



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:33 AM UTC

PDB ID : 6TRT / pdb_00006trt
Title : Chaetomium thermophilum UDP-Glucose Glucosyl Transferase (UGGT) double cysteine mutant S180C/T742C.
Authors : Roversi, P.; Zitzmann, N.; Ibba, R.; Hensen, M.
Deposited on : 2019-12-19
Resolution : 4.58 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

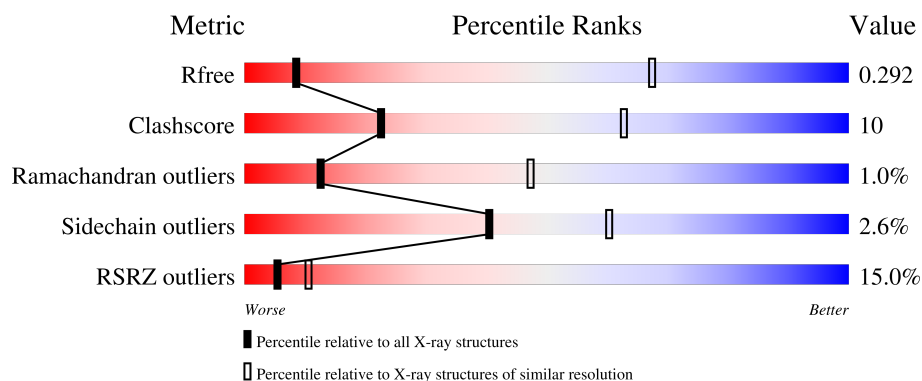
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.58 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	1003 (5.22-3.92)
Clashscore	190562	1019 (5.22-3.94)
Ramachandran outliers	187476	1068 (5.26-3.90)
Sidechain outliers	187428	1050 (5.26-3.90)
RSRZ outliers	180081	1139 (5.26-3.90)

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	14% 69% 21% 8%
2	B	3	33% 67%
2	D	3	33% 67%
3	C	8	88% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11210 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.

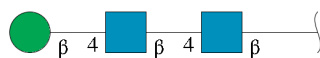
- Molecule 1 is a protein called UDP-glucose-glycoprotein glucosyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1369	Total	C	N	O	S	0	0	0
			11007	7045	1875	2053	34			

There are 14 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	180	CYS	SER	engineered mutation	UNP G0SB58
A	742	CYS	THR	engineered mutation	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 beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



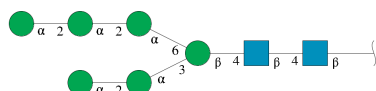
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.

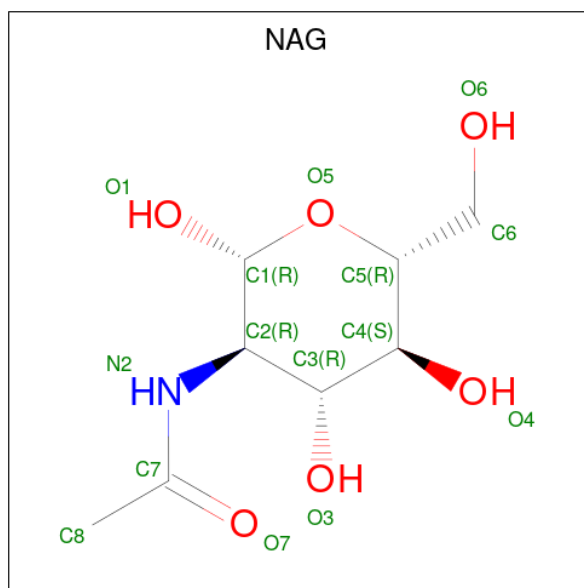


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 4 is TERBIUM(III) ION (CCD ID: Tb) (formula: Tb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Tb	0	0
			3	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

