



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:31 PM EDT

PDB ID : 6M55 / pdb_00006m55
Title : Crystal structure of the E496A mutant of HsBglA in complex with 4-galactosyllactose
Authors : Uehara, R.; Iwamoto, R.; Aoki, S.; Yoshizawa, T.; Takano, K.; Matsumura, H.; Tanaka, S.-i.
Deposited on : 2020-03-10
Resolution : 3.00 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

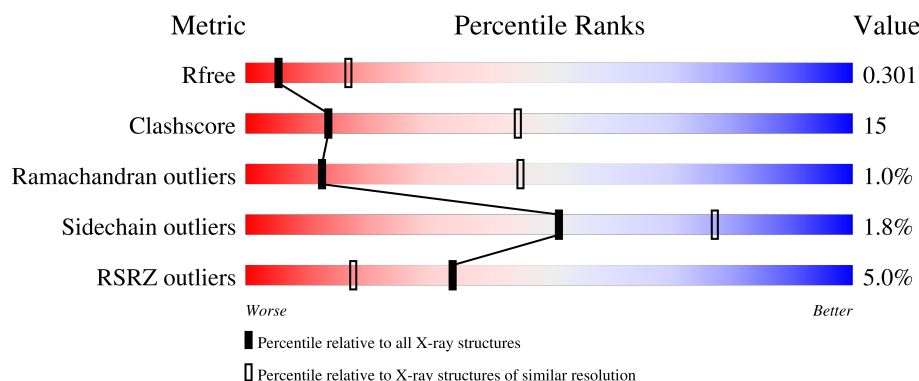
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	542	5% 76% 22% ..
1	D	542	5% 70% 26% .
2	C	3	100%
2	F	3	67% 33%
3	B	2	100%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8773 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

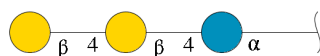
- Molecule 1 is a protein called Beta-galactosidase-like enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4284	2753	712	810	9			
1	D	542	Total	C	N	O	S	0	0	0
			4284	2753	712	810	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	ALA	GLU	engineered mutation	UNP Q564N5
A	595	HIS	-	expression tag	UNP Q564N5
A	596	HIS	-	expression tag	UNP Q564N5
D	496	ALA	GLU	engineered mutation	UNP Q564N5
D	595	HIS	-	expression tag	UNP Q564N5
D	596	HIS	-	expression tag	UNP Q564N5

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



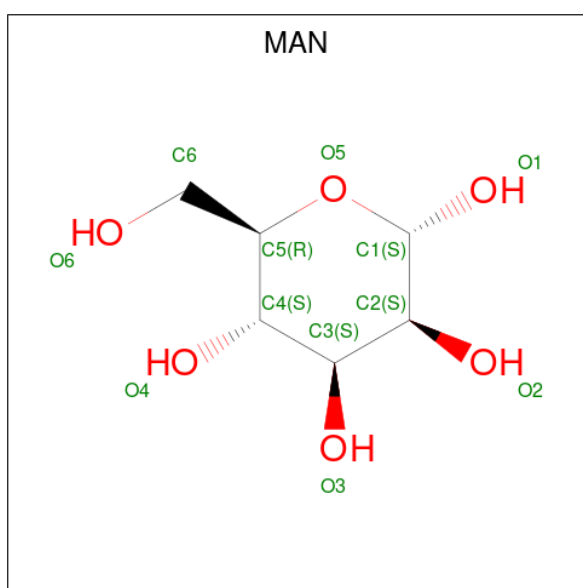
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			34	18	16			
2	F	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



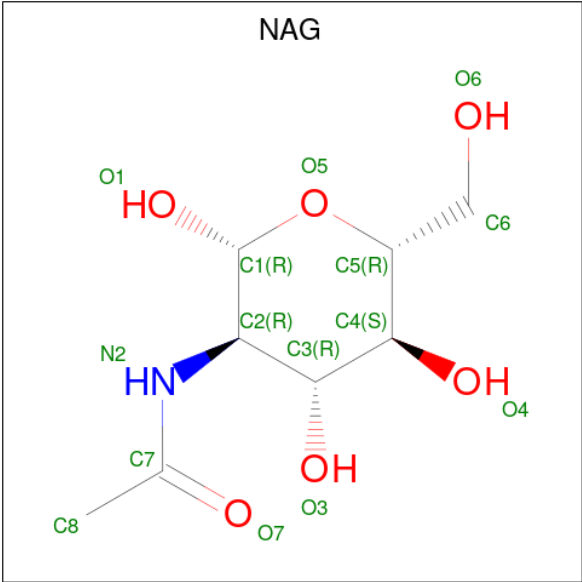
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

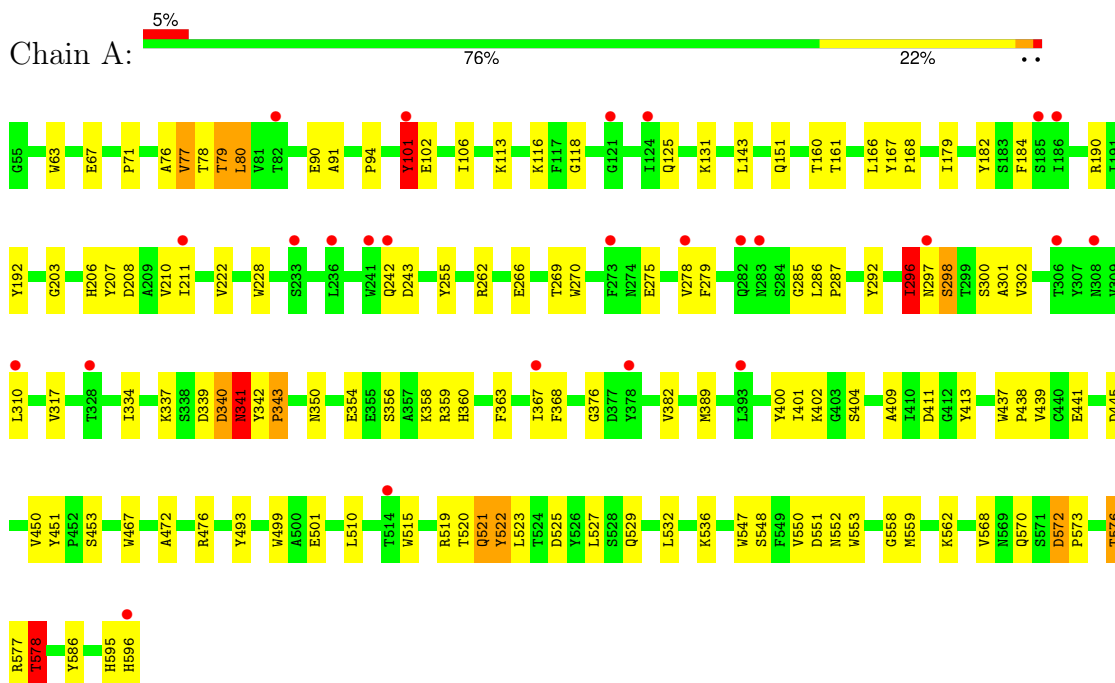
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	D	1	Total	O	0	0
			1	1		

