



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:39 PM UTC

PDB ID : 5MZO / pdb_00005mzo
Title : UDP-Glucose Glycoprotein Glucosyltransferase from Chaetomium thermophilum (open conformation)
Authors : Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.
Deposited on : 2017-02-01
Resolution : 3.48 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

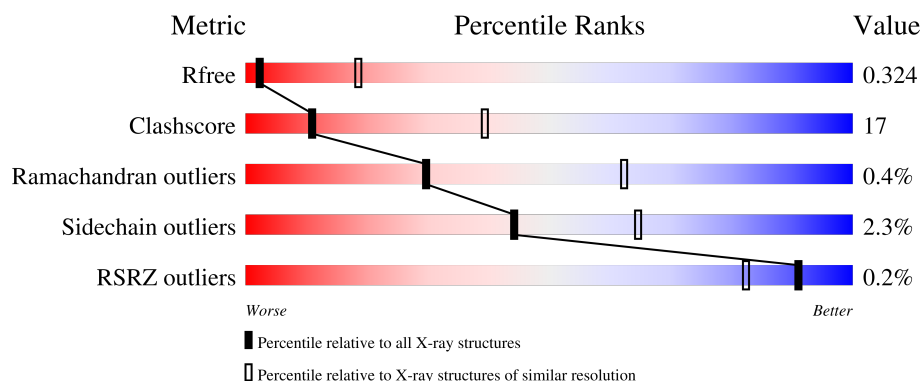
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	 62% 27% 8%
2	B	2	 50% 50%
2	D	2	 100%
2	E	2	 100%
3	C	5	 20% 40% 40%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11227 atoms, of which 12 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	1373	Total	C	N	O	S	0	0	0
			11035	7063	1879	2062	31			

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 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	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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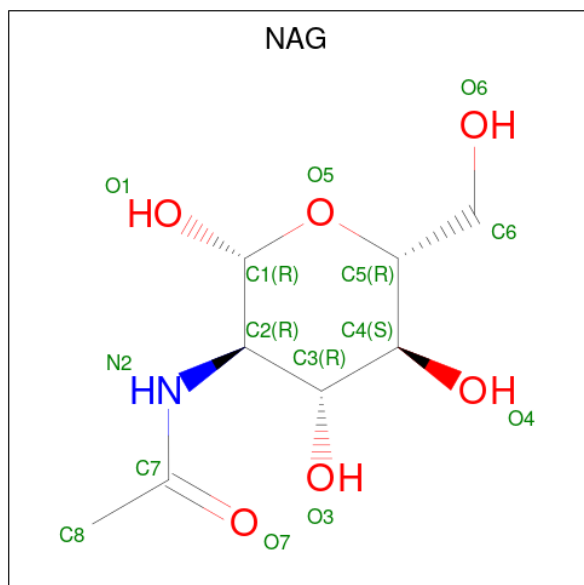
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 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
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

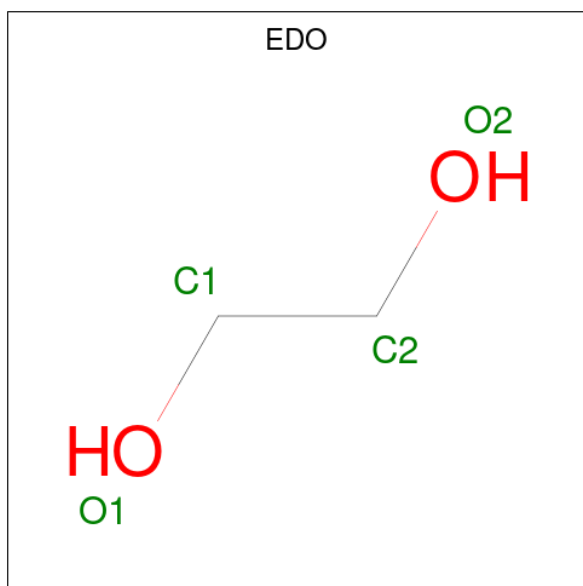


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 10 2 6 2	0	0
6	A	1	Total C H O 10 2 6 2	0	0

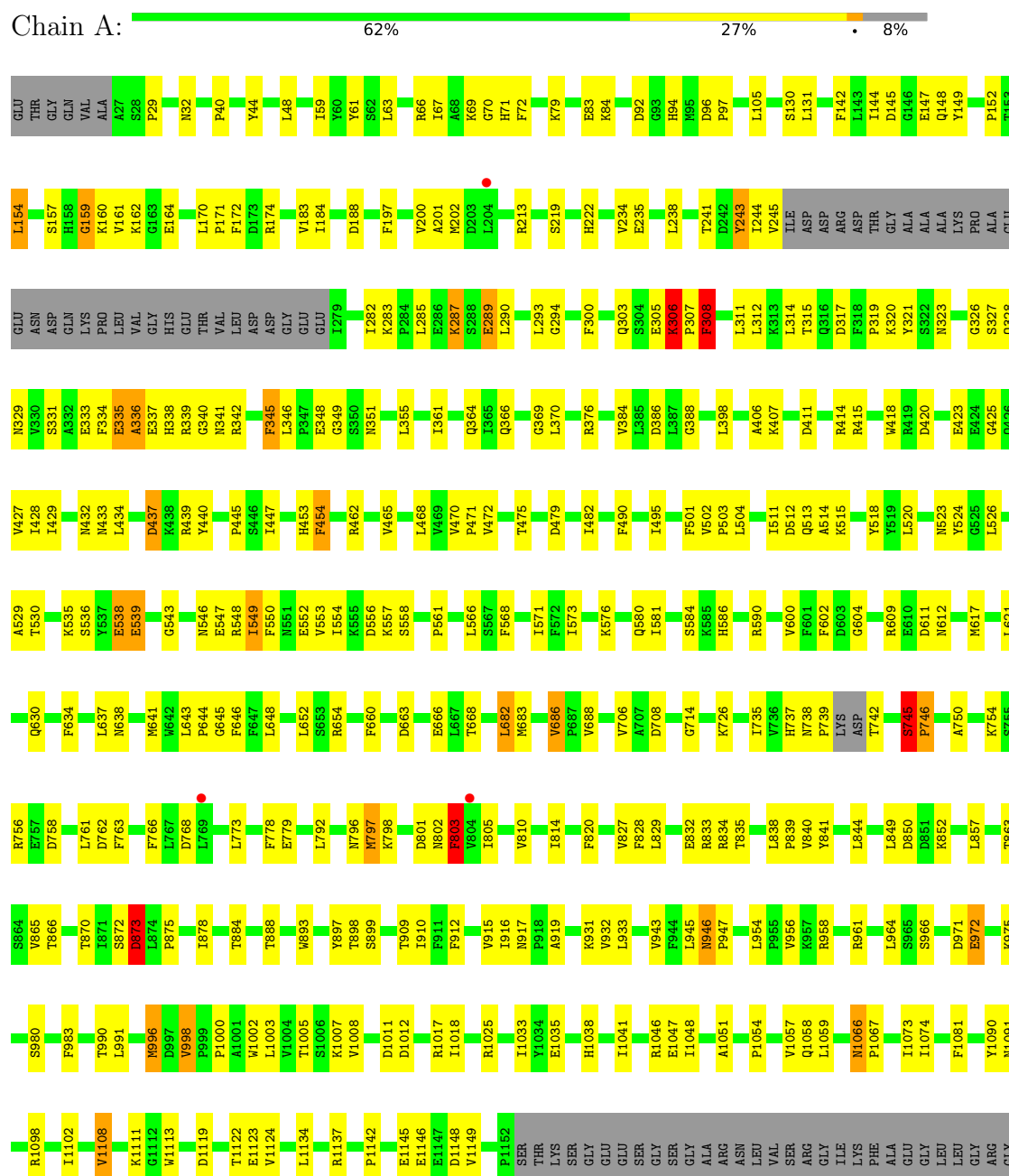
- Molecule 7 is water.

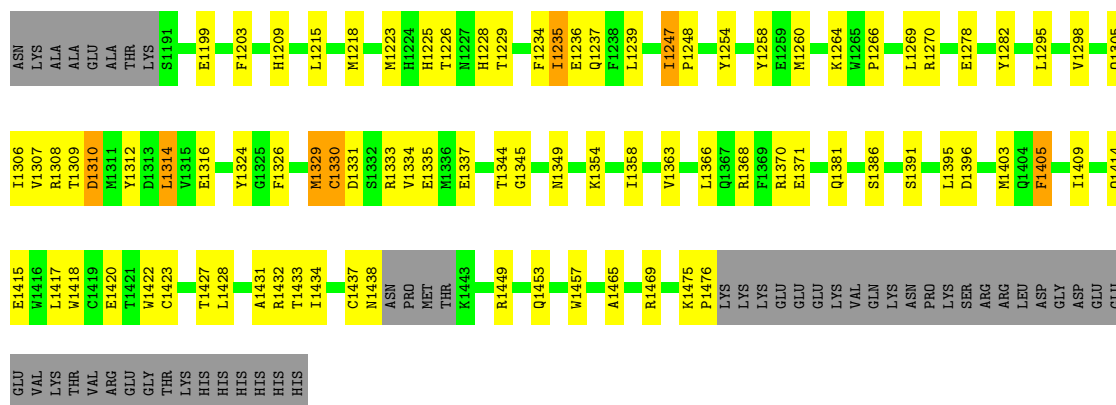
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	12	Total O 12 12	0	0