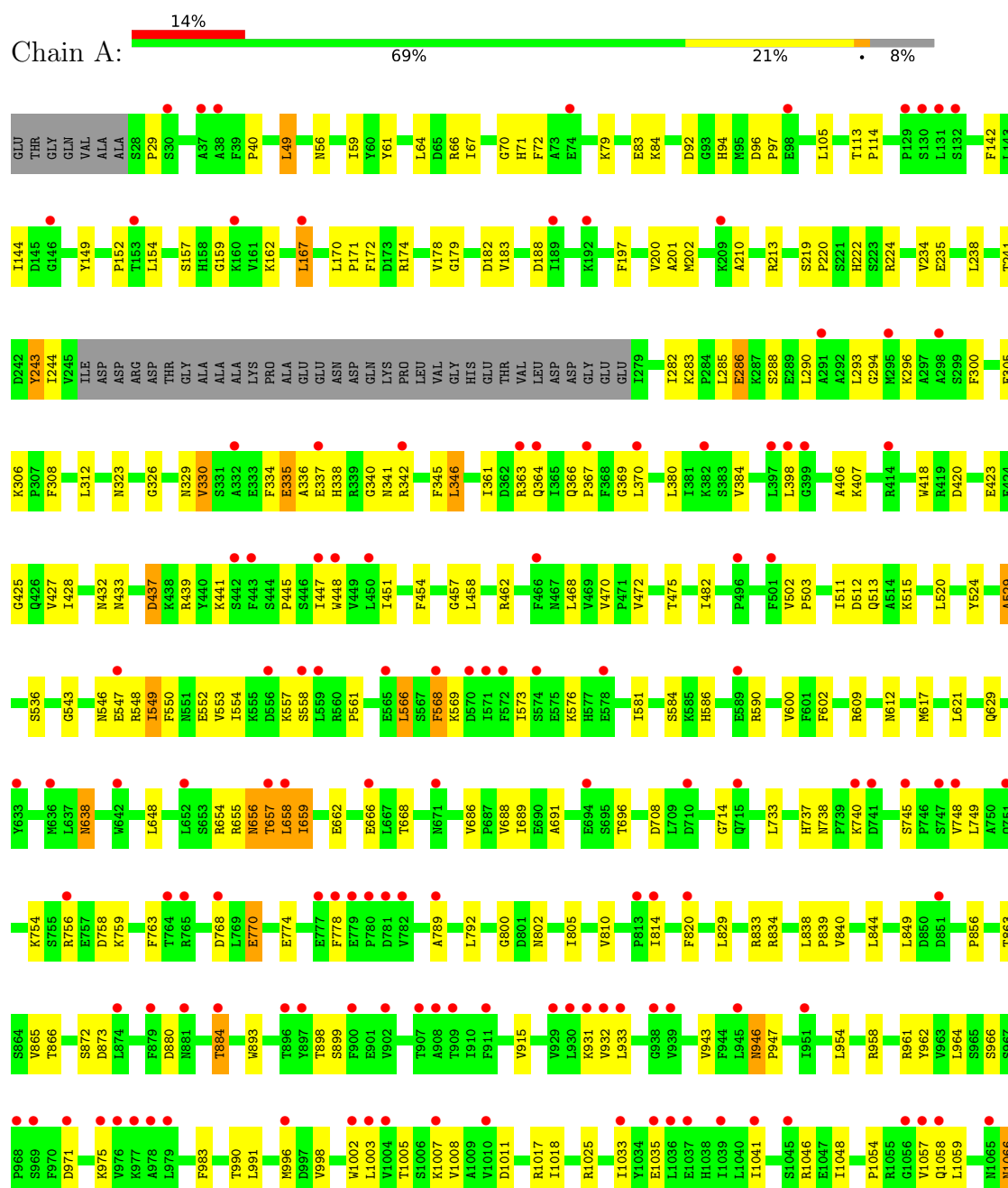


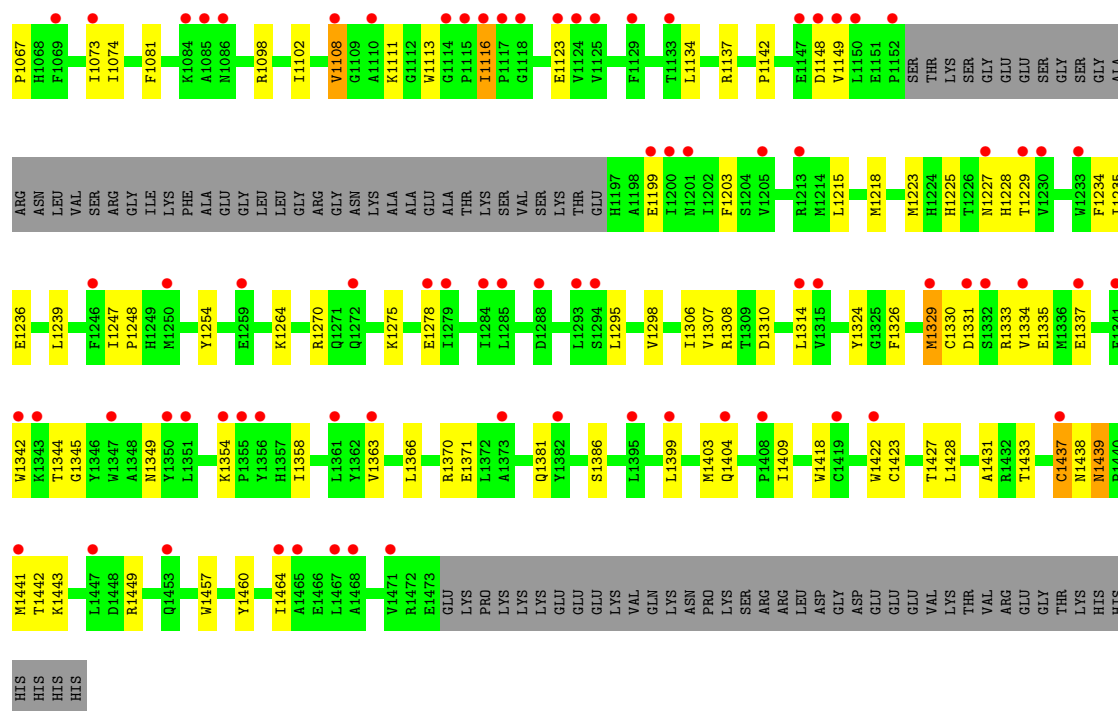
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 33% 67%



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 33% 67%



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 C: 88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	148.80Å 148.80Å 235.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	128.86 – 4.58 128.86 – 4.58	Depositor EDS
% Data completeness (in resolution range)	54.9 (128.86-4.58) 55.8 (128.86-4.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 4.47Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.291 , 0.297 0.283 , 0.292	Depositor DCC
R_{free} test set	418 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	263.8	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 369.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.083 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11210	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: NAG, BMA, TB, MAN

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	1/11272 (0.0%)	1.20	54/15289 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	ILE	CG1-CD1	-5.85	1.28	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ASN	CA-C-N	8.08	130.74	120.56
1	A	329	ASN	C-N-CA	8.08	130.74	120.56
1	A	243	TYR	CA-C-N	7.94	136.25	121.97
1	A	243	TYR	C-N-CA	7.94	136.25	121.97
1	A	1227	ASN	CA-CB-CG	7.59	120.19	112.60
1	A	638	ASN	CA-CB-CG	7.46	120.06	112.60
1	A	336	ALA	N-CA-C	-7.42	104.37	113.50
1	A	334	PHE	N-CA-C	-7.31	102.70	111.69
1	A	330	VAL	N-CA-C	7.29	117.42	110.42
1	A	568	PHE	CA-C-N	7.20	135.28	121.54
1	A	568	PHE	C-N-CA	7.20	135.28	121.54
1	A	305	GLU	CA-C-N	7.06	139.03	121.80
1	A	305	GLU	C-N-CA	7.06	139.03	121.80
1	A	1235	ILE	CA-C-N	6.94	131.23	120.82
1	A	1235	ILE	C-N-CA	6.94	131.23	120.82
1	A	335	GLU	CA-C-N	6.93	133.91	121.92
1	A	335	GLU	C-N-CA	6.93	133.91	121.92
1	A	1331	ASP	CA-C-N	6.71	129.57	120.38
1	A	1331	ASP	C-N-CA	6.71	129.57	120.38
1	A	159	GLY	N-CA-C	6.47	123.19	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	ARG	N-CA-C	-6.05	104.97	112.72
1	A	346	LEU	N-CA-C	5.97	118.56	110.31
1	A	432	ASN	CA-C-N	5.96	130.46	121.40
1	A	432	ASN	C-N-CA	5.96	130.46	121.40
1	A	778	PHE	CA-C-N	5.88	129.79	121.61
1	A	778	PHE	C-N-CA	5.88	129.79	121.61
1	A	340	GLY	N-CA-C	-5.75	105.66	113.37
1	A	49	LEU	N-CA-CB	5.70	119.08	110.30
1	A	336	ALA	CA-C-N	5.69	128.37	120.29
1	A	336	ALA	C-N-CA	5.69	128.37	120.29
1	A	300	PHE	CA-C-N	5.66	127.80	120.56
1	A	300	PHE	C-N-CA	5.66	127.80	120.56
1	A	286	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	1349	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	1108	VAL	N-CA-C	-5.39	99.99	107.80
1	A	1335	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	70	GLY	N-CA-C	-5.36	107.62	115.72
1	A	1310	ASP	N-CA-C	-5.33	100.40	108.67
1	A	1227	ASN	N-CA-C	-5.33	105.47	112.72
1	A	756	ARG	CA-C-N	5.32	127.67	120.38
1	A	756	ARG	C-N-CA	5.32	127.67	120.38
1	A	1334	VAL	N-CA-C	5.25	115.91	110.82
1	A	529	ALA	CA-C-N	5.11	127.08	120.44
1	A	529	ALA	C-N-CA	5.11	127.08	120.44
1	A	946	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	696	THR	CA-C-N	5.09	127.35	120.38
1	A	696	THR	C-N-CA	5.09	127.35	120.38
1	A	1041	ILE	N-CA-C	-5.07	99.86	107.37
1	A	340	GLY	CA-C-N	5.03	127.28	120.44
1	A	340	GLY	C-N-CA	5.03	127.28	120.44
1	A	655	ARG	CA-C-N	5.01	131.11	121.54
1	A	655	ARG	C-N-CA	5.01	131.11	121.54
1	A	241	THR	CA-C-N	5.01	127.24	120.38
1	A	241	THR	C-N-CA	5.01	127.24	120.38

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	11007	0	10875	230	6
2	B	39	0	34	0	0
2	D	39	0	34	0	0
3	C	94	0	79	3	0
4	A	3	0	0	0	0
5	A	28	0	26	0	0
All	All	11210	0	11048	233	6