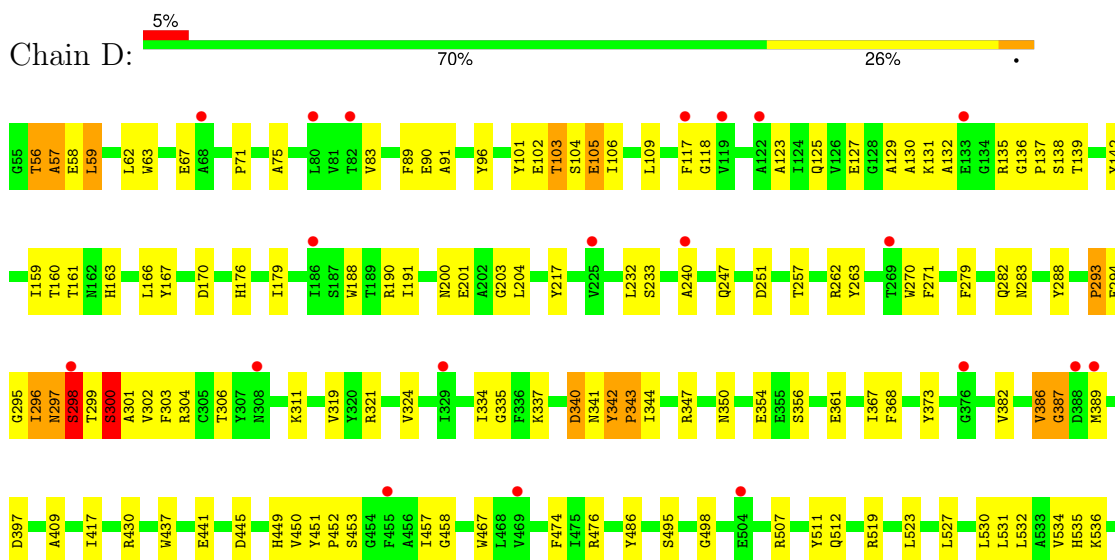
3 Residue-property plots [i](#)

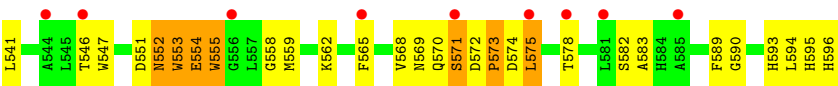
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Beta-galactosidase-like enzyme

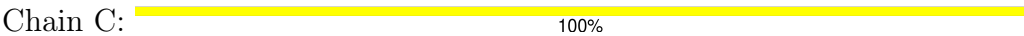


- Molecule 1: Beta-galactosidase-like enzyme





● Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



● Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.69Å 67.12Å 117.58Å 90.00° 128.54° 90.00°	Depositor
Resolution (Å)	45.21 – 3.00 45.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.21-3.00) 97.0 (45.21-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.265 , 0.298 0.268 , 0.301	Depositor DCC
R_{free} test set	1229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8773	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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, GLC, MAN, GAL

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	0.69	8/4418 (0.2%)	0.88	12/6029 (0.2%)
1	D	0.69	6/4418 (0.1%)	0.89	7/6029 (0.1%)
All	All	0.69	14/8836 (0.2%)	0.88	19/12058 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	553	TRP	CA-C	-7.46	1.43	1.52
1	D	554	GLU	CA-C	-6.41	1.45	1.52
1	A	578	THR	C-O	-6.37	1.16	1.23
1	A	101	TYR	CA-C	-6.06	1.44	1.52
1	A	76	ALA	CA-C	-6.03	1.44	1.52
1	D	573	PRO	C-O	-5.85	1.17	1.24
1	A	572	ASP	C-O	-5.66	1.18	1.24
1	A	341	ASN	C-O	-5.66	1.18	1.24
1	D	552	ASN	C-O	-5.65	1.18	1.24
1	A	79	THR	C-O	-5.57	1.17	1.23
1	D	293	PRO	C-O	-5.43	1.17	1.24
1	A	77	VAL	CA-CB	-5.36	1.48	1.54
1	A	79	THR	CA-C	-5.28	1.47	1.52
1	D	553	TRP	C-O	-5.13	1.18	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	296	ILE	N-CA-C	8.15	119.26	106.88
1	A	578	THR	CA-C-N	7.18	131.00	120.95
1	A	578	THR	C-N-CA	7.18	131.00	120.95
1	A	522	TYR	N-CA-C	-6.65	103.96	111.14
1	D	343	PRO	CB-CA-C	-6.52	100.80	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ALA	N-CA-C	-6.22	104.79	112.38
1	D	552	ASN	N-CA-C	6.12	117.91	109.29
1	A	343	PRO	N-CA-C	5.93	120.51	111.15
1	A	298	SER	N-CA-C	-5.88	105.42	113.30
1	A	77	VAL	N-CA-C	5.71	116.17	108.17
1	A	520	THR	CA-CB-OG1	-5.51	101.33	109.60
1	A	297	ASN	CA-CB-CG	5.45	118.05	112.60
1	A	296	ILE	CA-C-N	5.37	131.57	122.12
1	A	296	ILE	C-N-CA	5.37	131.57	122.12
1	D	101	TYR	N-CA-C	-5.33	104.44	111.96
1	D	59	LEU	N-CA-C	-5.28	105.52	111.28
1	A	297	ASN	CB-CA-C	-5.26	100.64	113.15
1	D	57	ALA	N-CA-C	-5.13	101.88	109.83
1	D	343	PRO	CA-N-CD	-5.08	104.89	112.00

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	4284	0	4028	110	0
1	D	4284	0	4026	144	0
2	C	34	0	30	6	0
2	F	34	0	30	5	0
3	B	28	0	25	3	0
3	E	28	0	25	2	0
4	A	11	0	10	0	0
4	D	11	0	10	0	0
5	D	56	0	52	0	0
6	A	2	0	0	0	0
6	D	1	0	0	0	0
All	All	8773	0	8236	248	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 15.

