HG13	2.20	0.42
1:A:475:GLN:CB	1:A:476:PRO:HD2	2.50	0.42
1:A:20:TRP:N	1:A:45:ALA:HA	2.35	0.41
1:A:233:VAL:HA	1:A:247:THR:O	2.19	0.41
1:A:484:ASP:OD1	1:A:485:HIS:HD2	2.03	0.41
1:A:69:ALA:HB1	1:A:125:TRP:CD1	2.55	0.41
1:A:291:ARG:HH11	1:A:291:ARG:HG2	1.85	0.41
1:A:27:PRO:O	1:A:284:PHE:HB2	2.21	0.41
1:A:266:MET:HE2	1:A:266:MET:HB3	1.88	0.41
1:A:298:THR:CG2	1:A:502:ARG:HD3	2.50	0.41
3:A:670:NAG:O3	3:A:670:NAG:H83	2.19	0.41
1:A:99:THR:CG2	1:A:148:ARG:HB2	2.42	0.41
1:A:531:ASN:HD22	1:A:531:ASN:N	2.14	0.41
1:A:181:LYS:HG2	1:A:185:LYS:HB2	2.02	0.41
1:A:89:LEU:O	1:A:91:ASN:N	2.44	0.41
1:A:388:ILE:HG23	1:A:434:PHE:CB	2.50	0.41
1:A:115:LYS:HD2	1:A:124:GLU:CB	2.46	0.41
1:A:413:PHE:C	1:A:430:TYR:HB2	2.46	0.41
1:A:415:LEU:O	1:A:428:SER:HA	2.21	0.41
1:A:482:LEU:C	1:A:483:ILE:HD13	2.45	0.41
1:A:38:TYR:CZ	1:A:53:ALA:HB3	2.56	0.41
1:A:51:VAL:HG11	1:A:68:PRO:HB3	2.03	0.41
1:A:152:THR:HB	4:A:861:HOH:O	2.20	0.41
1:A:360:ARG:HG3	1:A:360:ARG:HH11	1.86	0.41
1:A:386:ASP:HB2	1:A:434:PHE:HD1	1.86	0.41
1:A:114:PRO:CB	1:A:122:LEU:HD22	2.50	0.41
1:A:194:HIS:CG	1:A:195:TYR:N	2.88	0.41
1:A:293:ILE:CG2	1:A:319:PRO:HB3	2.51	0.41
1:A:298:THR:O	1:A:299:ASN:O	2.38	0.41
1:A:431:PHE:HA	1:A:446:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LYS:HG3	3:A:660:NAG:C8	2.47	0.40
1:A:277:LYS:HD2	1:A:299:ASN:HB2	2.02	0.40
1:A:39:GLN:OE1	1:A:50:ILE:HG21	2.22	0.40
1:A:59:ASP:OD1	1:A:59:ASP:N	2.54	0.40
1:A:63:TRP:CZ2	1:A:295:TRP:HH2	2.40	0.40
1:A:104:LYS:O	1:A:105:ASN:C	2.63	0.40
1:A:325:ASP:HB2	1:A:332:ILE:HD11	2.03	0.40
1:A:455:SER:H	1:A:462:LYS:NZ	2.19	0.40
1:A:8:TYR:O	1:A:486:SER:HB3	2.21	0.40
1:A:29:ILE:HD13	1:A:29:ILE:C	2.47	0.40
1:A:41:ASN:HA	1:A:42:PRO:HD2	1.95	0.40
1:A:348:LYS:HD3	1:A:349:ASN:N	2.37	0.40
1:A:388:ILE:H	1:A:388:ILE:HG13	1.78	0.40
1:A:495:GLY:C	1:A:497:ALA:N	2.77	0.40
1:A:496:ARG:HH11	1:A:496:ARG:HG3	1.85	0.40
1:A:366:VAL:O	1:A:368:ALA:N	2.55	0.40
1:A:446:LEU:HD21	1:A:448:CYS:SG	2.62	0.40
1:A:236:ILE:HG23	1:A:266:MET:HE1	2.03	0.40
1:A:282:LYS:HG3	1:A:283:THR:N	2.37	0.40
1:A:384:LYS:HG2	1:A:523:GLN:NE2	2.36	0.40
1:A:482:LEU:O	1:A:483:ILE:HD13	2.21	0.40
1:A:495:GLY:O	1:A:496:ARG:C	2.63	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	535/537 (100%)	426 (80%)	85 (16%)	24 (4%)	2 2