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 (233) 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:1225:HIS:ND1	1:A:1308:ARG:HA	1.64	1.11
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.24	1.02
3:C:3:BMA:H4	3:C:6:MAN:H61	1.44	0.97
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.95	0.94
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.05	0.91
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.56	0.88
1:A:67:ILE:HG22	1:A:72:PHE:CD2	2.12	0.84
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.12	0.82
1:A:1329:MET:HG2	1:A:1358:ILE:HD11	1.61	0.82
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.60	0.82
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.42	0.82
1:A:149:TYR:CE1	1:A:157:SER:HB3	2.16	0.80
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.64	0.79
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.82	0.78
1:A:338:HIS:O	1:A:341:ASN:HB2	1.81	0.78
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.66	0.78
1:A:72:PHE:CE1	1:A:84:LYS:HG3	2.20	0.77
1:A:59:ILE:HD13	1:A:94:HIS:ND1	2.00	0.76
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.66	0.76
1:A:244:ILE:HA	1:A:285:LEU:HB3	1.67	0.76
1:A:554:ILE:HG21	1:A:568:PHE:HE1	1.50	0.75
1:A:686:VAL:O	1:A:754:LYS:HE2	1.87	0.74
1:A:59:ILE:HD13	1:A:94:HIS:CG	2.22	0.74
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.70	0.72
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.71	0.72
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	2.07	0.71
1:A:407:LYS:NZ	1:A:884:THR:HB	2.04	0.71
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.71	0.71
1:A:283:LYS:HZ2	1:A:285:LEU:HD21	1.56	0.70
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.57	0.70
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.75	0.69
1:A:244:ILE:HD11	1:A:954:LEU:HD13	1.75	0.69
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.58	0.68
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.75	0.68
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.76	0.68
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.59	0.68
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.76	0.68
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.25	0.67
1:A:243:TYR:O	1:A:285:LEU:HG	1.95	0.67
1:A:244:ILE:HG12	1:A:285:LEU:HD12	1.75	0.67
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.77	0.67
1:A:433:ASN:O	1:A:437:ASP:HB2	1.95	0.66
1:A:407:LYS:HZ2	1:A:884:THR:HB	1.60	0.66
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.78	0.65
1:A:475:THR:HA	1:A:543:GLY:HA3	1.79	0.65
3:C:3:BMA:C4	3:C:6:MAN:H61	2.25	0.65
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.79	0.64
1:A:243:TYR:HD1	1:A:285:LEU:HD23	1.63	0.64
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.79	0.64
1:A:1354:LYS:HD2	1:A:1404:GLN:HG3	1.79	0.64
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.98	0.63
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.79	0.63
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.64	0.63
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.28	0.63
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.30	0.62
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.80	0.62
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.81	0.62
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.81	0.62
1:A:67:ILE:CG2	1:A:72:PHE:HD2	2.12	0.62
1:A:451:ILE:HA	1:A:629:GLN:HG2	1.81	0.61
1:A:447:ILE:HG23	1:A:448:TRP:CD1	2.36	0.61
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.52	0.60
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.31	0.60
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.84	0.60
1:A:66:ARG:O	1:A:71:HIS:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.33	0.59
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.85	0.59
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.86	0.58
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.89	0.58
1:A:1366:LEU:O	1:A:1370:ARG:HG3	2.04	0.57
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.85	0.57
1:A:174:ARG:O	1:A:213:ARG:HB3	2.05	0.57
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.85	0.57
1:A:1422:TRP:HZ3	1:A:1437:CYS:HB2	1.68	0.57
1:A:40:PRO:HB3	1:A:224:ARG:HD2	1.86	0.57
3:C:3:BMA:H4	3:C:6:MAN:C6	2.28	0.57
1:A:243:TYR:CD1	1:A:285:LEU:HD23	2.40	0.56
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.68	0.56
1:A:834:ARG:O	1:A:839:PRO:HD3	2.06	0.56
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.52	0.56
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.41	0.56
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.86	0.56
1:A:554:ILE:O	1:A:558:SER:HB2	2.06	0.55
1:A:554:ILE:O	1:A:558:SER:CB	2.55	0.55
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.87	0.55
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.88	0.54
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.89	0.54
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.37	0.54
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.71	0.54
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.90	0.54
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.89	0.54
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.34	0.54
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.43	0.54
1:A:418:TRP:H	1:A:418:TRP:CD1	2.25	0.54
1:A:656:ASN:O	1:A:657:THR:O	2.25	0.54
1:A:338:HIS:HD2	1:A:898:THR:CG2	2.11	0.53
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.73	0.53
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.38	0.53
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.91	0.53
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.73	0.53
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.21	0.52
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.27	0.52
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.34	0.52
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.39	0.52
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.92	0.52
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.92	0.51
1:A:872:SER:HB2	1:A:884:THR:OG1	2.10	0.51
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.92	0.51
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.36	0.51
1:A:657:THR:HG23	1:A:659:ILE:HG22	1.92	0.51
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.93	0.51
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.75	0.50
1:A:899:SER:HA	1:A:943:VAL:O	2.11	0.50
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.94	0.50
1:A:524:TYR:CE2	1:A:558:SER:HA	2.47	0.49
1:A:174:ARG:O	1:A:213:ARG:CB	2.60	0.49
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.13	0.49
1:A:546:ASN:O	1:A:549:ILE:HG22	2.13	0.49
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.95	0.49
1:A:1111:LYS:HB2	1:A:1116:ILE:HG13	1.94	0.49
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.93	0.49
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.94	0.49
1:A:656:ASN:HD21	1:A:662:GLU:H	1.61	0.48
1:A:178:VAL:HG22	1:A:789:ALA:CB	2.42	0.48
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.93	0.48
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.78	0.48
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.96	0.48
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.95	0.48
1:A:56:ASN:HB3	1:A:59:ILE:HG22	1.95	0.48
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.96	0.48
1:A:1329:MET:SD	1:A:1342:TRP:CH2	3.07	0.48
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.96	0.47
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.49	0.47
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.97	0.47
1:A:840:VAL:HG21	1:A:863:THR:HA	1.96	0.47
1:A:79:LYS:O	1:A:83:GLU:HG2	2.15	0.47
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.45	0.47
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.79	0.47
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.96	0.47
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.97	0.47
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.50	0.47
1:A:366:GLN:HG2	1:A:369:GLY:H	1.80	0.47
1:A:61:TYR:HB3	1:A:202:MET:HE1	1.97	0.46
1:A:1199:GLU:OE1	1:A:1228:HIS:ND1	2.48	0.46
1:A:536:SER:HA	1:A:549:ILE:HD13	1.96	0.46
1:A:668:THR:HG23	1:A:810:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:VAL:O	1:A:503:PRO:HA	2.15	0.46
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.79	0.46
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.16	0.46
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.50	0.46
1:A:654:ARG:HE	1:A:657:THR:HB	1.80	0.46
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.97	0.46
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	1.98	0.46
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.50	0.46
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.34	0.46
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.56	0.46
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.97	0.46
1:A:829:LEU:O	1:A:833:ARG:HB2	2.15	0.45
1:A:737:HIS:NE2	1:A:749:LEU:HD12	2.31	0.45
1:A:458:LEU:HD21	1:A:621:LEU:HD21	1.99	0.45
1:A:553:VAL:O	1:A:557:LYS:HB2	2.17	0.45
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.95	0.45
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.46	0.45
1:A:326:GLY:CA	1:A:330:VAL:HG11	2.43	0.45
1:A:573:ILE:HB	1:A:576:LYS:CB	2.47	0.45
1:A:740:LYS:HB2	1:A:800:GLY:HA3	1.98	0.45
1:A:745:SER:O	1:A:748:VAL:HG22	2.17	0.44
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.17	0.44
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.64	0.44
1:A:367:PRO:HD3	1:A:962:TYR:OH	2.18	0.44
1:A:656:ASN:ND2	1:A:662:GLU:H	2.16	0.44
1:A:691:ALA:HB3	1:A:856:PRO:HG2	2.00	0.44
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.51	0.44
1:A:105:LEU:HD13	1:A:966:SER:HA	1.99	0.43
1:A:179:GLY:HA3	1:A:210:ALA:HA	2.00	0.43
1:A:548:ARG:O	1:A:552:GLU:OE2	2.36	0.43
1:A:1116:ILE:HD13	1:A:1116:ILE:H	1.84	0.43
1:A:64:LEU:HD12	1:A:67:ILE:HD11	1.99	0.43
1:A:423:GLU:CD	1:A:590:ARG:HH11	2.25	0.43
1:A:561:PRO:CG	1:A:566:LEU:HD23	2.49	0.43
1:A:802:ASN:HB2	1:A:814:ILE:HB	2.00	0.43
1:A:441:LYS:HA	1:A:462:ARG:HD3	2.01	0.43
1:A:586:HIS:O	1:A:590:ARG:HB2	2.18	0.43
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.19	0.43
1:A:335:GLU:HA	1:A:337:GLU:HG2	2.00	0.43
1:A:468:LEU:HD22	1:A:617:MET:SD	2.58	0.43
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:NZ	1:A:285:LEU:HD21	2.27	0.43
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.19	0.43
1:A:1399:LEU:HD12	1:A:1399:LEU:HA	1.95	0.43
1:A:113:THR:OG1	1:A:114:PRO:HD3	2.19	0.43
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	3.06	0.43
1:A:370:LEU:HD13	1:A:933:LEU:HD11	2.00	0.43
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.84	0.43
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.94	0.42
1:A:770:GLU:OE2	1:A:774:GLU:OE2	2.37	0.42
1:A:445:PRO:HG3	1:A:462:ARG:NH2	2.35	0.42
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.47	0.42
1:A:1215:LEU:HD12	1:A:1218:MET:HE3	2.01	0.42
1:A:234:VAL:HG22	1:A:996:MET:CE	2.49	0.42
1:A:971:ASP:HB2	1:A:975:LYS:O	2.20	0.42
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.90	0.42
1:A:361:ILE:HG13	1:A:364:GLN:HG3	2.01	0.42
1:A:427:VAL:CG2	1:A:584:SER:HA	2.49	0.42
1:A:554:ILE:HD13	1:A:568:PHE:CE1	2.55	0.42
1:A:561:PRO:HG3	1:A:566:LEU:HD23	2.02	0.42
1:A:219:SER:HA	1:A:220:PRO:HD3	1.95	0.42
1:A:447:ILE:CG2	1:A:448:TRP:CD1	3.02	0.42
1:A:468:LEU:HD11	1:A:600:VAL:HG12	2.02	0.42
1:A:170:LEU:C	1:A:170:LEU:HD12	2.44	0.42
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.02	0.42
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.50	0.42
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	2.02	0.41
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.86	0.41
1:A:296:LYS:HD3	1:A:326:GLY:HA2	2.02	0.41
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	2.02	0.41
1:A:178:VAL:HG22	1:A:789:ALA:HB2	2.02	0.41
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.53	0.41
1:A:686:VAL:O	1:A:688:VAL:HG23	2.20	0.41
1:A:167:LEU:HD11	1:A:182:ASP:HB3	2.01	0.41
1:A:482:ILE:HD12	1:A:609:ARG:NH2	2.36	0.41
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.86	0.41
1:A:1460:TYR:O	1:A:1464:ILE:HG12	2.21	0.41
1:A:654:ARG:HH11	1:A:657:THR:H	1.68	0.41
1:A:708:ASP:O	1:A:714:GLY:HA3	2.21	0.41
1:A:1098:ARG:HG2	1:A:1148:ASP:HA	2.03	0.41
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.34	0.40
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.37	0.40
1:A:1275:LYS:O	1:A:1278:GLU:HB2	2.21	0.40
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.37	0.40