All (248) 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:D:572:ASP:OD1	1:D:573:PRO:HD2	1.23	1.26
1:D:467:TRP:CZ2	2:F:3:GAL:H5	1.95	1.01
1:D:294:GLU:CG	1:D:295:GLY:HA2	1.92	0.99
1:D:160:THR:HG22	1:D:161:THR:H	1.24	0.99
1:A:160:THR:HG22	1:A:161:THR:H	1.22	0.98
1:D:166:LEU:HD11	1:D:575:LEU:CD1	1.93	0.98
1:D:294:GLU:HG3	1:D:295:GLY:CA	1.95	0.97
1:D:294:GLU:HG3	1:D:295:GLY:HA2	0.99	0.96
1:D:574:ASP:O	1:D:575:LEU:HD12	1.64	0.95
1:D:572:ASP:OD1	1:D:573:PRO:CD	2.16	0.91
1:A:79:THR:O	1:A:80:LEU:C	2.19	0.84
1:D:59:LEU:HD11	1:D:136:GLY:HA2	1.60	0.82
1:D:386:VAL:HG23	1:D:387:GLY:H	1.44	0.82
1:D:57:ALA:C	1:D:59:LEU:H	1.89	0.80
1:A:467:TRP:CZ2	2:C:3:GAL:H5	2.19	0.77
1:D:294:GLU:HA	1:D:296:ILE:H	1.50	0.76
1:D:279:PHE:HA	1:D:282:GLN:NE2	2.00	0.76
1:D:166:LEU:HD11	1:D:575:LEU:HD13	1.66	0.75
1:A:476:ARG:HH22	1:A:536:LYS:HE2	1.51	0.74
1:A:367:ILE:HD13	1:A:382:VAL:HG11	1.70	0.74
1:A:356:SER:HB2	1:A:441:GLU:HB3	1.72	0.71
1:D:297:ASN:O	1:D:298:SER:C	2.33	0.71
1:D:337:LYS:HE3	1:D:495:SER:HB2	1.72	0.71
1:A:160:THR:HG22	1:A:161:THR:N	2.01	0.71
1:D:160:THR:HG22	1:D:161:THR:N	2.00	0.71
1:D:106:ILE:HD12	1:D:106:ILE:O	1.91	0.69
1:D:279:PHE:HA	1:D:282:GLN:HE21	1.58	0.69
1:D:553:TRP:CZ3	1:D:555:TRP:CE3	2.82	0.68
1:A:102:GLU:HG2	1:A:106:ILE:HD11	1.76	0.67
1:A:559:MET:HG2	1:A:570:GLN:NE2	2.10	0.67
1:D:342:TYR:CD2	1:D:361:GLU:HG3	2.31	0.66
1:A:339:ASP:HB3	1:A:411:ASP:HB2	1.78	0.66
1:A:106:ILE:HG22	1:A:532:LEU:HD11	1.77	0.66
1:D:163:HIS:ND1	1:D:170:ASP:OD2	2.28	0.65
1:D:553:TRP:HZ3	1:D:555:TRP:CE3	2.14	0.65
1:D:298:SER:O	1:D:301:ALA:HB3	1.97	0.65
1:D:554:GLU:O	1:D:558:GLY:N	2.30	0.65
1:D:467:TRP:HZ2	2:F:3:GAL:H5	1.60	0.64
1:D:191:ILE:HG23	1:D:204:LEU:HD11	1.80	0.64
1:A:275:GLU:HB3	1:A:339:ASP:OD2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:CG2	1:A:161:THR:H	2.07	0.63
1:D:106:ILE:HD12	1:D:593:HIS:CE1	2.34	0.63
1:D:595:HIS:O	1:D:596:HIS:HB2	1.98	0.63
1:A:572:ASP:OD2	1:A:576:THR:HG22	1.99	0.62
1:A:208:ASP:O	1:A:211:ILE:HG13	2.00	0.62
1:D:507:ARG:NE	1:D:512:GLN:HB3	2.15	0.61
1:D:166:LEU:HD11	1:D:575:LEU:HD12	1.83	0.61
1:A:363:PHE:CZ	1:A:438:PRO:HB2	2.36	0.61
1:A:467:TRP:HZ2	2:C:3:GAL:H5	1.66	0.61
1:D:467:TRP:CZ2	2:F:3:GAL:C5	2.78	0.61
1:D:311:LYS:HE3	1:D:397:ASP:OD1	2.01	0.60
1:D:297:ASN:O	1:D:300:SER:N	2.34	0.60
1:A:359:ARG:HD3	1:A:439:VAL:O	2.02	0.60
1:D:299:THR:C	1:D:301:ALA:H	2.10	0.60
1:A:77:VAL:HG13	1:A:77:VAL:O	2.00	0.59
1:A:510:LEU:HD13	3:E:1:NAG:H81	1.83	0.59
1:D:590:GLY:O	1:D:594:LEU:HB2	2.03	0.59
1:D:201:GLU:OE2	1:D:262:ARG:NH2	2.30	0.58
1:D:551:ASP:HB2	1:D:568:VAL:HG12	1.85	0.58
1:D:166:LEU:CD1	1:D:575:LEU:HD13	2.33	0.58
1:D:507:ARG:HE	1:D:512:GLN:HB3	1.69	0.58
1:D:534:VAL:HG23	1:D:535:HIS:CD2	2.39	0.57
1:D:102:GLU:OE1	1:D:593:HIS:NE2	2.37	0.57
1:A:118:GLY:HA2	1:A:179:ILE:HG23	1.85	0.57
1:A:90:GLU:OE2	1:A:578:THR:HA	2.03	0.57
1:D:138:SER:OG	1:D:139:THR:N	2.35	0.57
1:A:292:TYR:HB3	1:A:296:ILE:HG22	1.86	0.57
1:A:91:ALA:HB3	1:D:453:SER:HB2	1.86	0.57
1:A:367:ILE:CD1	1:A:382:VAL:HG11	2.36	0.56
1:A:510:LEU:HB2	3:E:1:NAG:H81	1.86	0.56
1:A:101:TYR:CE1	1:A:521:GLN:HG3	2.41	0.56
1:D:546:THR:HG21	1:D:565:PHE:HE2	1.69	0.56
1:D:57:ALA:C	1:D:59:LEU:N	2.63	0.55
1:D:83:VAL:HG21	1:D:217:TYR:OH	2.06	0.55
1:A:101:TYR:CD1	1:A:521:GLN:HG3	2.41	0.55
1:A:275:GLU:CG	1:A:339:ASP:OD2	2.54	0.55
1:A:270:TRP:O	1:A:334:ILE:HA	2.07	0.55
1:D:476:ARG:HH22	1:D:536:LYS:HE2	1.70	0.55
1:D:531:LEU:O	1:D:534:VAL:HG22	2.07	0.54
1:D:572:ASP:HB3	1:D:575:LEU:H	1.71	0.54
1:A:211:ILE:HD13	1:A:266:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:MET:HG2	1:D:570:GLN:NE2	2.23	0.53
1:A:94:PRO:HG3	1:D:451:TYR:CE2	2.43	0.53
1:A:367:ILE:HG23	1:A:368:PHE:CD2	2.44	0.53