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

Chain B: 50% 50%



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

Chain D: 100%



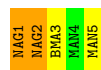
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



- Molecule 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 C: 20% 40% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	163.57Å 163.57Å 248.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	102.00 – 3.48 102.00 – 3.48	Depositor EDS
% Data completeness (in resolution range)	98.0 (102.00-3.48) 99.6 (102.00-3.48)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.49Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.251 , 0.278 0.285 , 0.324	Depositor DCC
R_{free} test set	1602 reflections (6.21%)	wwPDB-VP
Wilson B-factor (Å ²)	129.9	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 127.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11227	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, CA, BMA, NAG, EDO

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	0.75	5/11298 (0.0%)	1.42	80/15321 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1329	MET	SD-CE	-7.63	1.60	1.79
1	A	996	MET	SD-CE	-6.35	1.63	1.79
1	A	549	ILE	CG1-CD1	-6.19	1.27	1.51
1	A	1247	ILE	CG1-CD1	-5.74	1.29	1.51
1	A	1260	MET	SD-CE	-5.40	1.66	1.79

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ALA	N-CA-C	-12.58	96.63	114.12
1	A	411	ASP	N-CA-C	-11.70	99.14	113.41
1	A	334	PHE	N-CA-C	-10.86	98.33	111.69
1	A	796	ASN	CA-CB-CG	10.25	122.85	112.60
1	A	803	PHE	CA-CB-CG	9.49	123.29	113.80
1	A	287	LYS	CA-C-N	9.30	138.44	121.70
1	A	287	LYS	C-N-CA	9.30	138.44	121.70
1	A	340	GLY	N-CA-C	-9.04	101.26	113.37
1	A	308	PHE	CA-CB-CG	8.45	122.25	113.80
1	A	439	ARG	N-CA-C	-8.44	101.95	113.18
1	A	1415	GLU	N-CA-C	-8.24	102.33	112.38
1	A	243	TYR	CA-C-N	8.11	136.57	121.97
1	A	243	TYR	C-N-CA	8.11	136.57	121.97
1	A	159	GLY	N-CA-C	7.98	123.80	110.56
1	A	305	GLU	CA-C-N	7.65	140.47	121.80
1	A	305	GLU	C-N-CA	7.65	140.47	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLY	N-CA-C	-7.50	104.39	115.72
1	A	339	ARG	N-CA-C	-7.10	104.22	113.17
1	A	1235	ILE	CA-C-N	6.95	131.25	120.82
1	A	1235	ILE	C-N-CA	6.95	131.25	120.82
1	A	160	LYS	N-CA-C	-6.71	97.60	108.41
1	A	1041	ILE	N-CA-C	-6.53	97.71	107.37
1	A	556	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	69	LYS	N-CA-C	-6.47	104.31	111.36
1	A	1331	ASP	CA-C-N	6.42	129.21	120.54
1	A	1331	ASP	C-N-CA	6.42	129.21	120.54
1	A	638	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	766	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	1349	ASN	CA-CB-CG	6.27	118.87	112.60
1	A	454	PHE	CA-CB-CG	-6.26	107.54	113.80
1	A	1405	PHE	CA-C-N	6.12	128.76	120.44
1	A	1405	PHE	C-N-CA	6.12	128.76	120.44
1	A	145	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	154	LEU	CA-C-N	6.01	128.58	120.65
1	A	154	LEU	C-N-CA	6.01	128.58	120.65
1	A	300	PHE	CA-C-N	6.00	128.24	120.56
1	A	300	PHE	C-N-CA	6.00	128.24	120.56
1	A	1108	VAL	N-CA-C	-5.88	99.27	107.80
1	A	745	SER	CA-C-O	-5.87	112.11	120.16
1	A	1391	SER	N-CA-C	5.86	117.34	111.07
1	A	538	GLU	CA-C-N	5.80	128.30	120.65
1	A	538	GLU	C-N-CA	5.80	128.30	120.65
1	A	432	ASN	CA-C-N	5.78	130.94	121.58
1	A	432	ASN	C-N-CA	5.78	130.94	121.58
1	A	1310	ASP	N-CA-C	-5.77	99.73	108.67
1	A	646	PHE	N-CA-C	-5.72	105.03	112.23
1	A	909	THR	N-CA-C	-5.70	106.46	113.41
1	A	306	LYS	N-CA-C	-5.67	97.27	109.81
1	A	345	PHE	N-CA-C	5.63	119.66	112.12
1	A	762	ASP	N-CA-C	-5.62	104.65	112.30
1	A	1145	GLU	N-CA-C	-5.59	104.69	112.30
1	A	778	PHE	CA-C-N	5.51	131.35	121.76
1	A	778	PHE	C-N-CA	5.51	131.35	121.76
1	A	1334	VAL	N-CA-C	5.42	116.08	110.82
1	A	241	THR	CA-C-N	5.38	127.75	120.38
1	A	241	THR	C-N-CA	5.38	127.75	120.38
1	A	998	VAL	N-CA-CB	-5.37	103.70	111.21
1	A	946	ASN	CA-CB-CG	5.30	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1335	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	386	ASP	N-CA-C	-5.24	106.66	113.16
1	A	873	ASP	N-CA-C	-5.23	105.26	111.69
1	A	756	ARG	CA-C-N	5.22	127.53	120.38
1	A	756	ARG	C-N-CA	5.22	127.53	120.38
1	A	972	GLU	N-CA-C	-5.21	105.77	111.82
1	A	663	ASP	N-CA-C	-5.20	100.03	108.41
1	A	571	ILE	N-CA-C	5.20	115.45	108.17
1	A	779	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	1434	ILE	N-CA-C	5.15	115.27	107.75
1	A	850	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	514	ALA	N-CA-C	-5.13	105.60	111.14
1	A	326	GLY	CA-C-N	5.12	130.36	122.93
1	A	326	GLY	C-N-CA	5.12	130.36	122.93
1	A	319	PRO	CA-C-N	5.12	128.09	120.31
1	A	319	PRO	C-N-CA	5.12	128.09	120.31
1	A	335	GLU	CA-C-N	5.12	130.26	122.23
1	A	335	GLU	C-N-CA	5.12	130.26	122.23
1	A	1278	GLU	CA-C-N	5.09	127.16	120.60
1	A	1278	GLU	C-N-CA	5.09	127.16	120.60
1	A	888	THR	N-CA-C	-5.08	105.45	113.02
1	A	841	TYR	N-CA-C	5.05	116.47	111.07

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	11035	0	10907	366	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	C	61	0	52	2	0
4	A	14	0	13	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	12	12	0	0
7	A	12	0	0	1	0
All	All	11215	12	11059	368	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 17.