All (6) 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)
1:A:1442:THR:OG1	1:A:1442:THR:CG2[5_554]	1.39	0.81
1:A:1442:THR:CB	1:A:1442:THR:CB[5_554]	1.39	0.81
1:A:1442:THR:CB	1:A:1442:THR:CG2[5_554]	1.49	0.71
1:A:1442:THR:CG2	1:A:1442:THR:CG2[5_554]	1.51	0.69
1:A:1442:THR:CB	1:A:1442:THR:OG1[5_554]	1.55	0.65
1:A:1441:MET:CG	1:A:1441:MET:SD[5_554]	1.90	0.30

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	1363/1494 (91%)	1284 (94%)	65 (5%)	14 (1%)	12	47

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	SER
1	A	569	LYS
1	A	656	ASN
1	A	657	THR
1	A	659	ILE
1	A	1439	ASN
1	A	454	PHE
1	A	162	LYS

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Mol	Chain	Res	Type
1	A	666	GLU
1	A	1337	GLU
1	A	658	LEU
1	A	1142	PRO
1	A	306	LYS
1	A	457	GLY

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	1196/1297 (92%)	1165 (97%)	31 (3%)	40 60

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	154	LEU
1	A	167	LEU
1	A	222	HIS
1	A	286	GLU
1	A	308	PHE
1	A	323	ASN
1	A	342	ARG
1	A	363	ARG
1	A	437	ASP
1	A	513	GLN
1	A	566	LEU
1	A	612	ASN
1	A	638	ASN
1	A	658	LEU
1	A	758	ASP
1	A	759	LYS
1	A	770	GLU
1	A	820	PHE
1	A	873	ASP

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Mol	Chain	Res	Type
1	A	880	ASP
1	A	884	THR
1	A	1066	ASN
1	A	1116	ILE
1	A	1123	GLU
1	A	1203	PHE
1	A	1329	MET
1	A	1330	CYS
1	A	1437	CYS
1	A	1439	ASN
1	A	1443	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	GLN
1	A	513	GLN
1	A	540	GLN
1	A	546	ASN
1	A	656	ASN
1	A	728	ASN
1	A	1015	ASN
1	A	1068	HIS
1	A	1130	GLN
1	A	1201	ASN
1	A	1305	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

