



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:24 AM UTC

PDB ID : 6TRF / pdb_00006trf
Title : Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) purified from cells treated with kifunensine.
Authors : Roversi, P.; Zitzmann, N.
Deposited on : 2019-12-18
Resolution : 4.11 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

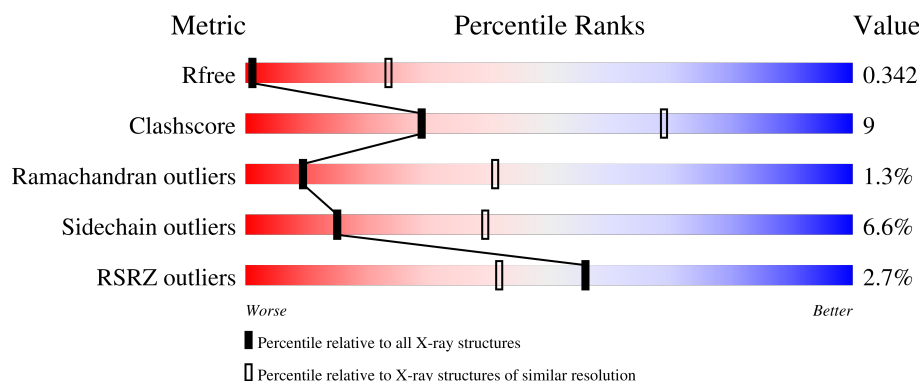
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.11 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	1494	 2% 66% 20% 12%
2	B	6	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10717 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.

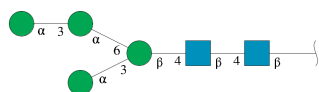
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1319	10616	6785	1806	1993	32	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58

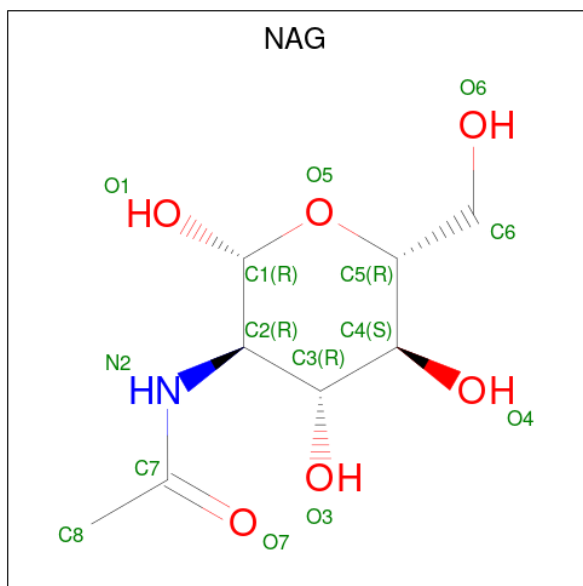
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	72	40	2	30	0	0	0