1:A:278:VAL:HG22	2:C:2:GAL:H2	1.91	0.53
1:A:292:TYR:HE2	1:A:298:SER:HB2	1.74	0.52
1:A:106:ILE:HG22	1:A:532:LEU:CD1	2.39	0.52
1:A:413:TYR:CE2	2:C:3:GAL:H3	2.45	0.52
1:D:117:PHE:CB	1:D:594:LEU:HD11	2.40	0.52
1:D:117:PHE:HB3	1:D:594:LEU:HD11	1.90	0.52
1:A:151:GLN:OE1	3:B:2:NAG:O7	2.27	0.52
1:D:344:ILE:HD13	1:D:474:PHE:CE2	2.45	0.52
1:A:472:ALA:CB	1:A:525:ASP:HB3	2.40	0.52
1:A:125:GLN:O	1:A:552:ASN:HB2	2.10	0.52
1:A:286:LEU:HD12	3:B:1:NAG:H62	1.92	0.52
1:A:595:HIS:O	1:A:596:HIS:ND1	2.42	0.52
1:D:303:PHE:O	1:D:306:THR:HG22	2.10	0.52
1:D:294:GLU:HA	1:D:296:ILE:N	2.21	0.52
1:A:350:ASN:O	1:A:354:GLU:HG3	2.10	0.51
1:A:453:SER:HB2	1:D:91:ALA:HB3	1.93	0.51
1:D:283:ASN:HA	1:D:288:TYR:CD2	2.44	0.51
1:A:63:TRP:CG	1:A:131:LYS:HZ3	2.28	0.51
1:A:400:TYR:O	1:A:404:SER:HB3	2.11	0.51
1:D:63:TRP:CE2	1:D:131:LYS:HG2	2.45	0.51
1:D:142:TYR:HB2	1:D:232:LEU:HD22	1.93	0.50
1:D:298:SER:O	1:D:301:ALA:CB	2.58	0.50
1:D:565:PHE:O	1:D:583:ALA:HB2	2.11	0.50
1:D:551:ASP:CG	1:D:562:LYS:HG3	2.36	0.50
1:A:413:TYR:HE2	2:C:3:GAL:HO3	1.57	0.50
1:A:190:ARG:HD2	1:A:207:TYR:CE1	2.47	0.50
1:D:160:THR:CG2	1:D:161:THR:N	2.72	0.50
1:D:553:TRP:HZ3	1:D:555:TRP:CZ3	2.30	0.50
1:D:450:VAL:HG12	1:D:451:TYR:O	2.12	0.50
1:D:321:ARG:HA	1:D:324:VAL:HG12	1.93	0.49
1:D:519:ARG:NH2	1:D:562:LYS:O	2.45	0.49
1:D:200:ASN:OD1	1:D:203:GLY:N	2.45	0.49
1:A:208:ASP:OD2	1:A:262:ARG:NH1	2.44	0.49
1:D:62:LEU:HB3	1:D:137:PRO:HG3	1.95	0.49
1:D:350:ASN:O	1:D:354:GLU:HG3	2.13	0.49
1:D:293:PRO:O	1:D:293:PRO:HG2	2.12	0.48
1:A:275:GLU:CB	1:A:339:ASP:OD2	2.61	0.48
1:A:190:ARG:HD2	1:A:207:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:C	1:A:342:TYR:CD1	2.92	0.48
1:D:389:MET:HE1	1:D:437:TRP:HH2	1.78	0.48
1:D:62:LEU:HD11	1:D:233:SER:HB3	1.94	0.48
1:D:298:SER:O	1:D:301:ALA:N	2.46	0.48
1:A:572:ASP:O	1:A:573:PRO:C	2.53	0.47
1:A:116:LYS:HD2	1:A:493:TYR:HE1	1.79	0.47
1:A:78:THR:O	1:A:78:THR:OG1	2.27	0.47
1:D:527:LEU:HB3	1:D:589:PHE:CE1	2.49	0.47
1:D:303:PHE:HA	1:D:306:THR:HG22	1.97	0.47
1:D:347:ARG:HH11	1:D:350:ASN:ND2	2.11	0.47
1:D:342:TYR:HD2	1:D:361:GLU:HG3	1.79	0.47
1:A:292:TYR:CE2	1:A:298:SER:HA	2.50	0.46
1:D:106:ILE:HG22	1:D:532:LEU:HG	1.96	0.46
1:A:78:THR:C	1:A:79:THR:HG23	2.41	0.46
1:A:296:ILE:HD12	1:A:296:ILE:HA	1.62	0.46
1:D:299:THR:C	1:D:301:ALA:N	2.73	0.46
1:D:347:ARG:HH11	1:D:350:ASN:HD21	1.64	0.46
1:A:166:LEU:HD12	1:A:577:ARG:CZ	2.46	0.46
1:A:472:ALA:O	1:A:529:GLN:HG3	2.16	0.46
1:D:574:ASP:C	1:D:575:LEU:HG	2.40	0.45
1:A:553:TRP:CD1	1:A:558:GLY:HA2	2.51	0.45
1:D:347:ARG:HG3	1:D:452:PRO:HG2	1.98	0.45
1:A:182:TYR:CE2	1:A:184:PHE:HB3	2.51	0.45
1:D:89:PHE:CZ	1:D:176:HIS:HB2	2.51	0.45
1:A:445:ASP:HB3	1:D:511:TYR:OH	2.17	0.45
1:D:340:ASP:HB3	1:D:341:ASN:H	1.56	0.45
1:A:101:TYR:HD1	1:A:101:TYR:HA	1.52	0.45
1:A:160:THR:CG2	1:A:161:THR:N	2.71	0.45
1:A:342:TYR:OH	1:A:358:LYS:HD2	2.17	0.45
1:D:367:ILE:HG23	1:D:368:PHE:CD2	2.51	0.45
1:A:510:LEU:HD21	1:A:578:THR:HG21	1.97	0.45
1:D:160:THR:CG2	1:D:161:THR:H	2.10	0.45
1:D:569:ASN:C	1:D:571:SER:H	2.25	0.45
1:D:498:GLY:HA3	1:D:547:TRP:O	2.17	0.44
1:D:271:PHE:HA	1:D:335:GLY:O	2.17	0.44
1:D:373:TYR:HB2	1:D:486:TYR:HB3	1.99	0.44
1:A:275:GLU:CD	1:A:339:ASP:OD2	2.60	0.44
1:D:135:ARG:HD2	1:D:190:ARG:CZ	2.47	0.44
1:A:78:THR:C	1:A:79:THR:CG2	2.90	0.44
1:D:523:LEU:HD12	1:D:582:SER:HB2	1.98	0.44
1:A:190:ARG:O	1:A:203:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:THR:O	1:D:302:VAL:HG12	2.18	0.44
1:D:90:GLU:OE2	1:D:578:THR:HA	2.17	0.44
1:D:129:ALA:HB1	1:D:132:ALA:HB3	2.00	0.44
1:D:534:VAL:HG23	1:D:535:HIS:HD2	1.81	0.44
1:A:499:TRP:HB3	1:A:519:ARG:HG3	2.00	0.44
1:D:96:TYR:CD1	1:D:96:TYR:O	2.70	0.44
1:D:163:HIS:CE1	1:D:167:TYR:HA	2.52	0.44
1:A:572:ASP:OD2	1:A:576:THR:CG2	2.64	0.43