14 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	0.34	0	17,19,21	1.14	2 (11%)
2	NAG	B	2	2	14,14,15	0.36	0	17,19,21	1.20	3 (17%)
2	BMA	B	3	2	11,11,12	0.26	0	15,15,17	0.51	0
3	NAG	C	1	1,3	14,14,15	0.33	0	17,19,21	1.11	1 (5%)
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	1.42	3 (17%)
3	BMA	C	3	3	11,11,12	0.29	0	15,15,17	0.46	0
3	MAN	C	4	3	11,11,12	0.46	0	15,15,17	1.27	3 (20%)
3	MAN	C	5	3	11,11,12	0.64	0	15,15,17	1.51	2 (13%)
3	MAN	C	6	3	11,11,12	0.27	0	15,15,17	0.89	1 (6%)
3	MAN	C	7	3	11,11,12	0.49	0	15,15,17	1.38	1 (6%)
3	MAN	C	8	3	11,11,12	0.29	0	15,15,17	0.78	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	1.55	3 (17%)
2	BMA	D	3	2	11,11,12	0.27	0	15,15,17	0.46	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	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	1/1/1/1
3	MAN	C	6	3	-	1/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	MAN	C1-O5-C5	4.94	118.81	112.19
3	C	7	MAN	C1-O5-C5	4.61	118.37	112.19
2	D	2	NAG	O5-C1-C2	4.05	117.56	111.29
2	D	2	NAG	C1-O5-C5	3.97	117.50	112.19
2	B	1	NAG	C1-O5-C5	3.72	117.17	112.19
3	C	1	NAG	C1-O5-C5	3.53	116.92	112.19
3	C	2	NAG	O5-C1-C2	-3.42	106.00	111.29
3	C	6	MAN	C1-O5-C5	3.34	116.67	112.19
3	C	2	NAG	C1-C2-N2	3.33	115.67	110.43
2	D	1	NAG	C1-O5-C5	2.95	116.15	112.19
3	C	8	MAN	C1-O5-C5	2.88	116.05	112.19
2	B	2	NAG	C1-C2-N2	2.75	114.76	110.43
3	C	4	MAN	C1-O5-C5	2.73	115.85	112.19
2	B	2	NAG	C1-O5-C5	2.65	115.74	112.19
2	B	2	NAG	C2-N2-C7	2.46	126.20	122.90
3	C	2	NAG	C2-N2-C7	2.46	126.20	122.90
3	C	5	MAN	C1-C2-C3	2.42	113.16	109.64
3	C	4	MAN	O2-C2-C3	2.29	114.90	110.15
3	C	4	MAN	O2-C2-C1	2.19	114.23	109.22
2	B	1	NAG	O5-C1-C2	2.14	114.60	111.29
2	D	2	NAG	C2-N2-C7	2.05	125.65	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	4	MAN	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
2	B	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7

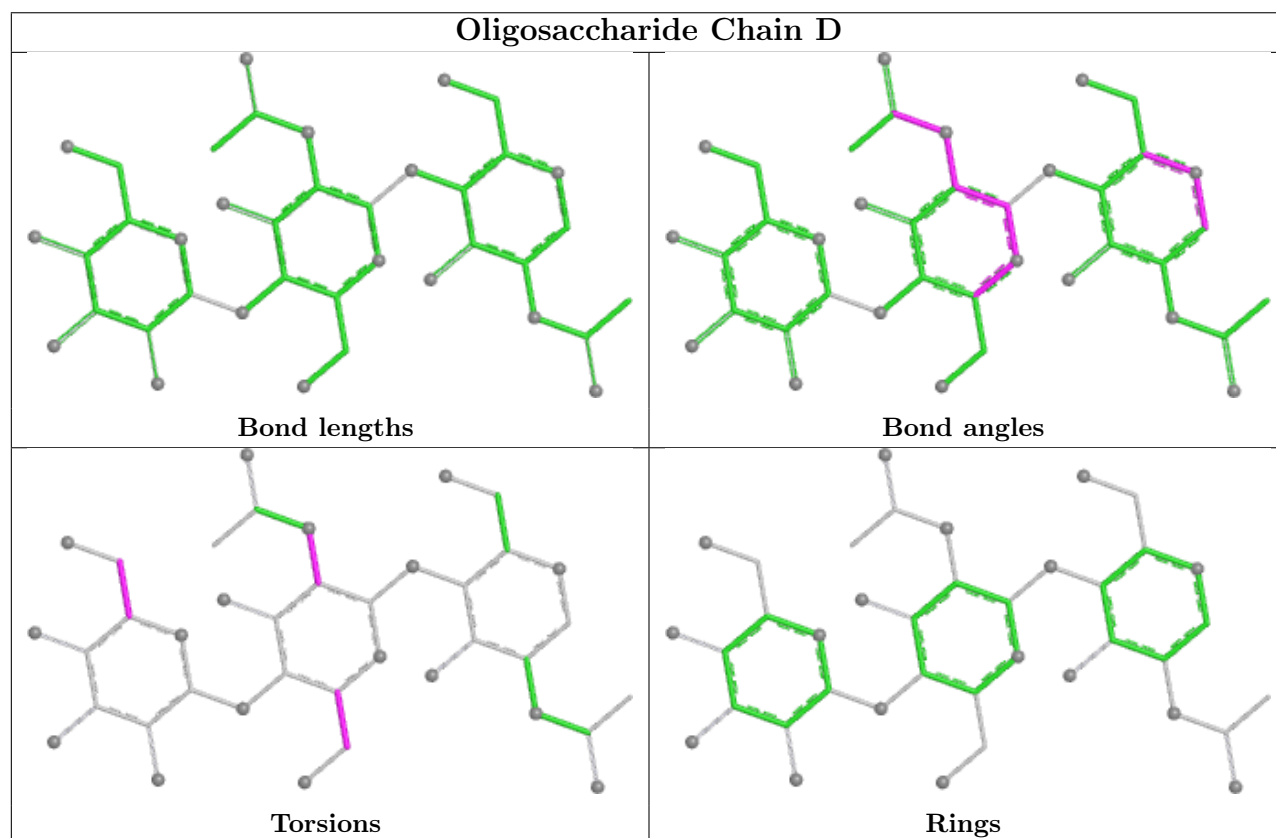
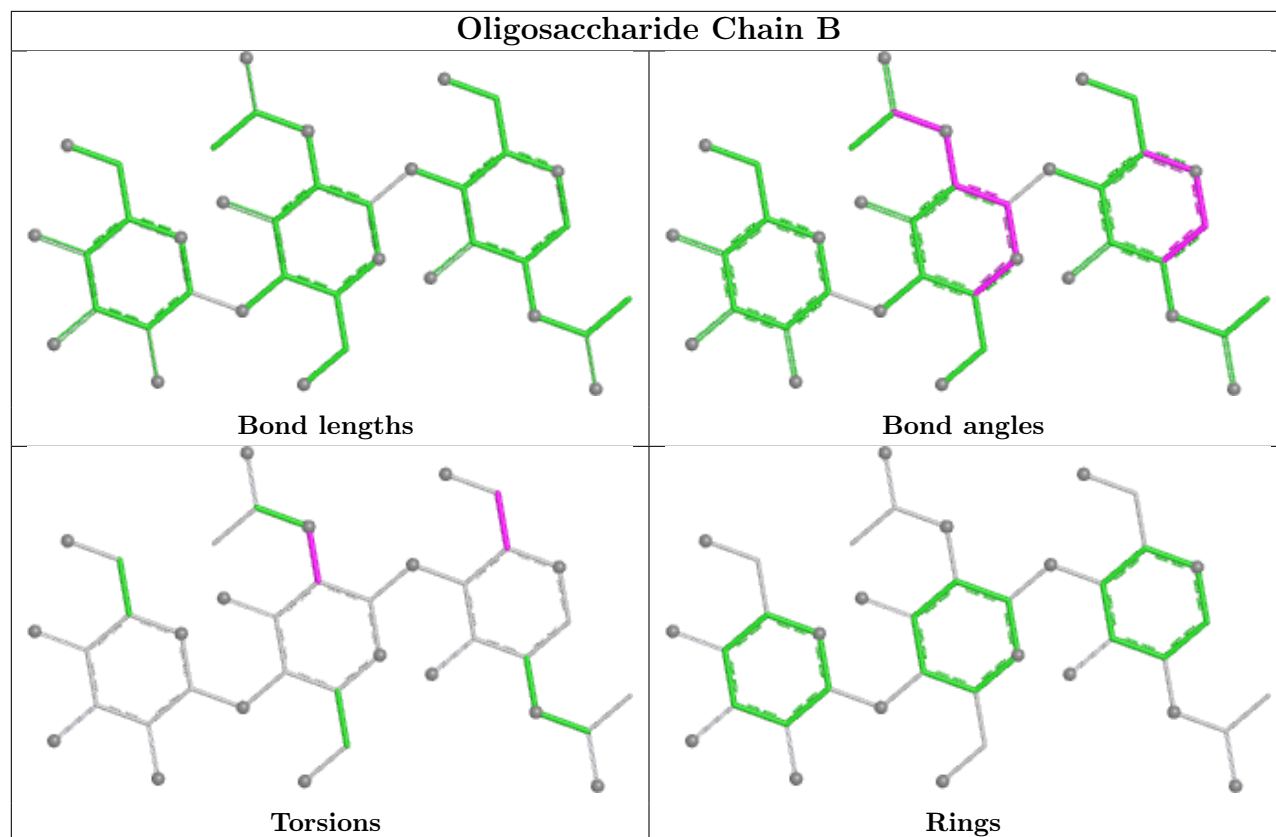
All (2) ring outliers are listed below:

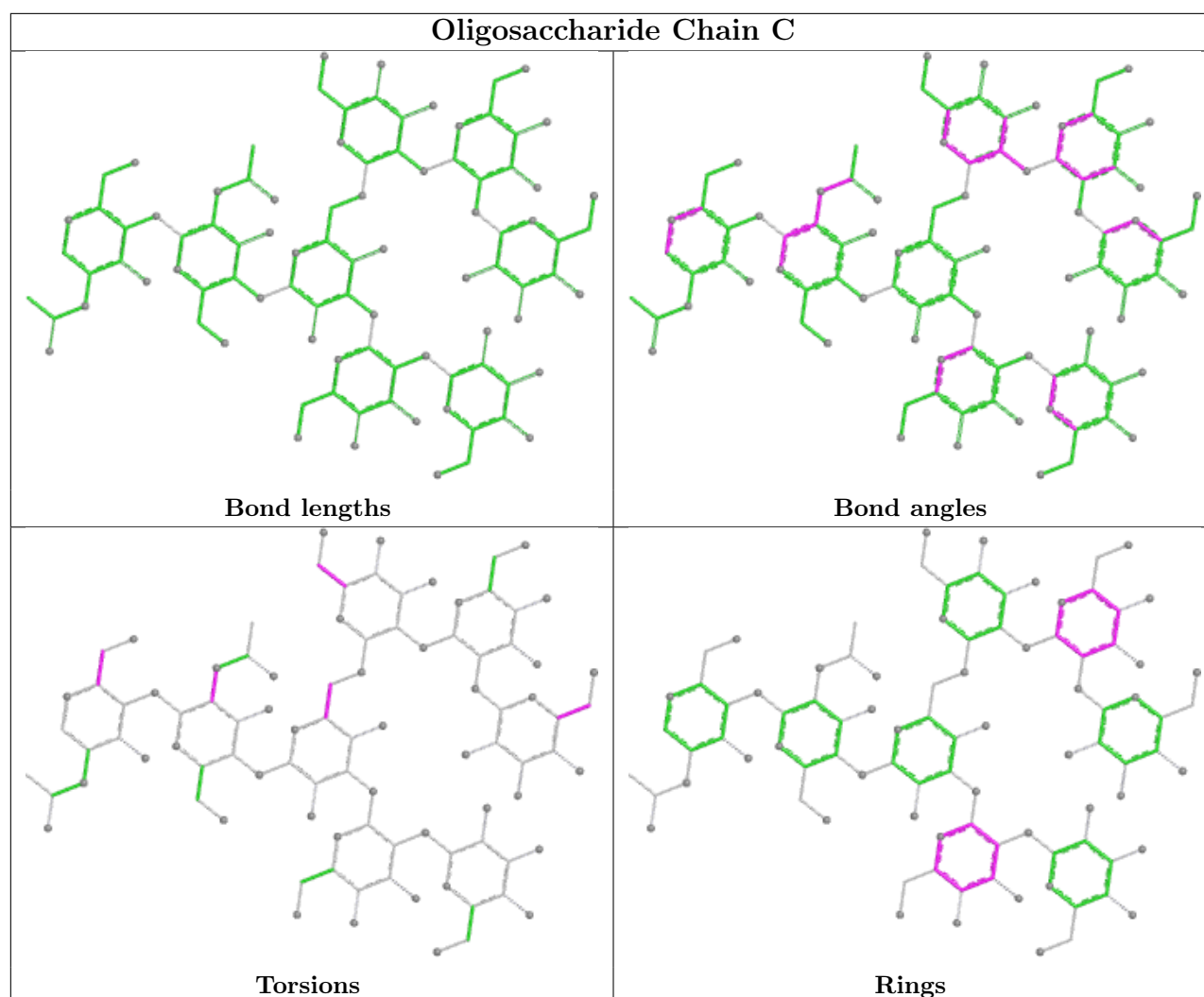
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	C1-C2-C3-C4-C5-O5
3	C	7	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	6	MAN	3	0
3	C	3	BMA	3	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 5 ligands modelled in this entry, 3 are 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	$\# Z > 2$
5	NAG	A	1607	1	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
5	NAG	A	1619	1	14,14,15	0.42	0	17,19,21	1.56	2 (11%)

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
5	NAG	A	1607	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1619	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1619	NAG	C1-O5-C5	5.36	119.37	112.19
5	A	1619	NAG	O5-C1-C2	3.14	116.15	111.29
5	A	1607	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1607	NAG	O5-C5-C6-O6
5	A	1619	NAG	O5-C5-C6-O6

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	1369/1494 (91%)	0.88	206 (15%) 5 10	54, 128, 265, 300	1 (0%)