- 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		

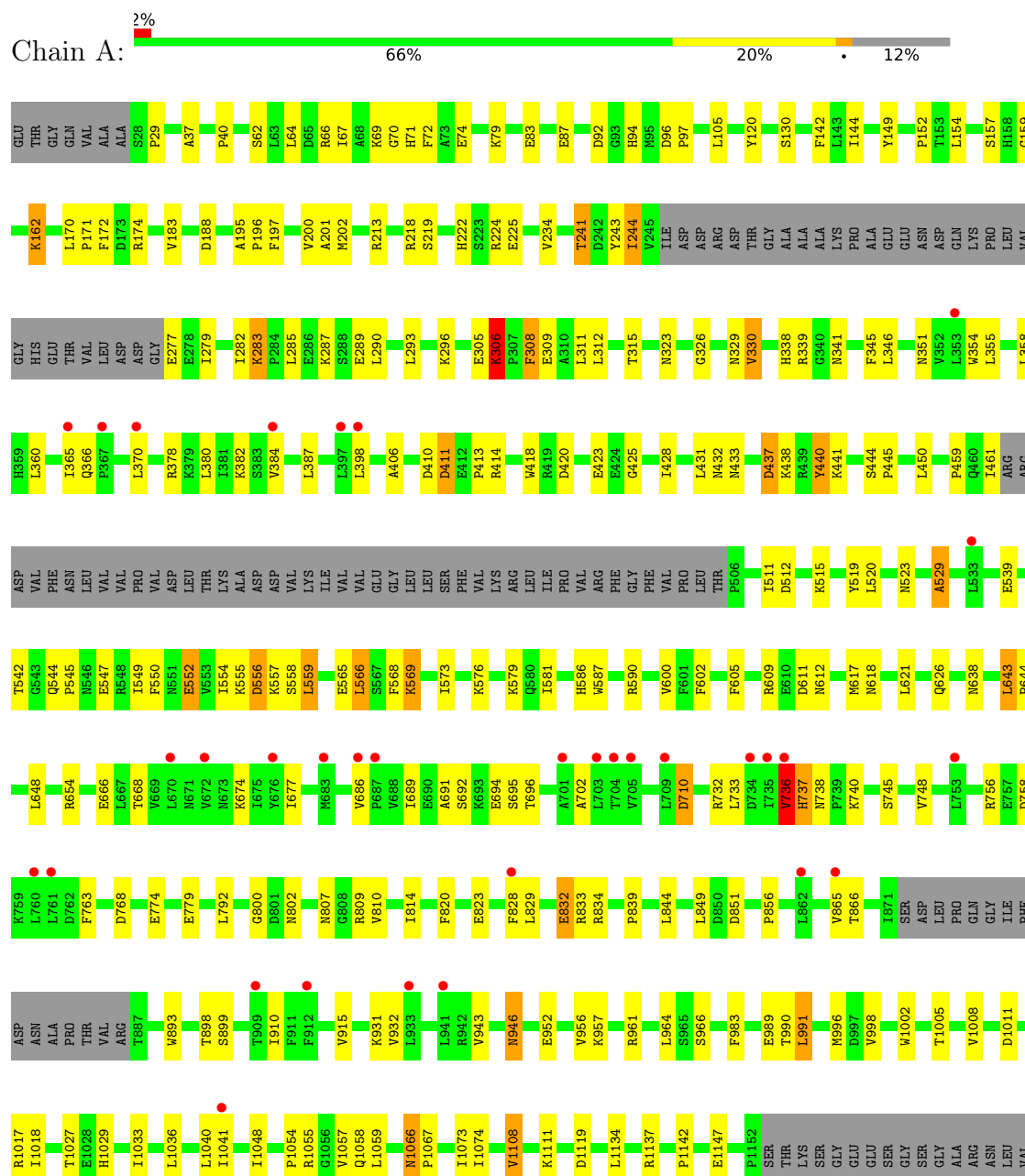
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

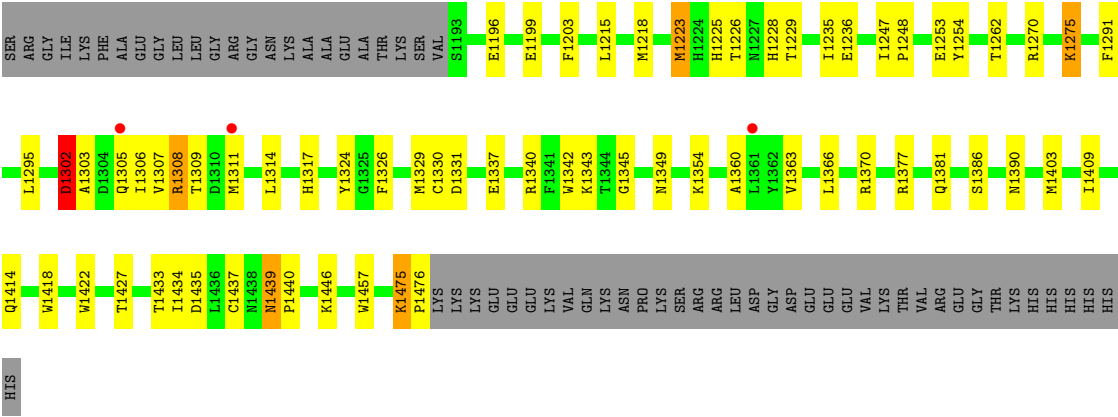
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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: UDP-glucose-glycoprotein glucosyltransferase-like protein





● Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 148.93Å 190.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.15 – 4.11 95.15 – 4.11	Depositor EDS
% Data completeness (in resolution range)	40.7 (95.15-4.11) 41.4 (95.15-4.11)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 4.15Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.255 , 0.315 0.285 , 0.342	Depositor DCC
R_{free} test set	351 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	207.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 260.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10717	wwPDB-VP
Average B, all atoms (Å ²)	270.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: MAN, NAG, BMA, 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	0.60	1/10870 (0.0%)	1.17	36/14734 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	736	VAL	CA-C	6.21	1.60	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLU	CA-C-N	7.61	140.36	121.80
1	A	305	GLU	C-N-CA	7.61	140.36	121.80
1	A	556	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	159	GLY	N-CA-C	6.65	123.47	111.03
1	A	1331	ASP	CA-C-N	6.63	129.46	120.38
1	A	1331	ASP	C-N-CA	6.63	129.46	120.38
1	A	568	PHE	CA-C-N	6.62	134.18	121.54
1	A	568	PHE	C-N-CA	6.62	134.18	121.54
1	A	710	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	330	VAL	N-CA-C	6.61	116.74	110.53
1	A	243	TYR	CA-C-N	6.47	133.62	121.97
1	A	243	TYR	C-N-CA	6.47	133.62	121.97
1	A	1302	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	411	ASP	N-CA-C	-5.71	104.67	111.69
1	A	329	ASN	CA-C-N	5.66	127.80	120.56
1	A	329	ASN	C-N-CA	5.66	127.80	120.56
1	A	411	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	1349	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	638	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	539	GLU	N-CA-C	5.29	116.86	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLY	N-CA-C	-5.26	107.53	115.32
1	A	756	ARG	CA-C-N	5.24	127.56	120.38
1	A	756	ARG	C-N-CA	5.24	127.56	120.38
1	A	308	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	1390	ASN	CA-C-N	5.21	127.21	120.44
1	A	1390	ASN	C-N-CA	5.21	127.21	120.44
1	A	1108	VAL	N-CA-C	-5.20	100.26	107.80
1	A	1040	LEU	N-CA-C	5.20	118.41	110.20
1	A	696	THR	CA-C-N	5.16	127.44	120.38
1	A	696	THR	C-N-CA	5.16	127.44	120.38
1	A	946	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	1235	ILE	CA-C-N	5.09	131.25	121.54
1	A	1235	ILE	C-N-CA	5.09	131.25	121.54
1	A	1041	ILE	N-CA-C	-5.06	99.89	107.37
1	A	529	ALA	CA-C-N	5.04	126.99	120.44
1	A	529	ALA	C-N-CA	5.04	126.99	120.44

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	10616	0	10457	184	0
2	B	72	0	61	1	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
All	All	10717	0	10544	185	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 9.