All (368) 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:1329:MET:SD	1:A:1358:ILE:HD11	1.65	1.36
1:A:337:GLU:OE1	1:A:897:TYR:HD2	1.15	1.26
1:A:1225:HIS:ND1	1:A:1308:ARG:HA	1.62	1.13
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	1.79	1.12
1:A:337:GLU:OE1	1:A:897:TYR:CD2	2.03	1.11
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.17	1.08
1:A:67:ILE:HG22	1:A:72:PHE:CD2	1.91	1.06
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.57	1.03
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	1.97	1.00
1:A:554:ILE:HG21	1:A:568:PHE:HE1	1.28	0.99
1:A:149:TYR:CE1	1:A:157:SER:HB2	1.98	0.98
1:A:1329:MET:SD	1:A:1358:ILE:CD1	2.51	0.98
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	1.85	0.94
1:A:524:TYR:HE2	1:A:558:SER:HG	1.05	0.94
1:A:524:TYR:OH	1:A:566:LEU:HD22	1.67	0.94
1:A:72:PHE:CE1	1:A:84:LYS:HG3	2.04	0.93
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.50	0.92
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.35	0.91
1:A:338:HIS:O	1:A:341:ASN:HB2	1.72	0.90
1:A:739:PRO:C	1:A:746:PRO:HD3	1.98	0.88
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.57	0.86
1:A:1058:GLN:HG2	1:A:1073:ILE:HG22	1.57	0.86
1:A:566:LEU:HD13	1:A:568:PHE:CD2	2.10	0.86
1:A:243:TYR:O	1:A:285:LEU:HG	1.76	0.85
1:A:554:ILE:HG21	1:A:568:PHE:CE1	2.12	0.85
1:A:482:ILE:HD12	1:A:609:ARG:HH22	1.42	0.85
1:A:328:GLN:H	1:A:329:ASN:HA	1.44	0.82
1:A:72:PHE:HE1	1:A:84:LYS:HG3	1.44	0.81
1:A:234:VAL:HG22	1:A:996:MET:HE2	1.62	0.81
1:A:67:ILE:CG2	1:A:72:PHE:HD2	1.91	0.81
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:PRO:HG3	1:A:566:LEU:HD23	1.62	0.80
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	1.64	0.79
1:A:346:LEU:HD12	1:A:893:TRP:HH2	1.48	0.79
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.65	0.79
1:A:1324:TYR:CD1	1:A:1326:PHE:CE1	2.70	0.79
1:A:686:VAL:O	1:A:754:LYS:HE2	1.82	0.78
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.13	0.78
1:A:1422:TRP:CZ3	1:A:1437:CYS:SG	2.78	0.77
1:A:1295:LEU:HD21	1:A:1298:VAL:HG23	1.67	0.76
1:A:433:ASN:O	1:A:437:ASP:HB2	1.85	0.76
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.21	0.76
1:A:311:LEU:O	1:A:315:THR:HG22	1.87	0.75
1:A:342:ARG:HD3	1:A:348:GLU:HB3	1.69	0.75
1:A:244:ILE:HA	1:A:285:LEU:HB3	1.67	0.75
1:A:475:THR:HA	1:A:543:GLY:HA3	1.69	0.75
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.47	0.74
1:A:797:MET:HB3	1:A:803:PHE:CZ	2.23	0.74
1:A:445:PRO:HG3	1:A:462:ARG:NH2	2.03	0.73
1:A:566:LEU:HD13	1:A:568:PHE:CE2	2.23	0.73
1:A:243:TYR:HD1	1:A:285:LEU:HD23	1.51	0.73
1:A:482:ILE:HD12	1:A:609:ARG:NH2	2.03	0.73
1:A:834:ARG:O	1:A:839:PRO:HD3	1.89	0.73
1:A:282:ILE:HG13	1:A:990:THR:HG22	1.70	0.73
1:A:346:LEU:HD12	1:A:893:TRP:CH2	2.23	0.73
1:A:144:ILE:HG12	1:A:183:VAL:HG12	1.71	0.72
1:A:546:ASN:HB3	1:A:549:ILE:CG2	2.17	0.72
1:A:67:ILE:CG2	1:A:72:PHE:CD2	2.68	0.72
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.71	0.72
1:A:245:VAL:HB	1:A:287:LYS:HB2	1.72	0.72
1:A:1098:ARG:HH21	1:A:1102:ILE:HD11	1.55	0.72
1:A:1324:TYR:CE1	1:A:1326:PHE:HE1	2.09	0.71
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.72	0.71
1:A:142:PHE:HE1	1:A:197:PHE:HD2	1.38	0.71
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.72	0.71
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.73	0.71
1:A:244:ILE:HD11	1:A:954:LEU:HD13	1.73	0.70
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.21	0.70
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.73	0.70
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.72	0.70
1:A:682:LEU:HD12	1:A:683:MET:HE2	1.72	0.70
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TYR:HE1	1:A:157:SER:HB2	1.53	0.69
1:A:130:SER:O	1:A:161:VAL:HG13	1.93	0.69
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.23	0.69
1:A:346:LEU:CD1	1:A:893:TRP:HH2	2.05	0.69
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.73	0.69
1:A:829:LEU:O	1:A:833:ARG:HB2	1.93	0.69
3:C:2:NAG:H62	3:C:3:BMA:H2	1.75	0.69
1:A:1366:LEU:O	1:A:1370:ARG:HG3	1.92	0.69
1:A:283:LYS:HZ2	1:A:285:LEU:HD21	1.58	0.68
1:A:188:ASP:OD1	1:A:219:SER:HB3	1.93	0.68
1:A:376:ARG:HH12	1:A:873:ASP:HB3	1.58	0.68
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.75	0.68
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.74	0.68
1:A:1247:ILE:HG13	1:A:1248:PRO:HD3	1.75	0.68
1:A:66:ARG:O	1:A:71:HIS:HB3	1.93	0.68
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.60	0.67
1:A:445:PRO:HG3	1:A:462:ARG:HH21	1.60	0.67
1:A:546:ASN:CB	1:A:549:ILE:HG22	2.22	0.67
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.77	0.66
1:A:523:ASN:OD1	1:A:566:LEU:HA	1.96	0.66
1:A:1428:LEU:HD12	1:A:1431:ALA:HB3	1.75	0.66
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.77	0.66
1:A:1324:TYR:CE1	1:A:1326:PHE:CE1	2.84	0.66
1:A:238:LEU:HD13	1:A:283:LYS:HE2	1.77	0.65
1:A:524:TYR:HE2	1:A:558:SER:OG	1.75	0.65
1:A:512:ASP:HA	1:A:515:LYS:HE3	1.78	0.65
1:A:142:PHE:CE1	1:A:197:PHE:HD2	2.14	0.65
1:A:872:SER:HB2	1:A:884:THR:OG1	1.96	0.65
1:A:335:GLU:HA	1:A:337:GLU:HG2	1.79	0.65
1:A:682:LEU:CD1	1:A:683:MET:HE2	2.27	0.65
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.23	0.64
1:A:1422:TRP:HZ3	1:A:1437:CYS:SG	2.19	0.64
1:A:243:TYR:CD1	1:A:285:LEU:HD23	2.32	0.64
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.29	0.63
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.28	0.63
1:A:244:ILE:HG12	1:A:285:LEU:HD12	1.81	0.63
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.29	0.62
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.34	0.62
1:A:706:VAL:HG11	1:A:803:PHE:CE1	2.34	0.62
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.34	0.62
1:A:1333:ARG:HH21	1:A:1420:GLU:HG2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.81	0.62
1:A:554:ILE:HG23	1:A:558:SER:CB	2.30	0.62
1:A:535:LYS:HE2	1:A:552:GLU:OE1	2.01	0.61
1:A:1438:ASN:HA	1:A:1449:ARG:HH22	1.66	0.61
1:A:524:TYR:HE2	1:A:558:SER:CB	2.14	0.61
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.30	0.61
1:A:1003:LEU:HD21	1:A:1264:LYS:HB2	1.83	0.60
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.84	0.60
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.64	0.60
1:A:289:GLU:HA	1:A:289:GLU:OE1	2.01	0.60
1:A:306:LYS:HG2	1:A:308:PHE:HE1	1.66	0.60
1:A:294:GLY:HA3	1:A:947:PRO:HB3	1.84	0.59
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.02	0.59
1:A:630:GLN:O	1:A:634:PHE:HD1	1.86	0.59
1:A:1295:LEU:HD21	1:A:1298:VAL:HG21	1.78	0.59
1:A:234:VAL:HG22	1:A:996:MET:CE	2.30	0.59
1:A:1324:TYR:HD1	1:A:1326:PHE:CE1	2.21	0.59
1:A:899:SER:HA	1:A:943:VAL:O	2.02	0.59
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.51	0.58
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.32	0.58
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.84	0.58
1:A:328:GLN:HB3	1:A:331:SER:H	1.68	0.58
1:A:590:ARG:HA	1:A:654:ARG:HH21	1.69	0.58
1:A:61:TYR:HB3	1:A:202:MET:HE1	1.86	0.58
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.03	0.58
1:A:142:PHE:HE2	1:A:201:ALA:HB2	1.67	0.58
1:A:553:VAL:O	1:A:557:LYS:HB2	2.04	0.58
1:A:561:PRO:CG	1:A:566:LEU:HD23	2.31	0.58
1:A:566:LEU:O	1:A:566:LEU:HD12	2.02	0.58
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.68	0.58
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.11	0.58
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.04	0.57
1:A:418:TRP:H	1:A:418:TRP:CD1	2.21	0.57
1:A:328:GLN:H	1:A:329:ASN:CA	2.15	0.57
1:A:472:VAL:O	1:A:503:PRO:HA	2.05	0.57
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.85	0.56
1:A:554:ILE:O	1:A:558:SER:CB	2.53	0.56
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.86	0.56
1:A:174:ARG:O	1:A:213:ARG:HB3	2.05	0.56
1:A:130:SER:HB3	1:A:162:LYS:O	2.06	0.56
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:CD1	1:A:609:ARG:NH2	2.69	0.56
1:A:147:GLU:HA	1:A:159:GLY:O	2.06	0.56
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.41	0.56
1:A:465:VAL:HG22	1:A:643:LEU:CD1	2.36	0.55
1:A:805:ILE:HG12	1:A:810:VAL:HG22	1.88	0.55
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.88	0.55
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.88	0.55
1:A:1295:LEU:CD2	1:A:1298:VAL:CG2	2.70	0.55
1:A:420:ASP:OD1	1:A:427:VAL:HG12	2.05	0.55
1:A:745:SER:HB2	1:A:746:PRO:HA	1.89	0.55
1:A:1054:PRO:HB2	1:A:1057:VAL:HG21	1.87	0.54
1:A:535:LYS:C	1:A:549:ILE:HD11	2.32	0.54
1:A:652:LEU:HD13	1:A:660:PHE:CZ	2.43	0.54
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.43	0.54
1:A:1058:GLN:CG	1:A:1073:ILE:HG22	2.34	0.54
1:A:1422:TRP:CE3	1:A:1437:CYS:SG	3.01	0.54
1:A:915:VAL:HG12	1:A:946:ASN:ND2	2.23	0.54
1:A:235:GLU:HB2	1:A:958:ARG:HD2	1.90	0.54
1:A:546:ASN:O	1:A:549:ILE:HG22	2.07	0.53
1:A:282:ILE:HG13	1:A:990:THR:CG2	2.38	0.53
1:A:290:LEU:HA	1:A:293:LEU:HD13	1.89	0.53
1:A:524:TYR:CD2	1:A:558:SER:HA	2.42	0.53
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.38	0.53
1:A:554:ILE:HD13	1:A:568:PHE:CE1	2.44	0.53
1:A:524:TYR:CE1	1:A:566:LEU:HB3	2.44	0.52