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	155	LEU
1	A	299	ASN
1	A	347	VAL
1	A	392	TRP
1	A	441	ASN
1	A	141	GLY
1	A	143	ASN
1	A	224	GLY
1	A	262	ASN
1	A	346	GLN
1	A	364	TYR
1	A	365	GLY
1	A	522	TYR
1	A	94	PRO
1	A	105	ASN
1	A	107	GLN
1	A	381	ASP
1	A	38	TYR
1	A	323	TRP
1	A	403	ASN
1	A	496	ARG
1	A	90	PRO
1	A	200	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	473/473 (100%)	431 (91%)	42 (9%)	9 20

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	MET
1	A	29	ILE
1	A	78	ILE

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Mol	Chain	Res	Type
1	A	117	LEU
1	A	142	ILE
1	A	143	ASN
1	A	146	SER
1	A	148	ARG
1	A	157	GLN
1	A	158	ASP
1	A	174	LEU
1	A	177	THR
1	A	227	ASN
1	A	236	ILE
1	A	240	ASP
1	A	247	THR
1	A	250	THR
1	A	253	ARG
1	A	256	ASP
1	A	262	ASN
1	A	284	PHE
1	A	318	ILE
1	A	324	LEU
1	A	329	LYS
1	A	346	GLN
1	A	353	LYS
1	A	356	LYS
1	A	376	LEU
1	A	382	LEU
1	A	388	ILE
1	A	397	LEU
1	A	401	LYS
1	A	421	LYS
1	A	441	ASN
1	A	450	ASP
1	A	453	ARG
1	A	463	THR
1	A	475	GLN
1	A	477	LEU
1	A	501	SER
1	A	502	ARG
1	A	518	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	6	GLN
1	A	15	GLN
1	A	19	ASN
1	A	22	ASN
1	A	62	ASN
1	A	106	GLN
1	A	216	ASN
1	A	262	ASN
1	A	290	ASN
1	A	330	GLN
1	A	346	GLN
1	A	349	ASN
1	A	396	GLN
1	A	439	ASN
1	A	451	GLN
1	A	472	ASN
1	A	474	HIS
1	A	475	GLN
1	A	523	GLN
1	A	529	ASN
1	A	531	ASN
1	A	536	ASN
1	A	539	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	1.17	1 (9%)	15,15,17	0.96	1 (6%)
2	FRU	B	2	2	11,12,12	1.43	2 (18%)	10,18,18	0.73	0

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	FRU	O2-C2	4.16	1.47	1.40
2	B	1	GLC	O5-C1	3.17	1.49	1.43
2	B	2	FRU	O5-C2	-2.01	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	C2-C3-C4	-2.24	106.92	110.86