All (185) 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:438:LYS:HA	1:A:441:LYS:HG2	1.31	1.12
1:A:643:LEU:HG	1:A:644:PRO:HD3	1.33	1.04
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.76	1.01
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.27	0.97
1:A:309:GLU:HG3	1:A:931:LYS:NZ	1.84	0.91
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.06	0.90
1:A:67:ILE:HG22	1:A:72:PHE:CD2	2.08	0.89
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.37	0.89
1:A:384:VAL:HG22	1:A:865:VAL:HG11	1.54	0.89
1:A:309:GLU:HG3	1:A:931:LYS:HZ3	1.37	0.85
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.14	0.82
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.63	0.80
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.63	0.79
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.66	0.78
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.66	0.76
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.71	0.72
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.72	0.72
1:A:66:ARG:HA	1:A:69:LYS:HE2	1.72	0.71
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	2.08	0.71
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.21	0.70
1:A:736:VAL:HG23	1:A:737:HIS:H	1.58	0.69
1:A:438:LYS:CA	1:A:441:LYS:HG2	2.17	0.69
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.58	0.69
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.59	0.68
1:A:433:ASN:O	1:A:437:ASP:HB2	1.94	0.67
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.77	0.67
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.76	0.67
1:A:445:PRO:HA	1:A:461:ILE:HG13	1.76	0.66
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.78	0.65
1:A:1226:THR:OG1	1:A:1228:HIS:ND1	2.28	0.64
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.79	0.64
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.27	0.64
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.59	0.64
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.62	0.63
1:A:554:ILE:O	1:A:558:SER:HB2	1.98	0.63
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.80	0.63
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.80	0.62
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.80	0.62
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.64	0.62
1:A:1305:GLN:HG2	1:A:1435:ASP:HA	1.82	0.62
1:A:188:ASP:OD1	1:A:219:SER:HB3	2.00	0.61
1:A:1291:PHE:HB3	1:A:1295:LEU:HD21	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:TRP:HB3	1:A:1434:ILE:CD1	2.30	0.61
1:A:668:THR:HG23	1:A:810:VAL:HG13	1.82	0.61
1:A:241:THR:HG21	1:A:957:LYS:HD3	1.82	0.60
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.84	0.60
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.48	0.60
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.84	0.60
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.32	0.59
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.90	0.59
1:A:702:ALA:HB1	1:A:732:ARG:HH21	1.68	0.59
1:A:309:GLU:HG3	1:A:931:LYS:HZ1	1.67	0.59
1:A:67:ILE:CG2	1:A:72:PHE:HD2	2.12	0.59
1:A:1340:ARG:HD2	1:A:1343:LYS:HZ2	1.68	0.58
1:A:365:ILE:HG23	1:A:370:LEU:HD11	1.85	0.58
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.85	0.58
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.67	0.58
1:A:1439:ASN:HB2	1:A:1440:PRO:HA	1.86	0.58
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.86	0.57
1:A:1055:ARG:HH12	1:A:1377:ARG:HH12	1.53	0.57
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.40	0.56
1:A:643:LEU:HG	1:A:644:PRO:CD	2.22	0.56
1:A:1307:VAL:HG21	1:A:1311:MET:HE2	1.87	0.56
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.88	0.56
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.23	0.56
1:A:149:TYR:CE1	1:A:157:SER:HB3	2.40	0.56
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.20	0.56
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.85	0.55
1:A:1475:LYS:HG3	1:A:1476:PRO:HD3	1.88	0.55
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.88	0.55
1:A:244:ILE:HG13	1:A:285:LEU:HD12	1.89	0.54
1:A:66:ARG:O	1:A:71:HIS:HB3	2.07	0.54
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.90	0.54
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.39	0.53
1:A:834:ARG:O	1:A:839:PRO:HD3	2.08	0.53
1:A:736:VAL:HG23	1:A:737:HIS:N	2.21	0.52
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.90	0.52
1:A:306:LYS:HA	1:A:306:LYS:NZ	2.25	0.52
1:A:686:VAL:HG11	1:A:736:VAL:HG12	1.92	0.52
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.74	0.51
1:A:418:TRP:H	1:A:418:TRP:CD1	2.28	0.51
1:A:1422:TRP:HZ3	1:A:1437:CYS:HB3	1.76	0.51
1:A:338:HIS:HD2	1:A:898:THR:CG2	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:SER:HA	1:A:943:VAL:O	2.11	0.51
1:A:174:ARG:O	1:A:213:ARG:HB3	2.11	0.50
1:A:309:GLU:HA	1:A:931:LYS:NZ	2.27	0.50
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.92	0.50
1:A:1302:ASP:OD1	1:A:1302:ASP:C	2.54	0.50
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.12	0.50