1:A:932:VAL:HG11	1:A:964:LEU:HG	1.91	0.52
1:A:1005:THR:HG21	1:A:1236:GLU:HG2	1.90	0.52
1:A:708:ASP:OD1	1:A:739:PRO:HD2	2.09	0.52
1:A:1223:MET:HG3	1:A:1254:TYR:HB3	1.91	0.52
1:A:428:ILE:HA	1:A:502:VAL:HG12	1.91	0.52
1:A:682:LEU:C	1:A:682:LEU:HD13	2.34	0.52
1:A:536:SER:HA	1:A:549:ILE:HD13	1.90	0.52
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.88	0.52
1:A:602:PHE:HZ	1:A:621:LEU:HD13	1.75	0.52
1:A:763:PHE:HD1	1:A:768:ASP:HB3	1.75	0.52
1:A:376:ARG:NH1	1:A:873:ASP:HB3	2.24	0.52
1:A:1058:GLN:HG2	1:A:1073:ILE:CG2	2.34	0.52
1:A:1048:ILE:HD11	1:A:1137:ARG:CD	2.35	0.52
1:A:434:LEU:HD23	1:A:440:TYR:CE2	2.45	0.52
1:A:554:ILE:O	1:A:558:SER:HB3	2.10	0.51
1:A:1247:ILE:HD12	1:A:1258:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.46	0.51
1:A:515:LYS:HG2	1:A:581:ILE:HD11	1.91	0.51
1:A:1225:HIS:HE1	1:A:1308:ARG:HG2	1.75	0.51
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.93	0.51
1:A:142:PHE:HE1	1:A:197:PHE:CD2	2.24	0.51
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.41	0.51
1:A:835:THR:O	1:A:839:PRO:HD2	2.11	0.51
1:A:414:ARG:HE	1:A:652:LEU:HD11	1.76	0.51
1:A:524:TYR:CE2	1:A:558:SER:HA	2.45	0.51
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.92	0.50
1:A:645:GLY:HA2	1:A:648:LEU:HB2	1.94	0.50
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	1.93	0.50
1:A:548:ARG:O	1:A:552:GLU:HG3	2.11	0.50
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.11	0.50
1:A:427:VAL:CG2	1:A:584:SER:HA	2.41	0.50
1:A:328:GLN:N	1:A:329:ASN:HA	2.21	0.49
1:A:1199:GLU:HG3	1:A:1229:THR:H	1.78	0.49
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.41	0.49
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.94	0.49
1:A:1247:ILE:HD12	1:A:1258:TYR:CE2	2.47	0.49
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.12	0.49
1:A:1008:VAL:HB	1:A:1033:ILE:HB	1.95	0.49
1:A:1368:ARG:O	1:A:1368:ARG:HD3	2.13	0.49
1:A:1465:ALA:HB1	1:A:1469:ARG:HH21	1.78	0.49
1:A:652:LEU:HD22	1:A:827:VAL:HG13	1.93	0.49
1:A:1215:LEU:HD12	1:A:1218:MET:HE3	1.95	0.49
1:A:415:ARG:HA	1:A:604:GLY:O	2.13	0.49
1:A:1381:GLN:HG3	1:A:1403:MET:SD	2.53	0.48
1:A:144:ILE:HB	1:A:149:TYR:HE2	1.78	0.48
1:A:919:ALA:O	1:A:956:VAL:HG23	2.13	0.48
1:A:745:SER:CB	1:A:746:PRO:HA	2.43	0.48
1:A:1199:GLU:CG	1:A:1229:THR:OG1	2.61	0.48
1:A:1247:ILE:CG1	1:A:1248:PRO:HD3	2.42	0.48
1:A:726:LYS:HE3	1:A:761:LEU:HB2	1.95	0.48
1:A:644:PRO:O	1:A:648:LEU:HD13	2.12	0.48
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.13	0.48
1:A:535:LYS:O	1:A:539:GLU:HB2	2.14	0.48
1:A:312:LEU:HD22	1:A:931:LYS:HD3	1.96	0.48
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.76	0.47
1:A:311:LEU:O	1:A:315:THR:CG2	2.60	0.47
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:VAL:HG22	1:A:735:ILE:O	2.14	0.47
1:A:333:GLU:HG2	1:A:336:ALA:HB2	1.96	0.47
1:A:453:HIS:C	1:A:454:PHE:CD2	2.92	0.47
1:A:366:GLN:OE1	1:A:1000:PRO:HD2	2.13	0.47
1:A:1102:ILE:HD13	1:A:1146:GLU:HB2	1.96	0.47
1:A:142:PHE:HZ	1:A:197:PHE:O	1.96	0.47
1:A:566:LEU:HD12	1:A:566:LEU:C	2.39	0.47
1:A:802:ASN:HB2	1:A:814:ILE:HB	1.97	0.47
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.29	0.47
1:A:174:ARG:O	1:A:213:ARG:CB	2.63	0.47
1:A:573:ILE:HB	1:A:576:LYS:CB	2.45	0.47
1:A:366:GLN:HG2	1:A:369:GLY:H	1.80	0.46
1:A:991:LEU:HD23	1:A:1017:ARG:HG3	1.97	0.46
1:A:600:VAL:HG23	1:A:609:ARG:HG3	1.96	0.46
1:A:59:ILE:O	1:A:63:LEU:HG	2.15	0.46
1:A:414:ARG:HE	1:A:652:LEU:CD1	2.28	0.46
1:A:471:PRO:HA	1:A:502:VAL:O	2.16	0.46
1:A:1005:THR:HG22	1:A:1237:GLN:HA	1.97	0.46
1:A:423:GLU:CD	1:A:590:ARG:HH11	2.24	0.46
1:A:686:VAL:O	1:A:688:VAL:HG23	2.15	0.46
3:C:1:NAG:H61	3:C:2:NAG:C7	2.46	0.46
1:A:414:ARG:NE	1:A:652:LEU:HD11	2.30	0.46
1:A:518:TYR:HB3	1:A:580:GLN:OE1	2.16	0.46
1:A:283:LYS:NZ	1:A:285:LEU:HD21	2.26	0.46
1:A:554:ILE:HD13	1:A:568:PHE:HE1	1.81	0.46
1:A:991:LEU:HG	1:A:1017:ARG:HD2	1.96	0.46
1:A:79:LYS:O	1:A:83:GLU:HG2	2.16	0.46
1:A:586:HIS:O	1:A:590:ARG:HB2	2.16	0.46
1:A:1306:ILE:HD11	1:A:1457:TRP:CD1	2.49	0.46
1:A:916:ILE:O	1:A:945:LEU:HA	2.16	0.45
1:A:1003:LEU:HD12	1:A:1038:HIS:HB2	1.98	0.45
1:A:306:LYS:N	1:A:307:PRO:HD3	2.31	0.45
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.30	0.45
1:A:566:LEU:CD1	1:A:568:PHE:CE2	2.97	0.45
1:A:708:ASP:O	1:A:714:GLY:HA3	2.16	0.45
1:A:511:ILE:HG22	1:A:515:LYS:HE2	1.96	0.45
1:A:590:ARG:HG2	1:A:654:ARG:HG3	1.99	0.45
1:A:40:PRO:HG2	7:A:1707:HOH:O	2.17	0.45
1:A:170:LEU:HB2	1:A:171:PRO:HD2	1.99	0.45
1:A:303:GLN:HE22	1:A:328:GLN:HE21	1.64	0.45
1:A:407:LYS:HD2	1:A:870:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ILE:HG13	1:A:364:GLN:HG3	1.98	0.45
1:A:406:ALA:CB	1:A:839:PRO:HG2	2.47	0.45
1:A:445:PRO:CG	1:A:462:ARG:HH21	2.29	0.45
1:A:1309:THR:OG1	1:A:1432:ARG:HB3	2.17	0.44
1:A:1066:ASN:HA	1:A:1067:PRO:HD3	1.76	0.44
1:A:142:PHE:CE2	1:A:201:ALA:HB2	2.51	0.44
1:A:915:VAL:HG12	1:A:946:ASN:HD22	1.80	0.44
1:A:1090:TYR:HB2	1:A:1124:VAL:HG23	2.00	0.44
1:A:1047:GLU:O	1:A:1051:ALA:HA	2.18	0.44
1:A:471:PRO:HB2	1:A:504:LEU:HD21	2.00	0.44
1:A:737:HIS:CE1	1:A:750:ALA:HA	2.53	0.44
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.32	0.44
1:A:351:ASN:HA	1:A:915:VAL:O	2.17	0.44
1:A:971:ASP:HB2	1:A:975:LYS:O	2.18	0.44
1:A:66:ARG:O	1:A:71:HIS:CB	2.63	0.44
1:A:465:VAL:HG22	1:A:643:LEU:HD12	1.99	0.44
1:A:641:MET:HE3	4:A:1601:NAG:H2	2.00	0.44
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.51	0.44
1:A:1330:CYS:HA	1:A:1414:GLN:OE1	2.18	0.44
1:A:682:LEU:CD1	1:A:682:LEU:C	2.91	0.43
1:A:338:HIS:HD2	1:A:898:THR:CG2	2.19	0.43
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.17	0.43
1:A:317:ASP:O	1:A:320:LYS:HB3	2.19	0.43
1:A:445:PRO:HD3	1:A:462:ARG:HH21	1.83	0.43
1:A:366:GLN:HE21	1:A:369:GLY:HA3	1.84	0.43
1:A:546:ASN:O	1:A:549:ILE:CG2	2.66	0.43
1:A:566:LEU:CD1	1:A:568:PHE:CD2	2.94	0.43
1:A:44:TYR:CE2	1:A:48:LEU:HD11	2.53	0.43
1:A:1098:ARG:HG3	1:A:1148:ASP:OD1	2.18	0.43
1:A:1012:ASP:HB2	1:A:1209:HIS:ND1	2.34	0.43
1:A:366:GLN:CG	1:A:369:GLY:H	2.31	0.43
1:A:1449:ARG:HB3	1:A:1453:GLN:OE1	2.19	0.43
1:A:32:ASN:OD1	1:A:980:SER:HB3	2.19	0.43
1:A:468:LEU:HD22	1:A:617:MET:SD	2.59	0.43
1:A:763:PHE:HD1	1:A:768:ASP:CB	2.32	0.43
1:A:1225:HIS:ND1	1:A:1308:ARG:C	2.77	0.43
1:A:429:ILE:HD11	1:A:501:PHE:CZ	2.54	0.43
1:A:314:LEU:HD12	1:A:321:TYR:HD2	1.84	0.42
1:A:355:LEU:HD13	1:A:912:PHE:CZ	2.54	0.42
1:A:737:HIS:CD2	1:A:737:HIS:N	2.87	0.42
1:A:840:VAL:HG21	1:A:863:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:ILE:HG13	1:A:1248:PRO:CD	2.47	0.42
1:A:536:SER:HA	1:A:549:ILE:CD1	2.49	0.42
1:A:1074:ILE:HD13	1:A:1081:PHE:HB3	2.01	0.42
1:A:1305:GLN:HE22	1:A:1417:LEU:HD11	1.83	0.42
1:A:154:LEU:HG	1:A:154:LEU:O	2.20	0.42
1:A:1235:ILE:HD13	1:A:1282:TYR:HB3	2.00	0.42
1:A:511:ILE:HG22	1:A:515:LYS:CE	2.49	0.42
1:A:1344:THR:HG22	1:A:1345:GLY:H	1.83	0.42
1:A:998:VAL:CG2	1:A:1002:TRP:HE3	2.33	0.42
1:A:243:TYR:CD1	1:A:285:LEU:CD2	3.03	0.42
1:A:384:VAL:HG22	1:A:865:VAL:HG11	1.99	0.42
1:A:576:LYS:O	1:A:580:GLN:HB2	2.19	0.42
1:A:1475:LYS:HA	1:A:1476:PRO:HD3	1.95	0.42
1:A:1111:LYS:HG3	1:A:1119:ASP:CB	2.50	0.42
1:A:349:GLY:HA2	1:A:917:ASN:HB2	2.01	0.42
1:A:1354:LYS:HD2	1:A:1405:PHE:CE1	2.55	0.42
1:A:524:TYR:OH	1:A:566:LEU:CD2	2.55	0.42
1:A:526:LEU:O	1:A:530:THR:HG23	2.20	0.41
1:A:828:PHE:O	1:A:832:GLU:HB2	2.20	0.41
1:A:798:LYS:HG2	1:A:801:ASP:OD2	2.20	0.41
1:A:468:LEU:HD11	1:A:600:VAL:HG12	2.03	0.41
1:A:1266:PRO:HD2	1:A:1269:LEU:HD23	2.02	0.41
1:A:142:PHE:HA	1:A:184:ILE:O	2.21	0.41
1:A:490:PHE:HA	1:A:495:ILE:HD12	2.02	0.41
1:A:520:LEU:CD2	1:A:529:ALA:HA	2.51	0.41
1:A:654:ARG:HB2	1:A:827:VAL:HG21	2.03	0.41
1:A:1330:CYS:HB3	1:A:1422:TRP:O	2.21	0.41
1:A:1226:THR:OG1	1:A:1228:HIS:HB2	2.21	0.41
1:A:835:THR:O	1:A:839:PRO:CD	2.69	0.41
1:A:1111:LYS:HG3	1:A:1119:ASP:HB3	2.01	0.41
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	2.03	0.41
1:A:668:THR:HG23	1:A:810:VAL:HB	2.02	0.41
1:A:1098:ARG:HG2	1:A:1148:ASP:HA	2.02	0.41
1:A:1312:TYR:CE1	1:A:1316:GLU:HG3	2.55	0.41
1:A:105:LEU:HD13	1:A:966:SER:HA	2.02	0.41
1:A:549:ILE:HD13	1:A:549:ILE:HG21	1.87	0.41
1:A:998:VAL:CG2	1:A:1002:TRP:CE3	3.04	0.41
1:A:998:VAL:HG23	1:A:1002:TRP:CE3	2.56	0.41
1:A:738:ASN:HD22	1:A:792:LEU:CD1	2.32	0.40
1:A:472:VAL:HG13	1:A:479:ASP:HB3	2.03	0.40
1:A:875:PRO:HB2	1:A:878:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:ARG:NH2	1:A:1420:GLU:HG2	2.32	0.40
1:A:1295:LEU:CD2	1:A:1298:VAL:HG23	2.42	0.40
1:A:303:GLN:NE2	1:A:328:GLN:HE21	2.20	0.40
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.50	0.40
1:A:388:GLY:O	1:A:852:LYS:HE2	2.22	0.40
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.54	0.40
1:A:244:ILE:CG1	1:A:285:LEU:HD12	2.49	0.40
1:A:285:LEU:HD13	1:A:285:LEU:HA	1.77	0.40
1:A:427:VAL:HG23	1:A:584:SER:HA	2.02	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	1363/1494 (91%)	1293 (95%)	64 (5%)	6 (0%)	30 62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	LYS
1	A	745	SER
1	A	666	GLU
1	A	746	PRO
1	A	1142	PRO
1	A	1337	GLU