1:D:296:ILE:HD11	1:D:304:ARG:HG3	1.99	0.43
1:D:574:ASP:O	1:D:575:LEU:CD1	2.52	0.43
1:A:515:TRP:CH2	1:D:458:GLY:HA2	2.51	0.43
1:D:386:VAL:HG23	1:D:387:GLY:N	2.23	0.43
1:D:530:LEU:HG	1:D:541:LEU:HD21	2.00	0.43
1:D:551:ASP:OD1	1:D:562:LYS:HG3	2.18	0.43
1:D:96:TYR:O	1:D:96:TYR:HD1	2.01	0.43
1:A:317:VAL:HG21	1:A:404:SER:O	2.18	0.43
1:A:337:LYS:HA	1:A:409:ALA:HB3	1.99	0.43
1:A:206:HIS:O	1:A:210:VAL:HG23	2.19	0.43
1:A:298:SER:O	1:A:298:SER:OG	2.35	0.43
1:A:550:VAL:HB	1:A:568:VAL:HG21	2.00	0.43
1:A:522:TYR:O	1:A:523:LEU:C	2.59	0.43
1:D:67:GLU:HB3	1:D:71:PRO:HA	2.00	0.43
1:D:467:TRP:HZ2	2:F:3:GAL:C5	2.26	0.43
1:A:341:ASN:C	1:A:343:PRO:HD3	2.43	0.43
1:D:445:ASP:OD1	1:D:449:HIS:HE1	2.02	0.43
1:D:574:ASP:C	1:D:575:LEU:CG	2.92	0.43
1:A:472:ALA:HB2	1:A:525:ASP:HB3	2.00	0.42
1:D:409:ALA:HB1	1:D:495:SER:HB3	2.01	0.42
1:D:553:TRP:CH2	1:D:555:TRP:HA	2.54	0.42
1:A:551:ASP:CG	1:A:562:LYS:HG3	2.44	0.42
1:D:109:LEU:HD22	1:D:535:HIS:CG	2.54	0.42
1:A:192:TYR:CE1	1:A:255:TYR:HA	2.55	0.42
1:D:247:GLN:NE2	1:D:251:ASP:OD1	2.48	0.42
1:A:167:TYR:CG	1:A:168:PRO:HD3	2.54	0.42
1:D:321:ARG:HA	1:D:324:VAL:CG1	2.48	0.42
1:A:310:LEU:HB3	1:A:401:ILE:HD13	2.02	0.42
1:D:59:LEU:HG	1:D:63:TRP:HD1	1.85	0.42
1:D:106:ILE:CD1	1:D:593:HIS:CE1	3.01	0.42
1:A:222:VAL:HG22	1:A:269:THR:HB	2.01	0.42
1:A:242:GLN:O	1:A:243:ASP:C	2.63	0.42
1:A:413:TYR:O	1:A:522:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:SER:HB2	1:D:441:GLU:HB3	2.02	0.42
1:D:303:PHE:CZ	1:D:386:VAL:HG11	2.54	0.42
1:D:417:ILE:HD11	1:D:457:ILE:HB	2.02	0.42
1:A:501:GLU:OE1	1:A:519:ARG:N	2.50	0.42
1:D:188:TRP:HD1	1:D:188:TRP:O	2.03	0.42
1:D:191:ILE:HG23	1:D:204:LEU:CD1	2.49	0.42
1:D:204:LEU:O	1:D:263:TYR:OH	2.35	0.42
1:A:547:TRP:HA	1:A:548:SER:HA	1.85	0.42
1:D:56:THR:CG2	1:D:57:ALA:H	2.32	0.42
1:D:382:VAL:O	1:D:386:VAL:HG22	2.20	0.42
1:A:79:THR:O	1:A:79:THR:OG1	2.35	0.41
1:A:527:LEU:HD11	1:A:586:TYR:CE1	2.55	0.41
1:D:56:THR:HG22	1:D:57:ALA:H	1.85	0.41
1:D:130:ALA:O	1:D:135:ARG:HD3	2.19	0.41
1:D:270:TRP:O	1:D:334:ILE:HA	2.20	0.41
1:D:594:LEU:HD23	1:D:594:LEU:HA	1.80	0.41
1:A:376:GLY:HA3	1:A:402:LYS:HD2	2.02	0.41
1:A:389:MET:HE1	1:A:437:TRP:HH2	1.85	0.41
1:A:285:GLY:HA2	3:B:1:NAG:O5	2.21	0.41
1:A:340:ASP:OD2	1:A:360:HIS:NE2	2.51	0.41
1:D:105:GLU:O	1:D:105:GLU:HG3	2.13	0.41
1:A:78:THR:O	1:A:79:THR:HG22	2.20	0.41
1:A:228:TRP:NE1	1:A:279:PHE:HB2	2.36	0.41
1:A:342:TYR:C	1:A:342:TYR:HD1	2.28	0.41
1:D:125:GLN:O	1:D:552:ASN:HB2	2.20	0.41
1:D:257:THR:OG1	1:D:319:VAL:HG11	2.20	0.41
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.88	0.41
1:A:113:LYS:HB3	1:A:113:LYS:HE3	1.81	0.41
1:A:67:GLU:HB3	1:A:71:PRO:HA	2.02	0.41
1:A:501:GLU:H	1:A:519:ARG:NH2	2.19	0.41
1:D:103:THR:OG1	1:D:104:SER:N	2.54	0.41
1:D:546:THR:HG21	1:D:565:PHE:CE2	2.53	0.41
1:A:296:ILE:HG22	1:A:296:ILE:O	2.20	0.41
1:D:467:TRP:HZ2	2:F:3:GAL:C6	2.33	0.41
1:A:94:PRO:HG3	1:D:451:TYR:HE2	1.86	0.41
1:A:300:SER:C	1:A:302:VAL:N	2.76	0.41
1:A:450:VAL:HG12	1:A:451:TYR:O	2.21	0.41
1:A:521:GLN:HE21	1:A:521:GLN:HB3	1.63	0.41
1:D:118:GLY:HA2	1:D:179:ILE:HG23	2.03	0.41
1:D:574:ASP:O	1:D:575:LEU:C	2.64	0.41
1:D:123:ALA:O	1:D:127:GLU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD13	1:A:287:PRO:HD3	2.04	0.40
1:D:75:ALA:HB2	1:D:159:ILE:HG23	2.02	0.40
1:A:413:TYR:CE2	2:C:3:GAL:C3	3.04	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	540/542 (100%)	515 (95%)	23 (4%)	2 (0%)	30	65
1	D	540/542 (100%)	509 (94%)	22 (4%)	9 (2%)	7	32
All	All	1080/1084 (100%)	1024 (95%)	45 (4%)	11 (1%)	12	45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	298	SER
1	D	555	TRP
1	D	240	ALA
1	D	56	THR
1	D	58	GLU
1	A	576	THR
1	D	300	SER
1	A	80	LEU
1	D	386	VAL
1	D	387	GLY
1	D	343	PRO