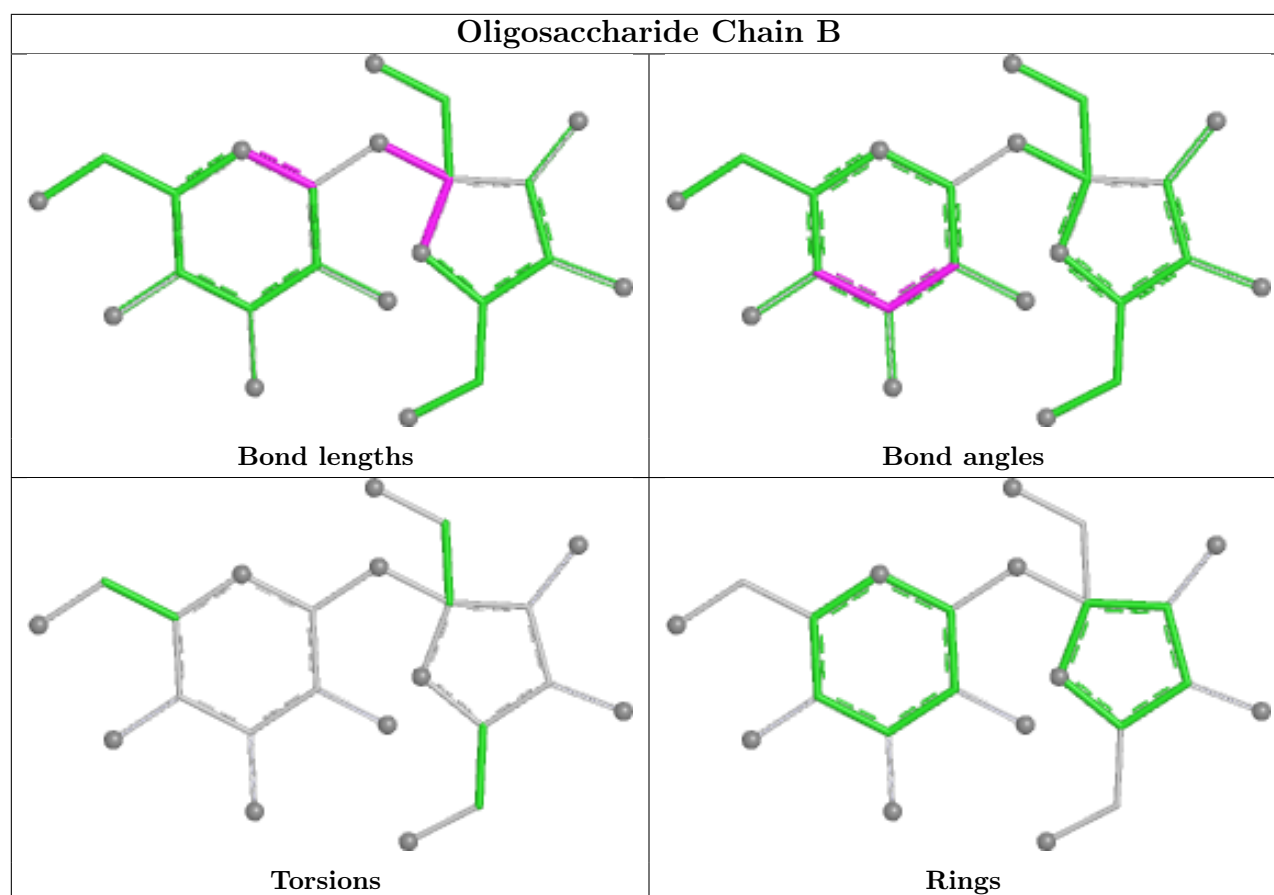
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

3 ligands 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	$\# Z > 2$
3	NAG	A	670	1	14,14,15	0.55	0	17,19,21	0.77	1 (5%)
3	NAG	A	660	1	14,14,15	0.60	0	17,19,21	1.00	0
3	NAG	A	680	1	14,14,15	0.65	0	17,19,21	0.67	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	670	1	-	5/6/23/26	0/1/1/1
3	NAG	A	660	1	-	3/6/23/26	0/1/1/1
3	NAG	A	680	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	680	NAG	C2-N2-C7	-2.17	119.99	122.90
3	A	670	NAG	C2-N2-C7	-2.13	120.05	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	660	NAG	C3-C2-N2-C7
3	A	660	NAG	C8-C7-N2-C2
3	A	660	NAG	O7-C7-N2-C2
3	A	670	NAG	C8-C7-N2-C2
3	A	670	NAG	O7-C7-N2-C2
3	A	680	NAG	C8-C7-N2-C2
3	A	680	NAG	O7-C7-N2-C2
3	A	670	NAG	O5-C5-C6-O6
3	A	680	NAG	O5-C5-C6-O6
3	A	680	NAG	C4-C5-C6-O6
3	A	670	NAG	C4-C5-C6-O6
3	A	670	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	670	NAG	1	0
3	A	660	NAG	2	0

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	537/537 (100%)	-1.83	0 100 100	10, 32, 49, 70	0

There are no RSRZ outliers to report.