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	1199/1297 (92%)	1171 (98%)	28 (2%)	44 64

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	GLU
1	A	222	HIS
1	A	289	GLU
1	A	308	PHE
1	A	323	ASN
1	A	327	SER
1	A	437	ASP
1	A	513	GLN
1	A	538	GLU
1	A	539	GLU
1	A	611	ASP
1	A	612	ASN
1	A	682	LEU
1	A	686	VAL
1	A	742	THR
1	A	758	ASP
1	A	773	LEU
1	A	797	MET
1	A	803	PHE
1	A	820	PHE
1	A	857	LEU
1	A	873	ASP
1	A	972	GLU
1	A	1066	ASN
1	A	1123	GLU
1	A	1203	PHE
1	A	1314	LEU
1	A	1330	CYS

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

Mol	Chain	Res	Type
1	A	328	GLN

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Mol	Chain	Res	Type
1	A	364	GLN
1	A	513	GLN
1	A	540	GLN
1	A	618	ASN
1	A	1015	ASN
1	A	1068	HIS
1	A	1130	GLN
1	A	1453	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 ⓘ

11 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	2,1	14,14,15	0.30	0	17,19,21	0.65	0
2	NAG	B	2	2	14,14,15	0.41	0	17,19,21	1.08	2 (11%)
3	NAG	C	1	1,3	14,14,15	0.35	0	17,19,21	1.37	1 (5%)
3	NAG	C	2	3	14,14,15	0.40	0	17,19,21	1.40	4 (23%)
3	BMA	C	3	3	11,11,12	0.35	0	15,15,17	0.57	0
3	MAN	C	4	3	11,11,12	0.45	0	15,15,17	0.84	0
3	MAN	C	5	3	11,11,12	0.44	0	15,15,17	1.10	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.39	0	17,19,21	1.98	2 (11%)
2	NAG	D	2	2	14,14,15	0.41	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	0.50	0	17,19,21	1.93	4 (23%)
2	NAG	E	2	2	14,14,15	0.36	0	17,19,21	0.87	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	1/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	6.62	121.05	112.19
2	D	1	NAG	C1-O5-C5	6.59	121.01	112.19
3	C	1	NAG	O5-C1-C2	-4.31	104.63	111.29
3	C	5	MAN	C1-O5-C5	3.96	117.49	112.19
2	D	1	NAG	O5-C1-C2	3.57	116.82	111.29
2	B	2	NAG	O5-C1-C2	2.96	115.87	111.29
3	C	2	NAG	C1-C2-N2	2.80	114.85	110.43
3	C	2	NAG	C1-O5-C5	2.78	115.92	112.19
3	C	2	NAG	C2-N2-C7	2.72	126.55	122.90
2	E	1	NAG	C1-C2-N2	2.70	114.69	110.43
2	D	2	NAG	C1-O5-C5	2.70	115.80	112.19
3	C	2	NAG	O5-C1-C2	-2.49	107.44	111.29
2	B	2	NAG	C1-O5-C5	2.46	115.48	112.19
2	E	2	NAG	C1-O5-C5	2.45	115.46	112.19
2	E	1	NAG	C2-N2-C7	2.41	126.13	122.90
2	E	1	NAG	O5-C1-C2	2.02	114.42	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	MAN	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C1-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7
2	D	1	NAG	C4-C5-C6-O6