1:A:1340:ARG:HD2	1:A:1343:LYS:NZ	2.26	0.50
1:A:413:PRO:HB3	1:A:605:PHE:HE1	1.77	0.50
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.94	0.50
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.94	0.49
1:A:1360:ALA:HB1	1:A:1435:ASP:OD1	2.11	0.49
1:A:829:LEU:O	1:A:833:ARG:HB2	2.13	0.49
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.48	0.49
1:A:1027:THR:HG22	1:A:1029:HIS:H	1.78	0.49
1:A:1223:MET:SD	1:A:1254:TYR:HB3	2.53	0.48
1:A:432:ASN:ND2	1:A:440:TYR:OH	2.46	0.48
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.94	0.48
1:A:130:SER:HB3	1:A:162:LYS:O	2.12	0.48
1:A:828:PHE:O	1:A:832:GLU:HB2	2.13	0.48
1:A:600:VAL:CG2	1:A:609:ARG:HG3	2.43	0.48
1:A:1418:TRP:HB3	1:A:1434:ILE:HD13	1.94	0.48
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.96	0.48
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.95	0.47
1:A:1418:TRP:HB3	1:A:1434:ILE:HD12	1.96	0.47
1:A:62:SER:OG	1:A:66:ARG:NH1	2.48	0.47
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.97	0.46
1:A:702:ALA:H	1:A:807:ASN:ND2	2.13	0.46
1:A:296:LYS:HG2	1:A:330:VAL:HG22	1.97	0.46
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.81	0.46
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.86	0.46
2:B:2:NAG:H62	2:B:3:BMA:C1	2.45	0.46
1:A:79:LYS:O	1:A:83:GLU:HG2	2.16	0.46
1:A:306:LYS:HA	1:A:306:LYS:HZ3	1.81	0.46
1:A:174:ARG:O	1:A:213:ARG:CB	2.64	0.46
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.51	0.45
1:A:542:THR:HG22	1:A:544:GLN:H	1.81	0.45
1:A:552:GLU:HA	1:A:555:LYS:NZ	2.32	0.45
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.99	0.45
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.99	0.45
1:A:544:GLN:HG3	1:A:545:PRO:HD2	1.98	0.45
1:A:654:ARG:HH11	1:A:823:GLU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.98	0.45
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.35	0.45
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.99	0.45
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.33	0.45
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.99	0.45
1:A:586:HIS:O	1:A:590:ARG:HB2	2.17	0.45
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.52	0.45
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.99	0.45
1:A:691:ALA:HB3	1:A:856:PRO:HG2	1.98	0.44
1:A:736:VAL:CG2	1:A:737:HIS:H	2.25	0.44
1:A:338:HIS:O	1:A:341:ASN:HB2	2.17	0.44
1:A:600:VAL:HG23	1:A:609:ARG:HG3	2.00	0.44
1:A:1314:LEU:HG	1:A:1363:VAL:HG21	1.99	0.44
1:A:428:ILE:HD11	1:A:587:TRP:NE1	2.33	0.44
1:A:692:SER:O	1:A:695:SER:OG	2.33	0.44
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.99	0.44
1:A:1439:ASN:HB2	1:A:1440:PRO:CA	2.48	0.43
1:A:64:LEU:HD12	1:A:67:ILE:HD11	2.00	0.43
1:A:69:LYS:HE3	1:A:71:HIS:HB2	2.01	0.43
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.83	0.43
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.18	0.43
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	2.01	0.43
1:A:1329:MET:SD	1:A:1342:TRP:NE1	2.92	0.43
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.53	0.43
1:A:552:GLU:HA	1:A:555:LYS:HZ1	1.84	0.43
1:A:740:LYS:HB2	1:A:800:GLY:HA3	2.00	0.43
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.42	0.43
1:A:961:ARG:HA	1:A:961:ARG:HD3	1.92	0.43
1:A:195:ALA:HB3	1:A:196:PRO:HD3	2.00	0.42
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.47	0.42
1:A:1306:ILE:CD1	1:A:1457:TRP:HD1	2.30	0.42
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	3.07	0.42
1:A:311:LEU:O	1:A:315:THR:HG22	2.18	0.42
1:A:573:ILE:HB	1:A:576:LYS:CB	2.47	0.42
1:A:120:TYR:CG	1:A:218:ARG:HG2	2.55	0.42
1:A:519:TYR:HD1	1:A:576:LYS:HZ2	1.63	0.42
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.39	0.42
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.02	0.42
1:A:745:SER:O	1:A:748:VAL:HG22	2.20	0.42
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.52	0.41
1:A:234:VAL:HG22	1:A:996:MET:CE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ALA:H	1:A:807:ASN:HD21	1.68	0.41
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.34	0.41
1:A:105:LEU:HD13	1:A:966:SER:HA	2.03	0.41
1:A:296:LYS:HE2	1:A:330:VAL:HG13	2.01	0.41
1:A:355:LEU:HD11	1:A:910:ILE:HG23	2.03	0.41
1:A:1275:LYS:HB3	1:A:1275:LYS:HE2	1.92	0.41
1:A:1340:ARG:HD3	1:A:1342:TRP:CZ2	2.56	0.41
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.85	0.41
1:A:1215:LEU:HD12	1:A:1218:MET:HE3	2.03	0.41
1:A:413:PRO:HB3	1:A:605:PHE:CE1	2.56	0.41
1:A:523:ASN:OD1	1:A:566:LEU:HA	2.20	0.41
1:A:283:LYS:HD2	1:A:283:LYS:O	2.22	0.40
1:A:406:ALA:HB2	1:A:839:PRO:HG2	2.04	0.40
1:A:423:GLU:CD	1:A:590:ARG:HH11	2.29	0.40
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.61	0.40
1:A:346:LEU:HD11	1:A:354:TRP:HH2	1.87	0.40
1:A:450:LEU:HD23	1:A:459:PRO:HB2	2.04	0.40
1:A:351:ASN:HA	1:A:915:VAL:O	2.21	0.40
1:A:37:ALA:HA	1:A:1036:LEU:HB3	2.03	0.40
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.37	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	1309/1494 (88%)	1235 (94%)	57 (4%)	17 (1%)	9 41