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1468	ALA	11.5
1	A	1331	ASP	10.8
1	A	1115	PRO	10.6
1	A	1464	ILE	8.2
1	A	1332	SER	7.1
1	A	1036	LEU	6.4
1	A	570	ASP	6.3
1	A	933	LEU	6.2
1	A	764	THR	5.9
1	A	779	GLU	5.8
1	A	978	ALA	5.8
1	A	658	LEU	5.8
1	A	1085	ALA	5.8
1	A	897	TYR	5.7
1	A	652	LEU	5.5
1	A	1354	LYS	5.4
1	A	1065	ASN	5.4
1	A	710	ASP	5.2
1	A	1329	MET	5.1
1	A	130	SER	5.1
1	A	879	PHE	5.0
1	A	1110	ALA	4.8
1	A	694	GLU	4.8
1	A	1230	VAL	4.8
1	A	1108	VAL	4.8
1	A	1200	ILE	4.8
1	A	938	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1007	LYS	4.7
1	A	1453	GLN	4.7
1	A	1343	LYS	4.6
1	A	642	TRP	4.6
1	A	295	MET	4.5
1	A	1147	GLU	4.5
1	A	1114	GLY	4.5
1	A	1037	GLU	4.5
1	A	1294	SER	4.4
1	A	782	VAL	4.4
1	A	1246	PHE	4.4
1	A	1227	ASN	4.4
1	A	1314	LEU	4.4
1	A	1315	VAL	4.3
1	A	450	LEU	4.3
1	A	1363	VAL	4.3
1	A	748	VAL	4.2
1	A	896	THR	4.2
1	A	768	ASP	4.1
1	A	851	ASP	4.1
1	A	1123	GLU	4.1
1	A	364	GLN	4.1
1	A	907	THR	4.1
1	A	1284	ILE	4.1
1	A	778	PHE	4.1
1	A	909	THR	4.0
1	A	979	LEU	4.0
1	A	1086	ASN	4.0
1	A	129	PRO	4.0
1	A	765	ARG	4.0
1	A	1058	GLN	3.9
1	A	1056	GLY	3.8
1	A	382	LYS	3.8
1	A	1117	PRO	3.8
1	A	1465	ALA	3.7
1	A	1069	PHE	3.7
1	A	1337	GLU	3.7
1	A	969	SER	3.7
1	A	1437	CYS	3.7
1	A	1361	LEU	3.6
1	A	1341	PHE	3.6
1	A	367	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	74	GLU	3.6
1	A	1447	LEU	3.6
1	A	756	ARG	3.5
1	A	1057	VAL	3.5
1	A	908	ALA	3.5
1	A	745	SER	3.5
1	A	442	SER	3.4
1	A	1039	ILE	3.4
1	A	1033	ILE	3.4
1	A	902	VAL	3.4
1	A	1342	TRP	3.4
1	A	38	ALA	3.4
1	A	1124	VAL	3.3
1	A	1471	VAL	3.3
1	A	1395	LEU	3.3
1	A	1229	THR	3.2
1	A	131	LEU	3.2
1	A	1116	ILE	3.2
1	A	1467	LEU	3.2
1	A	900	PHE	3.2
1	A	929	VAL	3.2
1	A	740	LYS	3.2
1	A	1041	ILE	3.1
1	A	1259	GLU	3.1
1	A	547	GLU	3.1
1	A	813	PRO	3.1
1	A	574	SER	3.0
1	A	447	ILE	3.0
1	A	1035	GLU	3.0
1	A	1422	TRP	3.0
1	A	1399	LEU	3.0
1	A	37	ALA	3.0
1	A	741	ASP	2.9
1	A	337	GLU	2.9
1	A	565	GLU	2.9
1	A	1118	GLY	2.9
1	A	884	THR	2.9
1	A	715	GLN	2.9
1	A	559	LEU	2.9
1	A	1150	LEU	2.9
1	A	951	ILE	2.8
1	A	666	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	945	LEU	2.8
1	A	1233	TRP	2.8
1	A	496	PRO	2.8
1	A	363	ARG	2.8
1	A	1213	ARG	2.8
1	A	1347	TRP	2.8
1	A	977	LYS	2.8
1	A	1293	LEU	2.8
1	A	976	VAL	2.7
1	A	1084	LYS	2.7
1	A	671	ASN	2.7
1	A	1278	GLU	2.7
1	A	1045	SER	2.7
1	A	342	ARG	2.7
1	A	160	LYS	2.7
1	A	298	ALA	2.7
1	A	777	GLU	2.7
1	A	1205	VAL	2.7
1	A	1441	MET	2.7
1	A	1152	PRO	2.7
1	A	636	MET	2.7
1	A	911	PHE	2.6
1	A	1149	VAL	2.6
1	A	780	PRO	2.6
1	A	820	PHE	2.6
1	A	153	THR	2.6
1	A	789	ALA	2.6
1	A	571	ILE	2.6
1	A	1073	ILE	2.6
1	A	1334	VAL	2.5
1	A	1382	TYR	2.5
1	A	501	PHE	2.5
1	A	1002	TRP	2.5
1	A	968	PRO	2.5
1	A	1003	LEU	2.5
1	A	1279	ILE	2.5
1	A	1010	VAL	2.5
1	A	657	THR	2.5
1	A	747	SER	2.5
1	A	1272	GLN	2.5
1	A	448	TRP	2.5
1	A	132	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1408	PRO	2.4
1	A	1129	PHE	2.4
1	A	939	VAL	2.4
1	A	98	GLU	2.4
1	A	466	PHE	2.4
1	A	971	ASP	2.4
1	A	996	MET	2.4
1	A	1199	GLU	2.3
1	A	443	PHE	2.3
1	A	1350	TYR	2.3
1	A	414	ARG	2.3
1	A	633	TYR	2.3
1	A	589	GLU	2.3
1	A	881	ASN	2.3
1	A	572	PHE	2.3
1	A	814	ILE	2.3
1	A	1355	PRO	2.3
1	A	931	LYS	2.3
1	A	556	ASP	2.3
1	A	189	ILE	2.2
1	A	397	LEU	2.2
1	A	932	VAL	2.2
1	A	370	LEU	2.2
1	A	399	GLY	2.2
1	A	1125	VAL	2.2
1	A	1351	LEU	2.2
1	A	291	ALA	2.2
1	A	1419	CYS	2.2
1	A	568	PHE	2.2
1	A	874	LEU	2.2
1	A	1004	VAL	2.2
1	A	578	GLU	2.2
1	A	167	LEU	2.2
1	A	781	ASP	2.1
1	A	1285	LEU	2.1
1	A	1250	MET	2.1
1	A	1404	GLN	2.1
1	A	1148	ASP	2.1
1	A	1288	ASP	2.1
1	A	192	LYS	2.1
1	A	1201	ASN	2.1
1	A	146	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	LYS	2.1
1	A	751	GLN	2.1
1	A	558	SER	2.1
1	A	975	LYS	2.0
1	A	1356	TYR	2.0
1	A	1133	THR	2.0
1	A	30	SER	2.0
1	A	1373	ALA	2.0
1	A	398	LEU	2.0
1	A	930	LEU	2.0
1	A	332	ALA	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](#)