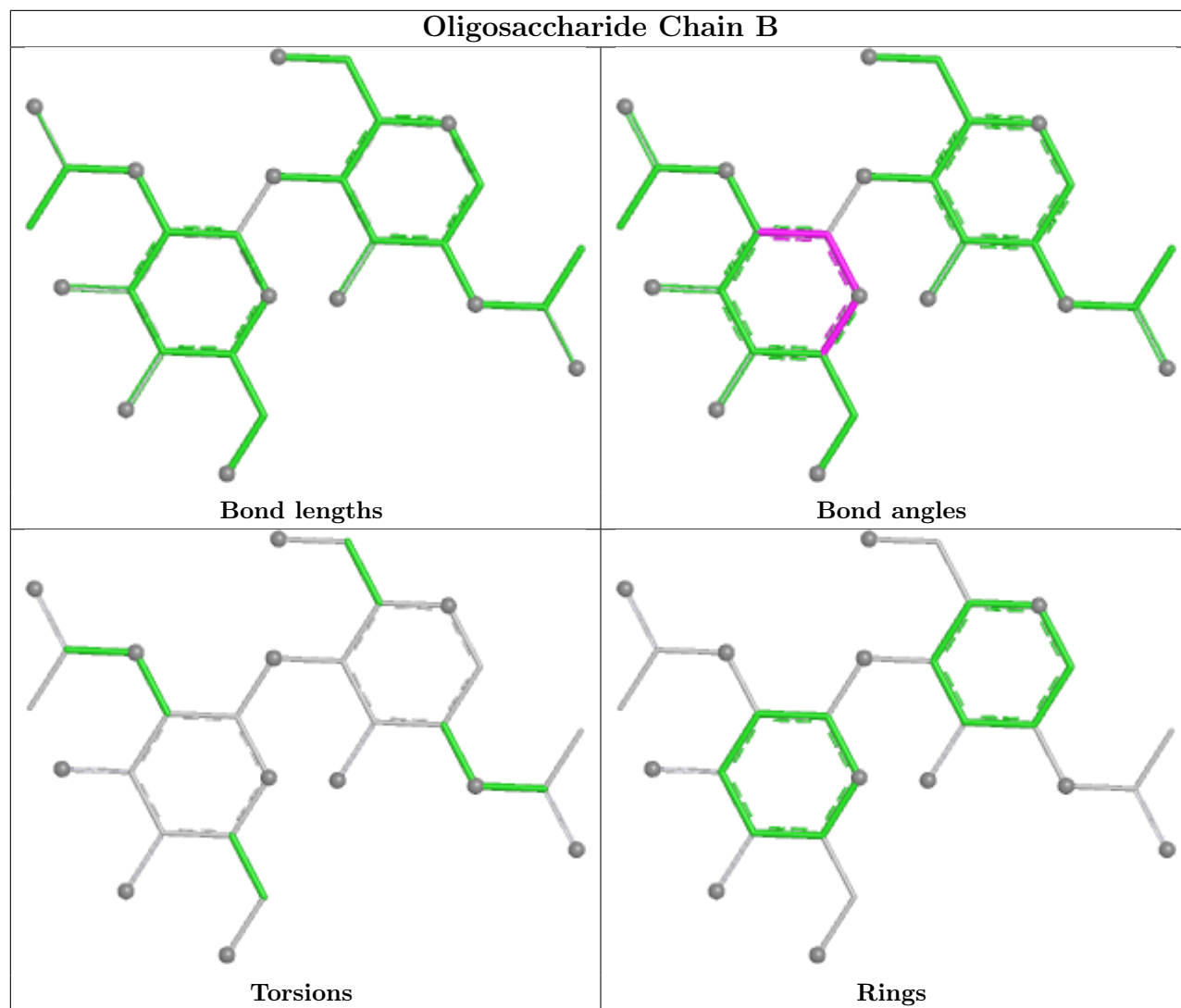
All (1) ring outliers are listed below:

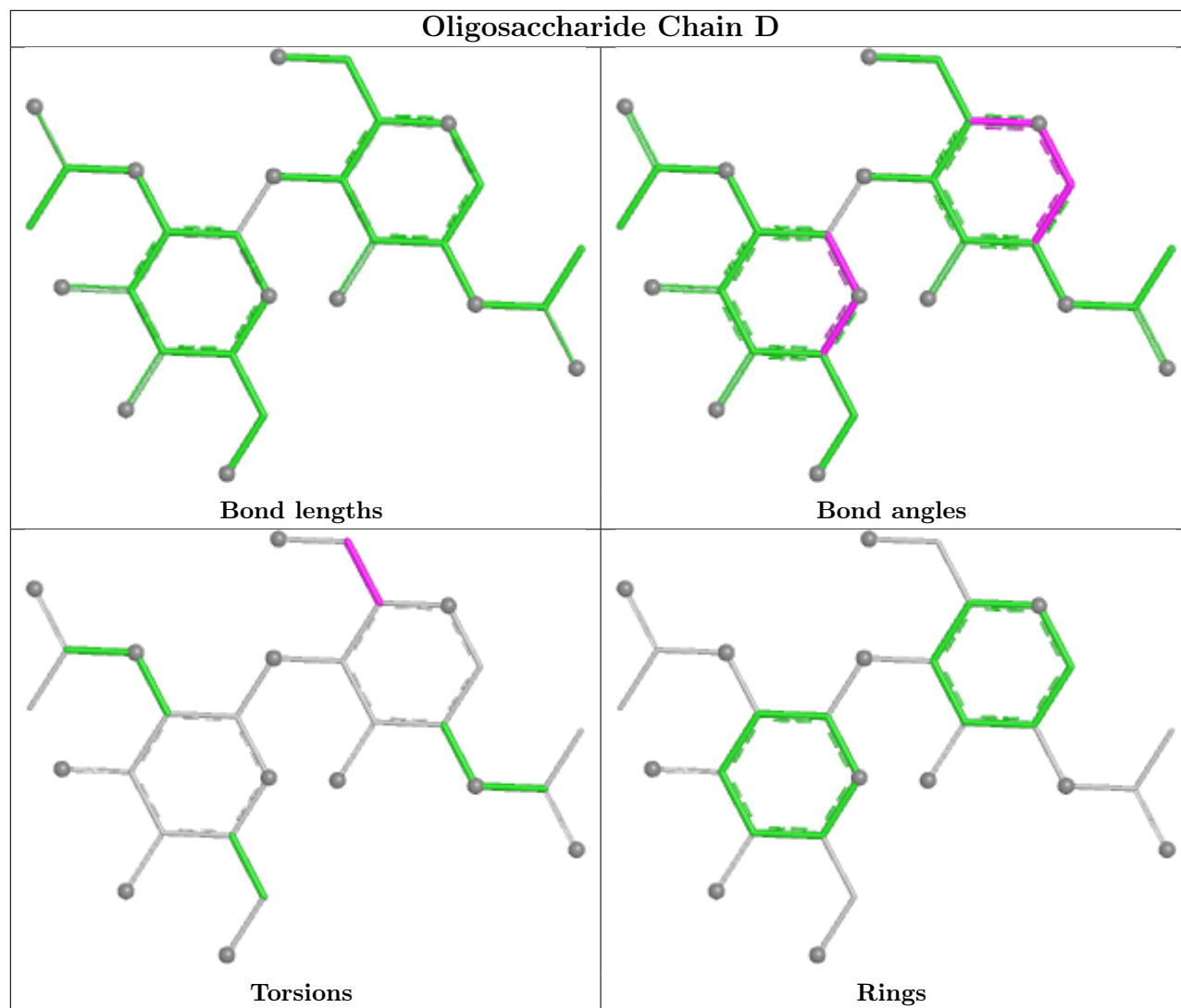
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	C1-C2-C3-C4-C5-O5