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

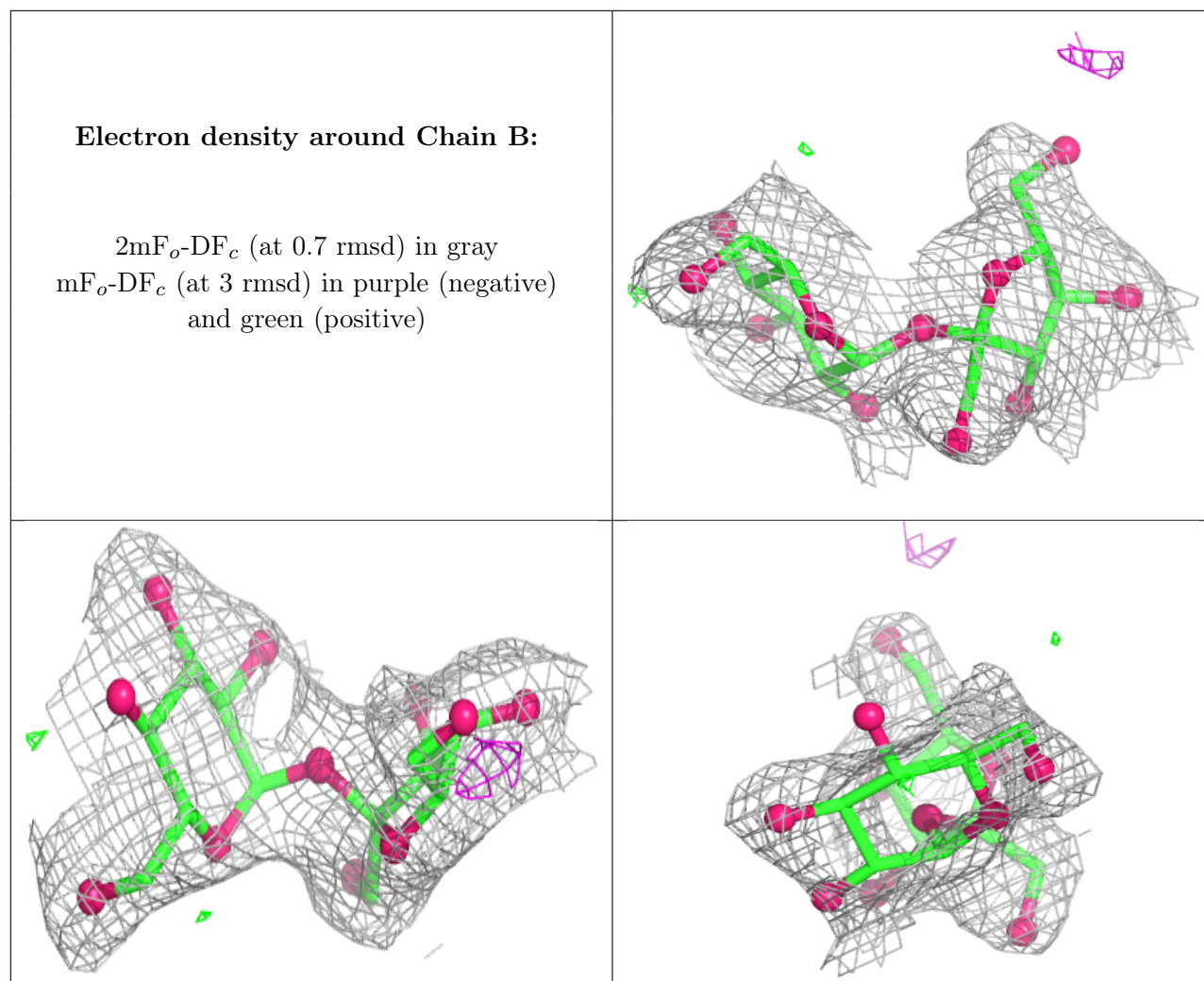
There are no non-standard protein/DNA/RNA residues in this entry.

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	56,60,63,67	0
2	FRU	B	2	12/12	0.99	0.03	46,49,52,53	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($\text{\AA}^2$)	Q<0.9
3	NAG	A	660	14/15	0.99	0.03	40,42,45,46	0
3	NAG	A	670	14/15	0.99	0.04	65,66,67,68	0
3	NAG	A	680	14/15	0.99	0.03	44,52,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.