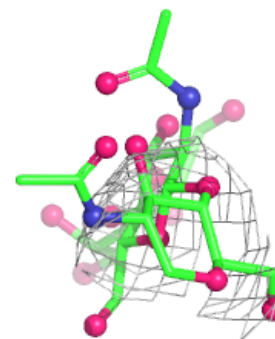
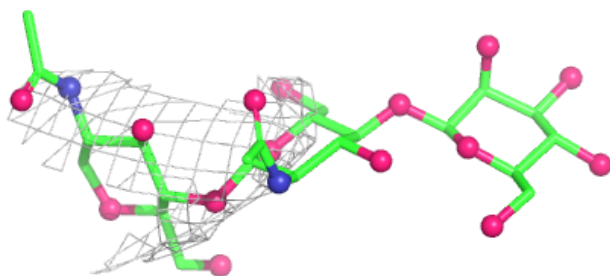
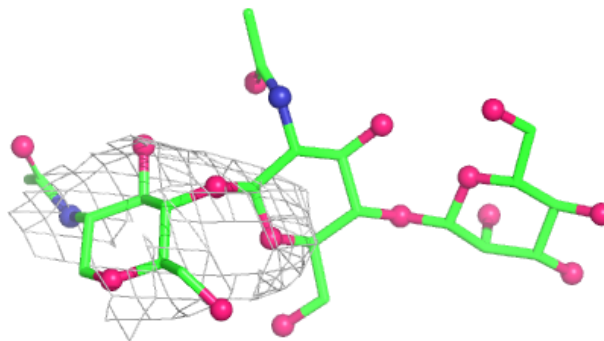
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BMA	D	3	11/12	0.06	0.18	291,292,292,293	0
3	MAN	C	5	11/12	0.10	0.14	300,300,300,300	0
3	MAN	C	8	11/12	0.12	0.16	298,298,299,299	0
3	MAN	C	4	11/12	0.13	0.21	300,300,300,300	0
3	BMA	C	3	11/12	0.34	0.16	291,296,298,298	0
2	BMA	B	3	11/12	0.35	0.15	167,261,296,297	0
3	MAN	C	6	11/12	0.41	0.10	300,300,300,300	0
3	MAN	C	7	11/12	0.61	0.14	297,298,299,299	0
2	NAG	D	2	14/15	0.61	0.15	290,292,295,296	0
2	NAG	D	1	14/15	0.77	0.16	286,292,293,294	0
2	NAG	B	2	14/15	0.78	0.13	113,153,272,293	0
3	NAG	C	2	14/15	0.80	0.18	191,214,266,286	0
2	NAG	B	1	14/15	0.87	0.10	95,109,135,138	0
3	NAG	C	1	14/15	0.93	0.16	132,156,192,273	0

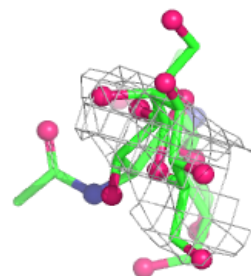
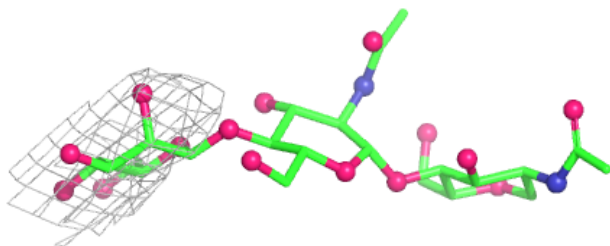
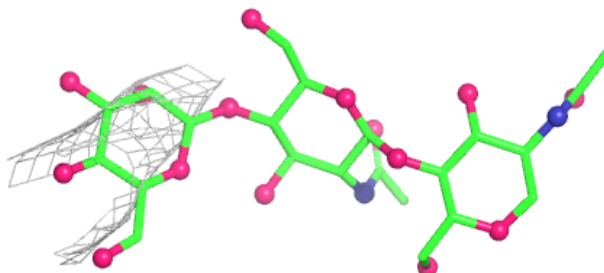
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

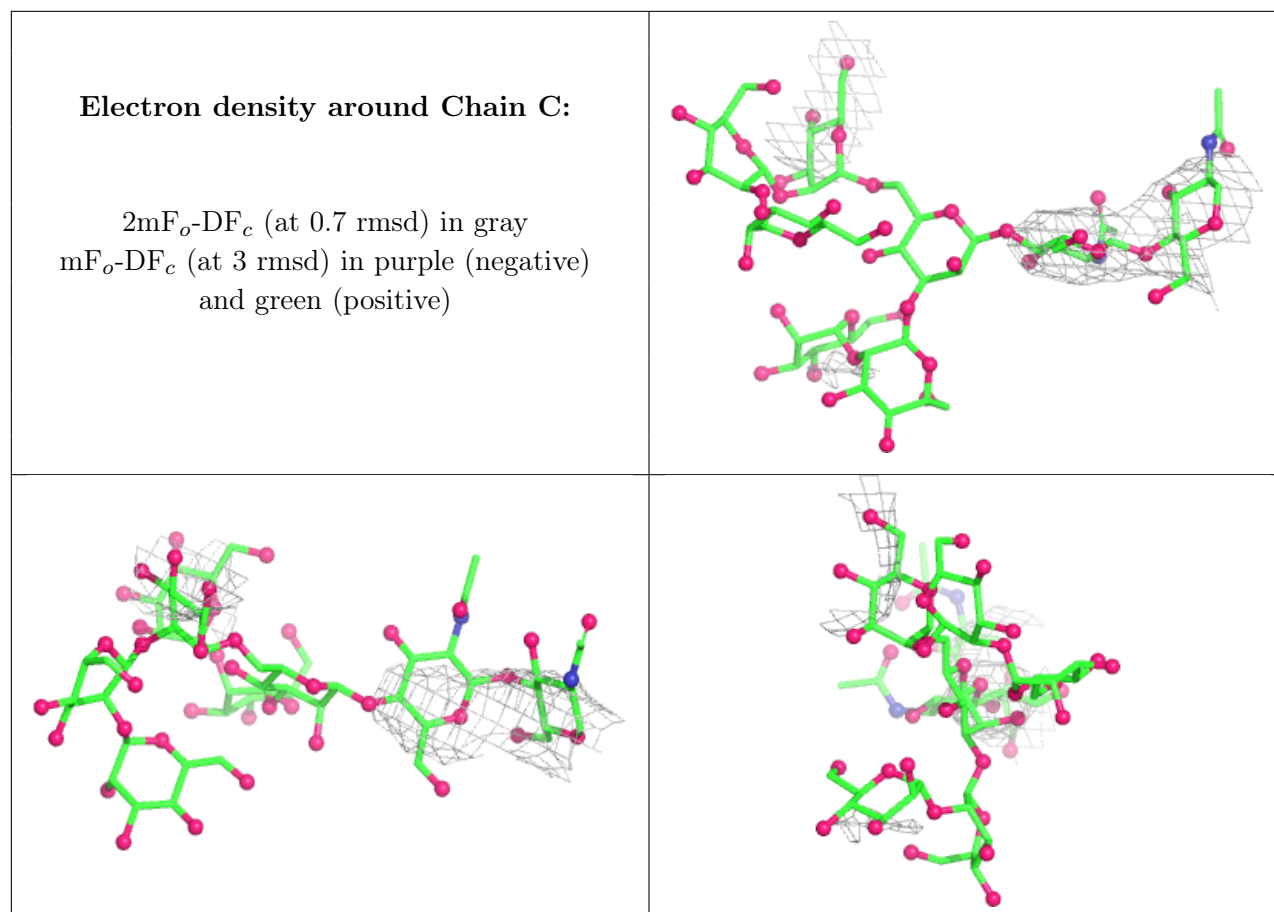
Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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
5	NAG	A	1619	14/15	0.66	0.21	289,290,291,291	0
5	NAG	A	1607	14/15	0.78	0.19	114,191,280,293	0
4	TB	A	1601	1/1	0.93	0.17	213,213,213,213	0
4	TB	A	1602	1/1	0.99	0.05	166,166,166,166	0
4	TB	A	1603	1/1	1.00	0.05	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.