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ILE

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Mol	Chain	Res	Type
1	A	287	LYS
1	A	306	LYS
1	A	444	SER
1	A	737	HIS
1	A	1303	ALA
1	A	1439	ASN
1	A	569	LYS
1	A	736	VAL
1	A	1345	GLY
1	A	559	LEU
1	A	666	GLU
1	A	611	ASP
1	A	1475	LYS
1	A	279	ILE
1	A	1142	PRO
1	A	1337	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	1151/1297 (89%)	1075 (93%)	76 (7%)	15 39

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	87	GLU
1	A	154	LEU
1	A	162	LYS
1	A	202	MET
1	A	222	HIS
1	A	225	GLU
1	A	241	THR
1	A	277	GLU
1	A	283	LYS

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Mol	Chain	Res	Type
1	A	289	GLU
1	A	306	LYS
1	A	308	PHE
1	A	323	ASN
1	A	339	ARG
1	A	358	LEU
1	A	360	LEU
1	A	366	GLN
1	A	378	ARG
1	A	380	LEU
1	A	382	LYS
1	A	387	LEU
1	A	410	ASP
1	A	411	ASP
1	A	414	ARG
1	A	431	LEU
1	A	437	ASP
1	A	440	TYR
1	A	549	ILE
1	A	552	GLU
1	A	556	ASP
1	A	557	LYS
1	A	559	LEU
1	A	565	GLU
1	A	566	LEU
1	A	569	LYS
1	A	579	LYS
1	A	612	ASN
1	A	617	MET
1	A	618	ASN
1	A	626	GLN
1	A	643	LEU
1	A	674	LYS
1	A	677	ILE
1	A	694	GLU
1	A	710	ASP
1	A	758	ASP
1	A	774	GLU
1	A	779	GLU
1	A	809	ARG
1	A	820	PHE
1	A	832	GLU

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Mol	Chain	Res	Type
1	A	851	ASP
1	A	952	GLU
1	A	956	VAL
1	A	989	GLU
1	A	991	LEU
1	A	1011	ASP
1	A	1066	ASN
1	A	1147	GLU
1	A	1196	GLU
1	A	1203	PHE
1	A	1223	MET
1	A	1253	GLU
1	A	1262	THR
1	A	1275	LYS
1	A	1302	ASP
1	A	1308	ARG
1	A	1309	THR
1	A	1317	HIS
1	A	1330	CYS
1	A	1354	LYS
1	A	1366	LEU
1	A	1370	ARG
1	A	1414	GLN
1	A	1446	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	323	ASN
1	A	432	ASN
1	A	460	GLN
1	A	626	GLN
1	A	679	ASN
1	A	1015	ASN
1	A	1201	ASN
1	A	1267	HIS
1	A	1414	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 ⓘ

6 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	NAG	B	1	1,2	14,14,15	0.35	0	17,19,21	1.52	1 (5%)
2	NAG	B	2	2	14,14,15	0.31	0	17,19,21	0.65	0
2	BMA	B	3	2	11,11,12	0.30	0	15,15,17	0.44	0
2	MAN	B	4	2	11,11,12	0.41	0	15,15,17	1.30	1 (6%)
2	MAN	B	5	2	11,11,12	0.32	0	15,15,17	0.77	1 (6%)
2	MAN	B	6	2	11,11,12	0.55	0	15,15,17	1.13	2 (13%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	1/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-5.27	103.14	111.29
2	B	4	MAN	C1-O5-C5	4.41	118.09	112.19
2	B	6	MAN	C1-O5-C5	3.35	116.68	112.19
2	B	5	MAN	C1-O5-C5	2.76	115.88	112.19
2	B	6	MAN	C1-C2-C3	2.29	112.98	109.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6