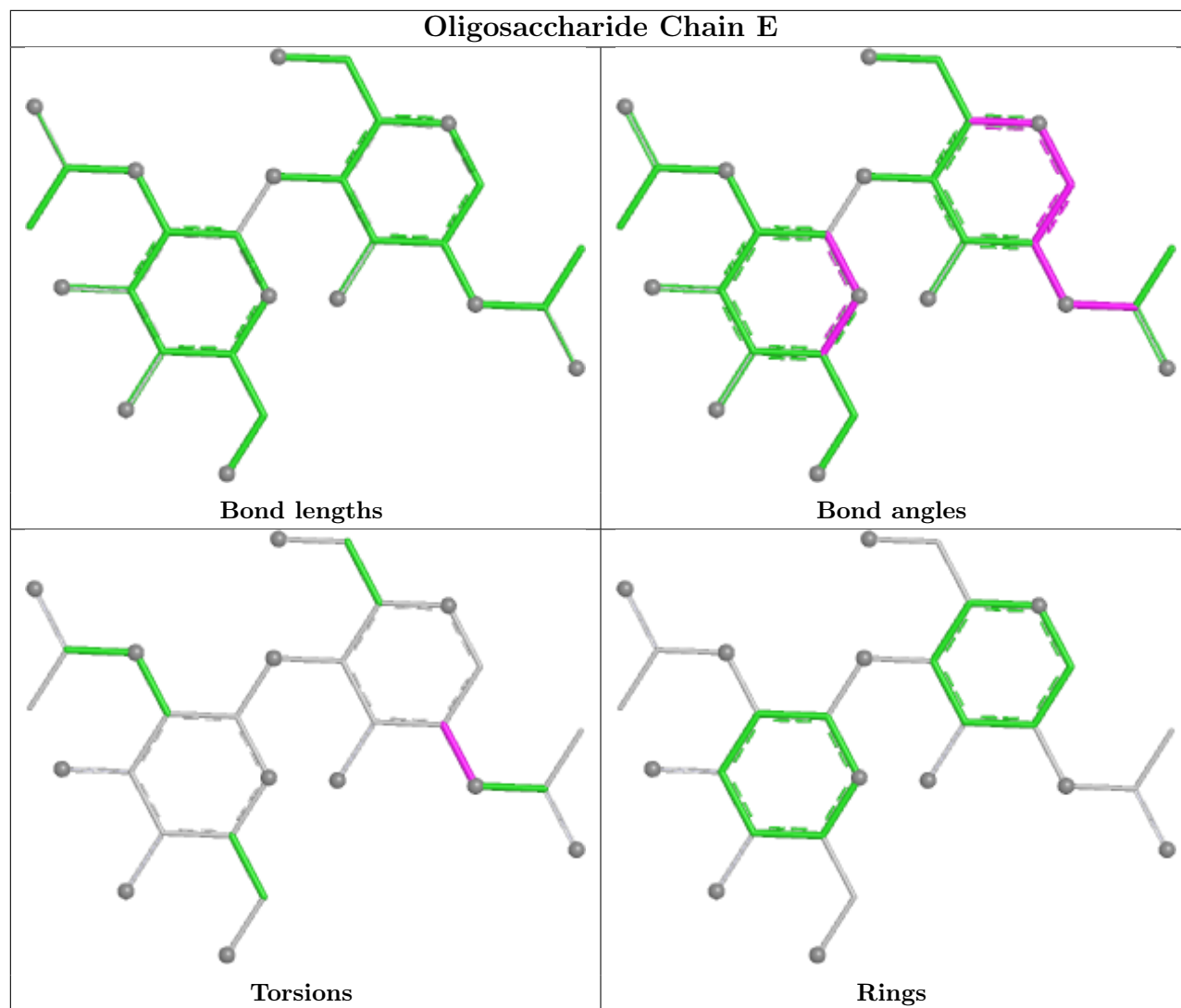
3 monomers are involved in 2 short contacts:

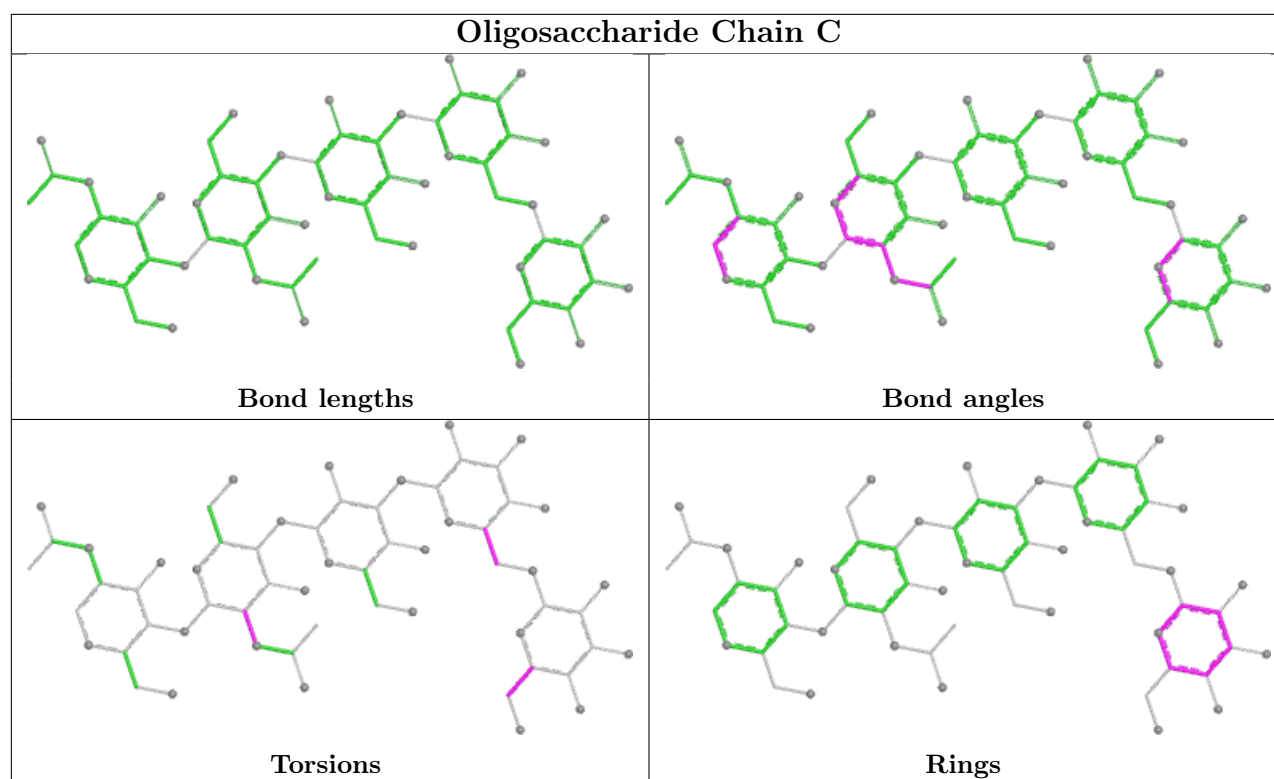
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	3	BMA	1	0
3	C	2	NAG	2	0

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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
6	EDO	A	1614	-	3,3,3	0.49	0	2,2,2	0.40	0
6	EDO	A	1615	-	3,3,3	0.48	0	2,2,2	0.42	0
4	NAG	A	1601	1	14,14,15	0.41	0	17,19,21	0.78	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
6	EDO	A	1614	-	-	0/1/1/1	-
6	EDO	A	1615	-	-	0/1/1/1	-
4	NAG	A	1601	1	-	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(°)	Ideal(°)
4	A	1601	NAG	C2-N2-C7	2.08	125.69	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1601	NAG	1	0

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 [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	1373/1494 (91%)	-0.25	3 (0%) 91 82	101, 167, 228, 269	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	804	VAL	3.1
1	A	769	LEU	2.9
1	A	204	LEU	2.5

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.

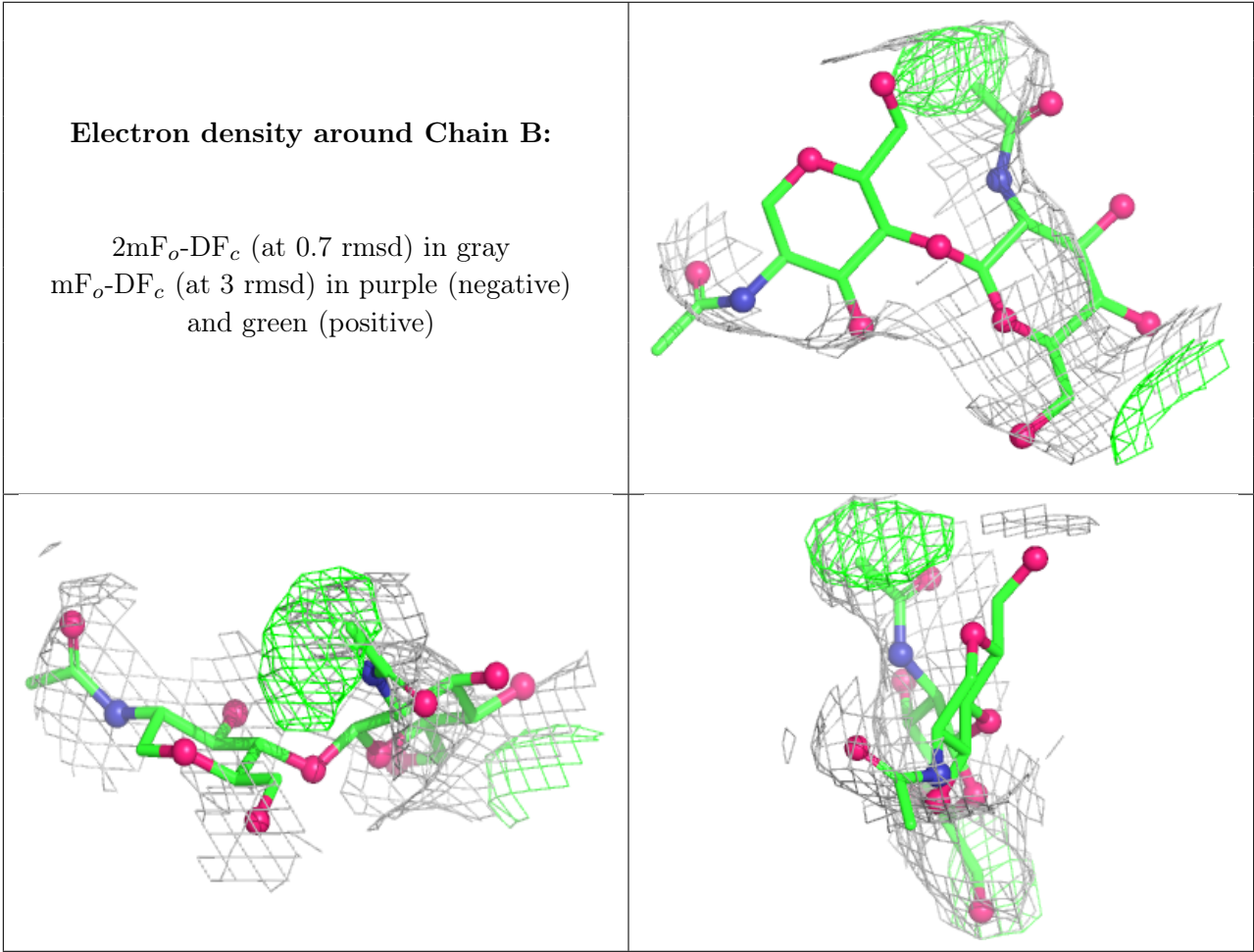
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	-0.24	0.13	235,238,240,242	0
2	NAG	E	1	14/15	-0.11	0.11	238,242,245,245	0
3	BMA	C	3	11/12	-0.06	0.10	238,240,243,246	0
2	NAG	D	2	14/15	0.07	0.10	227,232,234,235	0
2	NAG	D	1	14/15	0.19	0.11	207,217,224,228	0
2	NAG	E	2	14/15	0.20	0.09	243,245,246,246	0
3	MAN	C	4	11/12	0.22	0.08	247,249,252,252	0
3	MAN	C	5	11/12	0.33	0.07	243,247,248,249	0
3	NAG	C	2	14/15	0.50	0.08	203,214,225,232	0