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	442/442 (100%)	436 (99%)	6 (1%)	59	80
1	D	442/442 (100%)	432 (98%)	10 (2%)	44	74
All	All	884/884 (100%)	868 (98%)	16 (2%)	51	77

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

Mol	Chain	Res	Type
1	A	101	TYR
1	A	296	ILE
1	A	340	ASP
1	A	341	ASN
1	A	521	GLN
1	A	578	THR
1	D	103	THR
1	D	105	GLU
1	D	297	ASN
1	D	298	SER
1	D	300	SER
1	D	340	ASP
1	D	342	TYR
1	D	430	ARG
1	D	571	SER
1	D	575	LEU

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	151	GLN
1	A	154	ASN
1	A	176	HIS
1	A	274	ASN
1	A	521	GLN
1	A	570	GLN

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Mol	Chain	Res	Type
1	D	370	GLN
1	D	427	ASN
1	D	436	ASN
1	D	449	HIS
1	D	570	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 ⓘ

10 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	$\# Z > 2$
3	NAG	B	1	3,1	14,14,15	1.06	2 (14%)	17,19,21	2.53	6 (35%)
3	NAG	B	2	3	14,14,15	0.81	0	17,19,21	1.69	4 (23%)
2	GLC	C	1	2	12,12,12	0.68	0	17,17,17	1.78	4 (23%)
2	GAL	C	2	2	11,11,12	0.26	0	15,15,17	0.54	0
2	GAL	C	3	2	11,11,12	0.26	0	15,15,17	0.52	0
3	NAG	E	1	3,1	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.58	0
2	GLC	F	1	2	12,12,12	0.46	0	17,17,17	0.53	0
2	GAL	F	2	2	11,11,12	0.26	0	15,15,17	0.48	0
2	GAL	F	3	2	11,11,12	0.27	0	15,15,17	0.53	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	B	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	GAL	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	GAL	F	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	NAG	C2-N2	-2.18	1.42	1.46
3	B	1	NAG	O7-C7	-2.06	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	-5.59	104.69	112.19
3	B	2	NAG	C2-N2-C7	4.81	129.35	122.90
3	B	1	NAG	O5-C5-C6	4.49	116.39	107.66
3	B	1	NAG	C1-C2-N2	-4.35	103.57	110.43
3	B	1	NAG	C3-C4-C5	-3.98	103.01	110.23
2	C	1	GLC	C3-C4-C5	-3.60	103.71	110.23
2	C	1	GLC	O3-C3-C2	-3.53	102.06	110.38
2	C	1	GLC	C1-O5-C5	2.81	119.08	113.65
2	C	1	GLC	O4-C4-C3	2.51	116.28	110.38
3	B	1	NAG	O4-C4-C5	-2.25	103.78	109.32
3	B	2	NAG	C1-O5-C5	2.23	115.18	112.19
3	B	2	NAG	C3-C4-C5	-2.23	106.19	110.23
3	B	2	NAG	O5-C5-C4	-2.20	105.49	110.83
3	B	1	NAG	O7-C7-N2	-2.16	118.16	121.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	B	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
2	C	3	GAL	O5-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

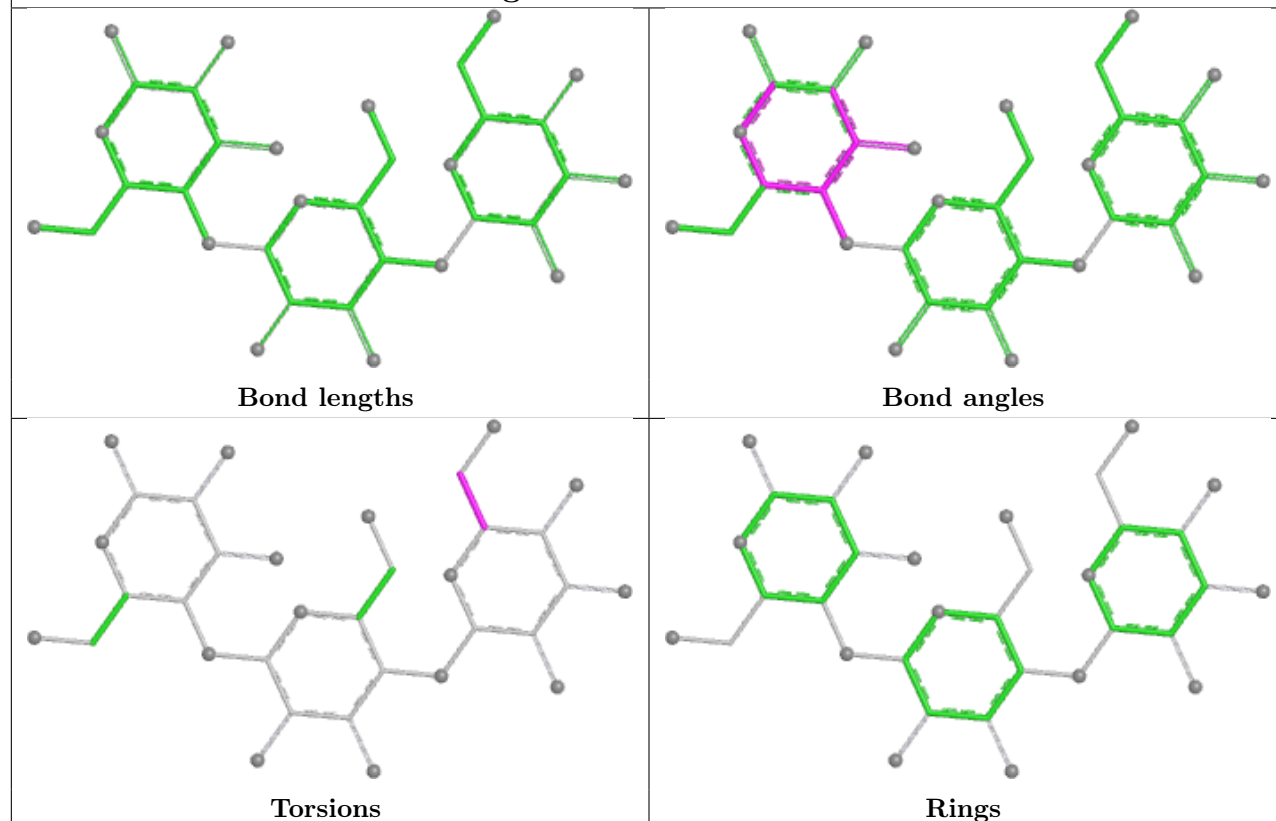
There are no ring outliers.

6 monomers are involved in 16 short contacts:

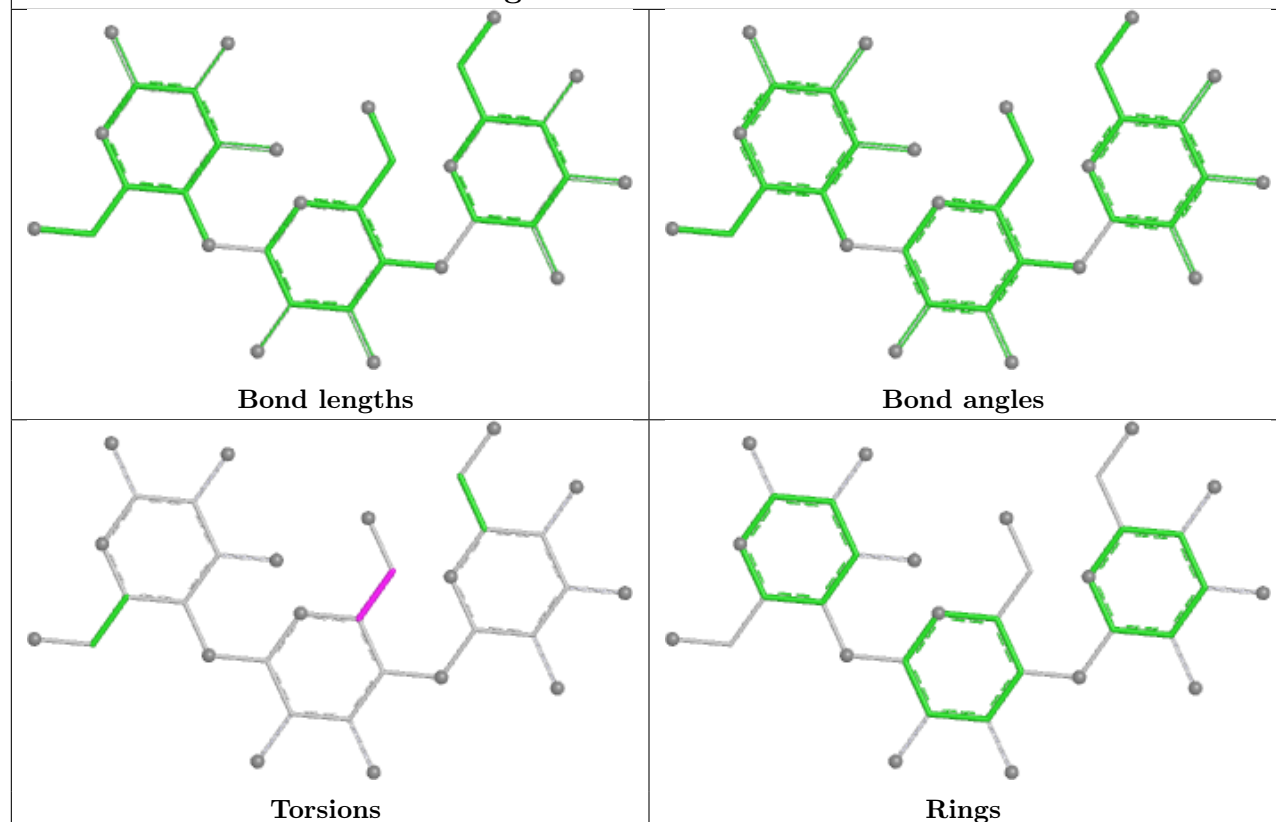
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	GAL	5	0
2	C	3	GAL	5	0
3	B	1	NAG	2	0
3	B	2	NAG	1	0
2	C	2	GAL	1	0
3	E	1	NAG	2	0

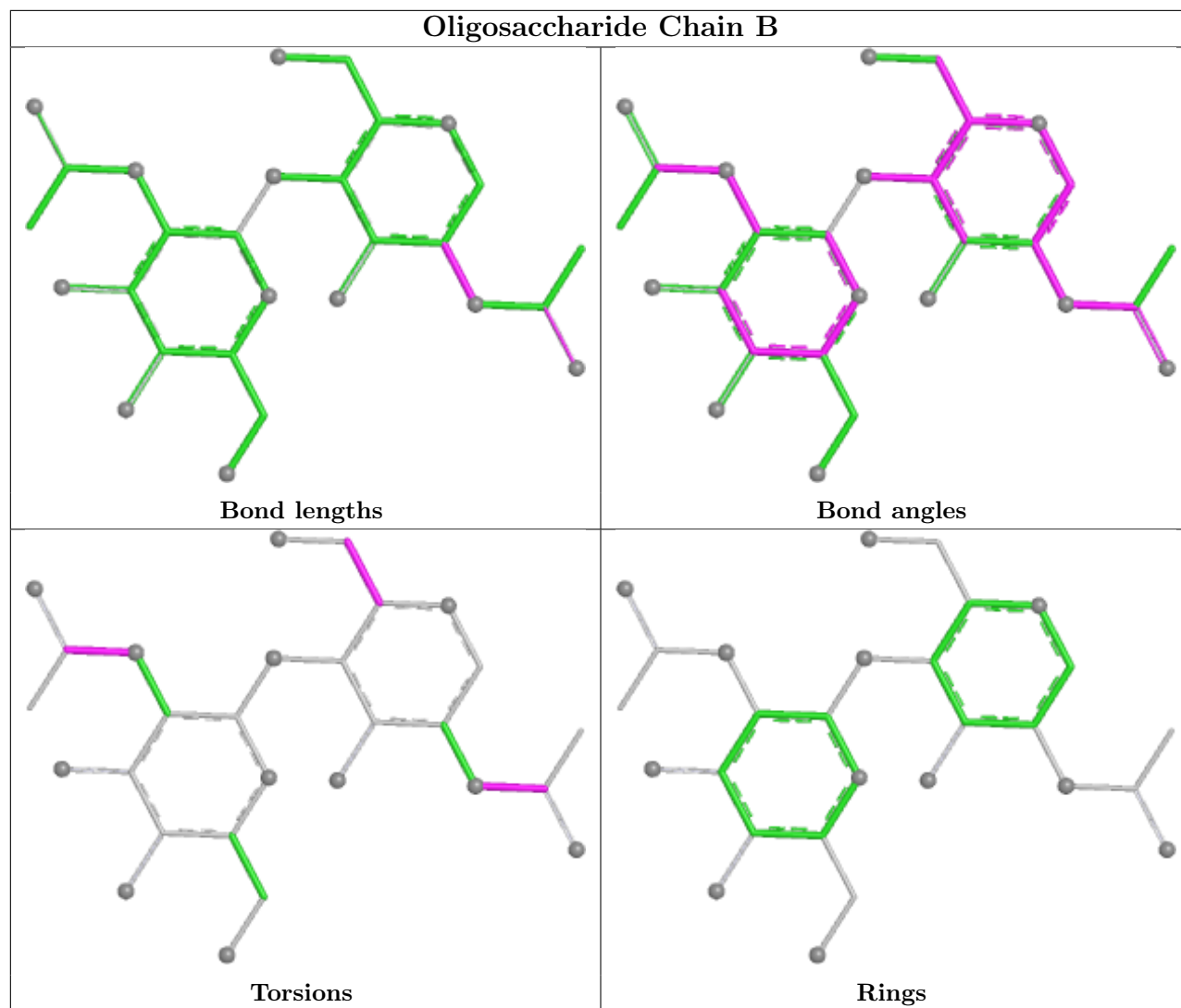
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