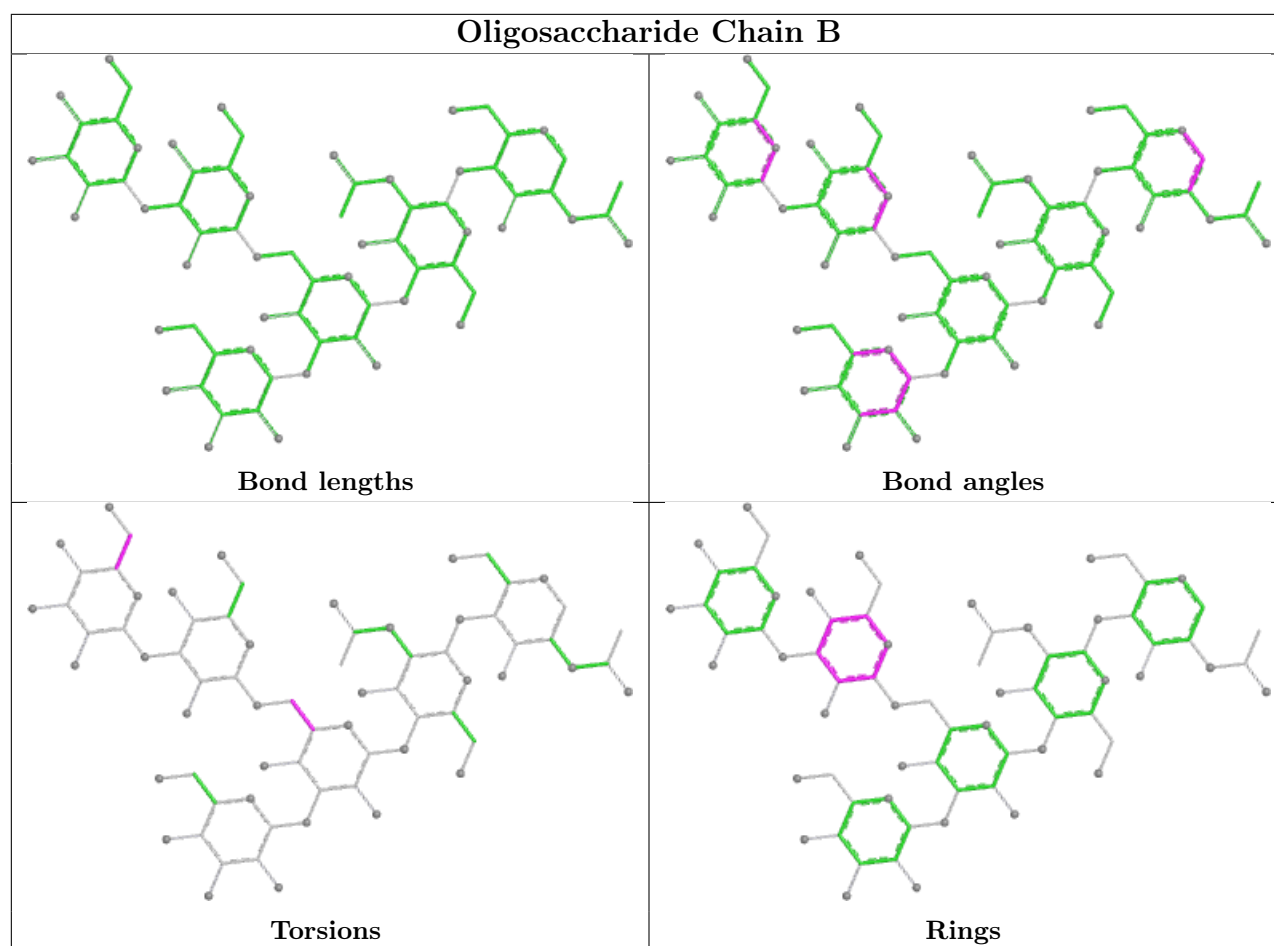
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	3	BMA	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1601	1	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
3	NAG	A	1602	-	14,14,15	0.31	0	17,19,21	0.51	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
3	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1602	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1601	NAG	C1-O5-C5	2.36	115.34	112.19

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 [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	1319/1494 (88%)	-0.30	36 (2%) 56 42	94, 284, 300, 300	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	ILE	5.3
1	A	912	PHE	4.9
1	A	734	ASP	4.5
1	A	941	LEU	4.1
1	A	686	VAL	3.7
1	A	862	LEU	3.7
1	A	683	MET	3.6
1	A	705	VAL	3.5
1	A	704	THR	3.5
1	A	397	LEU	3.5
1	A	760	LEU	3.4
1	A	370	LEU	3.2
1	A	365	ILE	3.2
1	A	384	VAL	3.1
1	A	687	PRO	2.8
1	A	933	LEU	2.8
1	A	736	VAL	2.7
1	A	1361	LEU	2.7
1	A	398	LEU	2.7
1	A	676	TYR	2.7
1	A	672	VAL	2.6
1	A	353	LEU	2.6
1	A	1041	ILE	2.6
1	A	865	VAL	2.4
1	A	367	PRO	2.4
1	A	533	LEU	2.4
1	A	709	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	703	LEU	2.4
1	A	909	THR	2.3
1	A	1311	MET	2.2
1	A	1305	GLN	2.2
1	A	701	ALA	2.1
1	A	761	LEU	2.1
1	A	670	LEU	2.1
1	A	753	LEU	2.0
1	A	828	PHE	2.0