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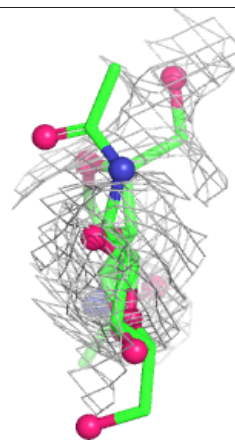
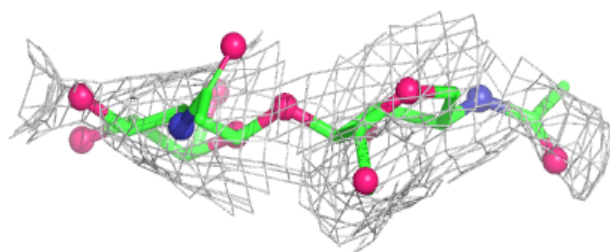
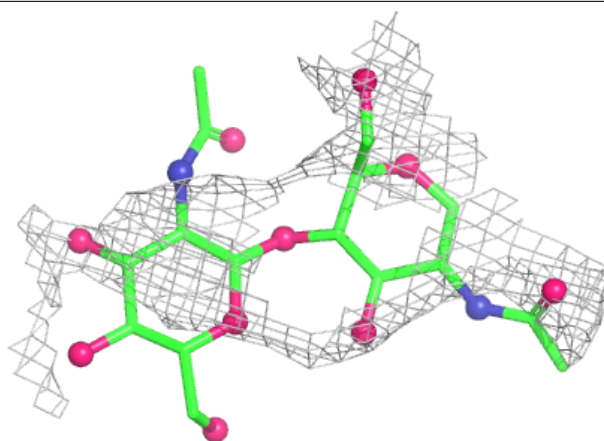
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	1	14/15	0.71	0.07	213,218,226,231	0
3	NAG	C	1	14/15	0.84	0.07	171,184,192,199	0

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.



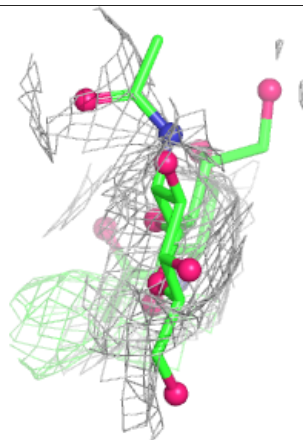
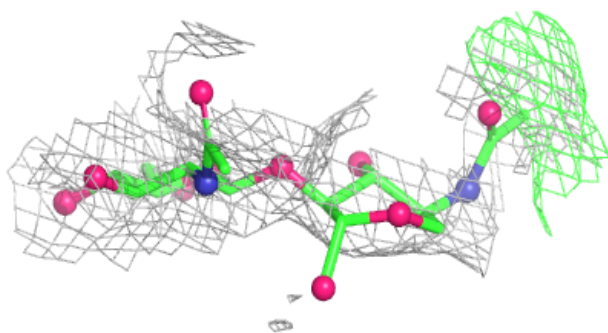
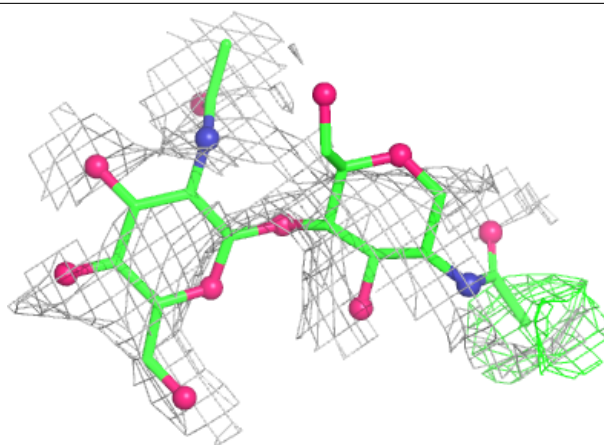
Electron density around Chain D:

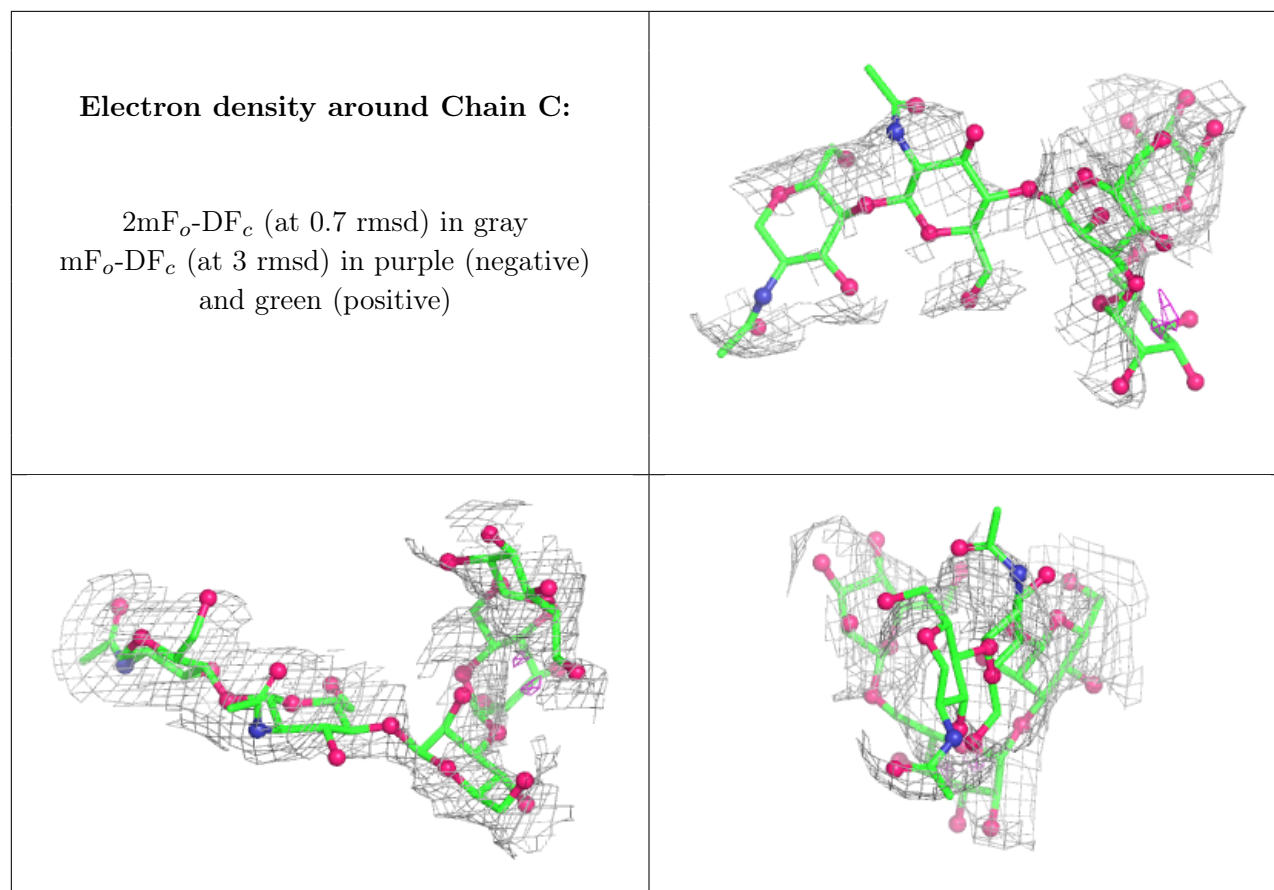
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
5	CA	A	1613	1/1	0.14	0.09	167,167,167,167	1
4	NAG	A	1601	14/15	0.59	0.10	215,219,223,223	0
6	EDO	A	1614	4/4	0.85	0.18	121,122,122,122	0
6	EDO	A	1615	4/4	0.90	0.08	137,137,137,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.