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

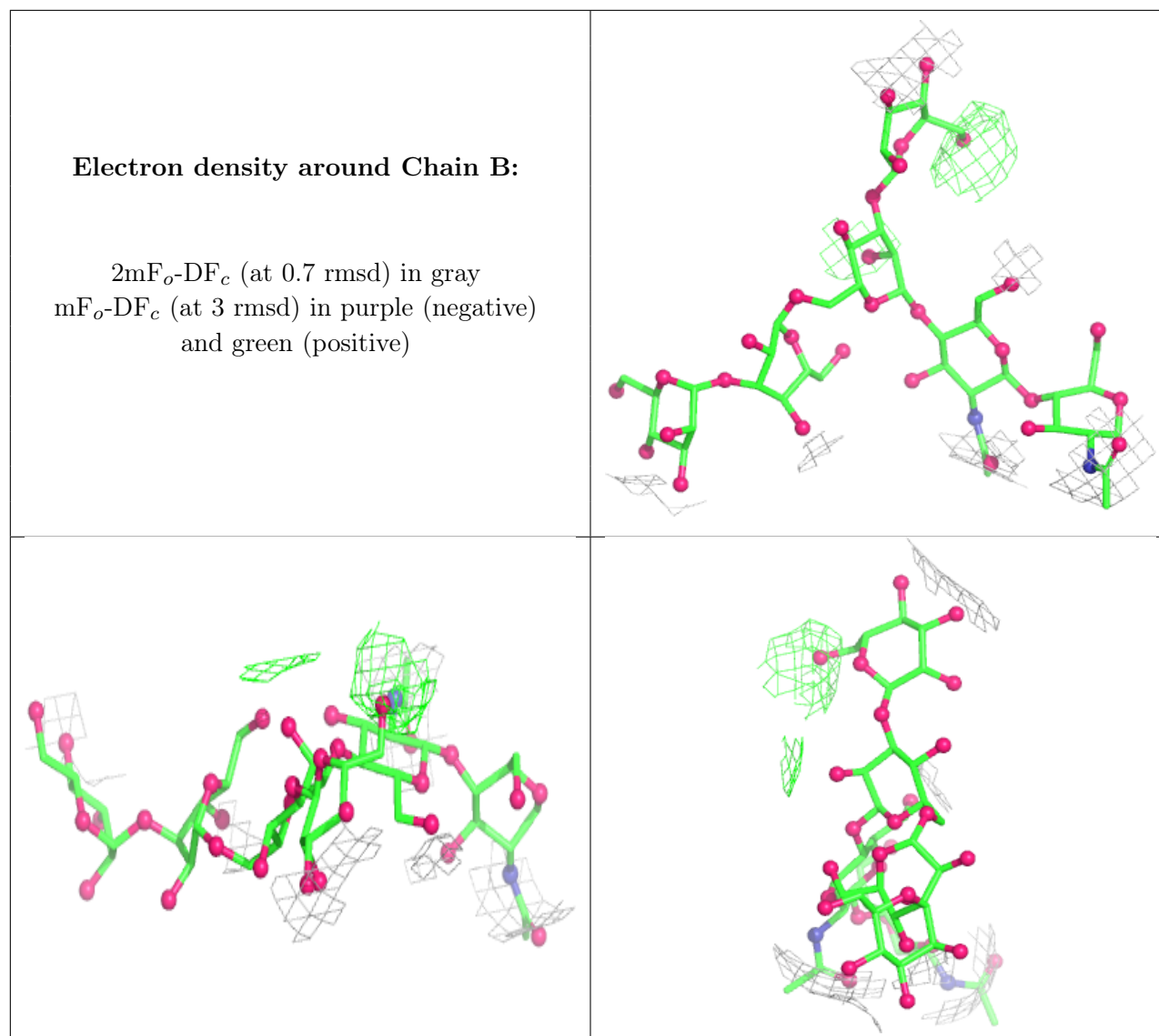
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
2	MAN	B	5	11/12	0.15	0.07	292,293,295,295	0
2	MAN	B	6	11/12	0.16	0.10	300,300,300,300	0
2	BMA	B	3	11/12	0.55	0.06	298,300,300,300	0
2	MAN	B	4	11/12	0.74	0.06	293,295,297,297	0
2	NAG	B	2	14/15	0.76	0.08	290,295,300,300	0
2	NAG	B	1	14/15	0.91	0.12	286,292,296,298	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
3	NAG	A	1602	14/15	0.73	0.08	300,300,300,300	0
3	NAG	A	1601	14/15	0.80	0.04	240,268,285,290	0
4	CA	A	1603	1/1	0.91	0.19	298,298,298,298	1

6.5 Other polymers [i](#)

There are no such residues in this entry.