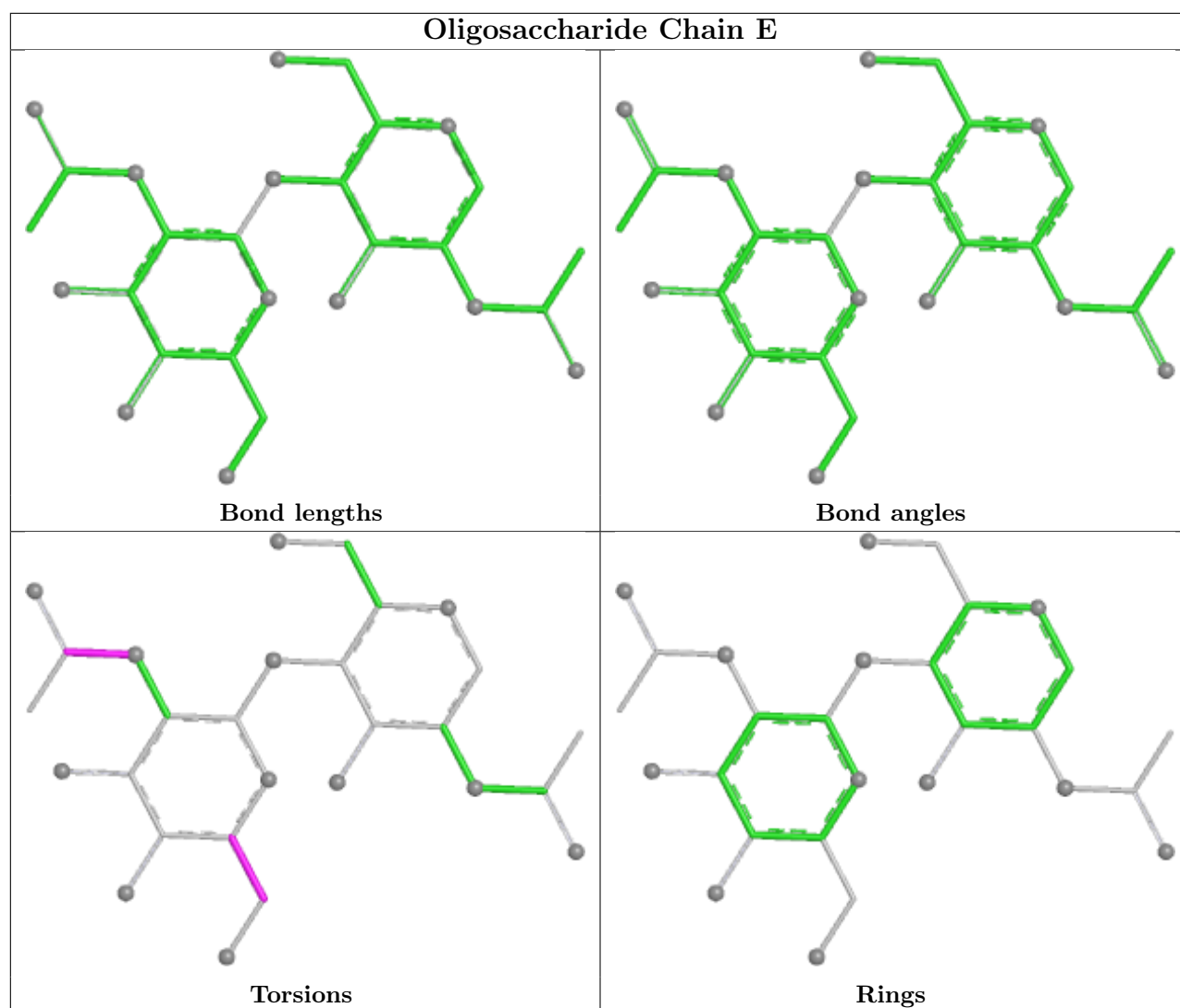
Oligosaccharide Chain C



Oligosaccharide Chain F







5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MAN	A	601	1	11,11,12	0.26	0	15,15,17	0.53	0
5	NAG	D	605	1	14,14,15	0.31	0	17,19,21	0.55	0
5	NAG	D	604	1	14,14,15	1.47	1 (7%)	17,19,21	2.63	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	603	1	14,14,15	0.95	2 (14%)	17,19,21	2.38	6 (35%)
5	NAG	D	602	1	14,14,15	1.41	3 (21%)	17,19,21	3.15	6 (35%)
4	MAN	D	601	1	11,11,12	0.40	0	15,15,17	1.09	1 (6%)

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
4	MAN	A	601	1	-	2/2/19/22	0/1/1/1
5	NAG	D	605	1	-	4/6/23/26	0/1/1/1
5	NAG	D	604	1	-	2/6/23/26	0/1/1/1
5	NAG	D	603	1	-	2/6/23/26	0/1/1/1
5	NAG	D	602	1	-	5/6/23/26	0/1/1/1
4	MAN	D	601	1	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	604	NAG	C4-C5	-2.82	1.47	1.53
5	D	603	NAG	O5-C5	-2.26	1.39	1.43
5	D	603	NAG	O5-C1	-2.24	1.39	1.43
5	D	602	NAG	C2-N2	-2.06	1.42	1.46
5	D	602	NAG	C4-C3	-2.01	1.47	1.52
5	D	602	NAG	C1-C2	-2.01	1.49	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	602	NAG	O5-C1-C2	-8.70	97.83	111.29
5	D	602	NAG	C1-O5-C5	6.37	120.72	112.19
5	D	604	NAG	O5-C1-C2	-5.37	102.98	111.29
5	D	603	NAG	C2-N2-C7	5.32	130.03	122.90
5	D	602	NAG	C4-C3-C2	-4.37	104.61	111.02
5	D	604	NAG	C2-N2-C7	-4.16	117.32	122.90
5	D	604	NAG	C6-C5-C4	-4.11	102.92	113.02
5	D	604	NAG	C3-C4-C5	-3.87	103.22	110.23
5	D	603	NAG	O5-C1-C2	-3.84	105.35	111.29
5	D	604	NAG	C4-C3-C2	-3.79	105.46	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	603	NAG	O5-C5-C4	-3.52	102.25	110.83
4	D	601	MAN	C1-O5-C5	-3.44	107.58	112.19
5	D	603	NAG	O5-C5-C6	-3.17	101.50	107.66
5	D	602	NAG	C3-C4-C5	-2.94	104.91	110.23
5	D	602	NAG	O3-C3-C4	-2.88	103.59	110.38
5	D	603	NAG	C3-C4-C5	-2.71	105.33	110.23
5	D	603	NAG	C1-O5-C5	2.52	115.56	112.19
5	D	602	NAG	C6-C5-C4	-2.39	107.16	113.02
5	D	604	NAG	O3-C3-C4	-2.30	104.96	110.38
5	D	604	NAG	O7-C7-N2	-2.21	118.08	121.98
5	D	604	NAG	O5-C5-C4	-2.10	105.71	110.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	602	NAG	O7-C7-N2-C2
5	D	603	NAG	C8-C7-N2-C2
5	D	603	NAG	O7-C7-N2-C2
5	D	602	NAG	C8-C7-N2-C2
4	A	601	MAN	O5-C5-C6-O6
5	D	604	NAG	C8-C7-N2-C2
5	D	605	NAG	C8-C7-N2-C2
5	D	604	NAG	O7-C7-N2-C2
5	D	605	NAG	O7-C7-N2-C2
4	A	601	MAN	C4-C5-C6-O6
5	D	605	NAG	C4-C5-C6-O6
5	D	605	NAG	O5-C5-C6-O6
5	D	602	NAG	C1-C2-N2-C7
5	D	602	NAG	C3-C2-N2-C7
5	D	602	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	542/542 (100%)	0.89	25 (4%)	37 20	55, 56, 57, 58	0
1	D	542/542 (100%)	0.88	29 (5%)	31 16	54, 55, 56, 57	0
All	All	1084/1084 (100%)	0.88	54 (4%)	34 18	54, 55, 57, 58	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	VAL	3.5
1	D	82	THR	3.4
1	D	240	ALA	3.2
1	A	283	ASN	3.0
1	D	269	THR	3.0
1	D	546	THR	2.9
1	D	585	ALA	2.9
1	A	211	ILE	2.8
1	A	378	TYR	2.8
1	D	565	PHE	2.7
1	A	124	ILE	2.7
1	A	278	VAL	2.7
1	A	308	ASN	2.7
1	A	306	THR	2.6
1	A	241	TRP	2.6
1	D	68	ALA	2.6
1	A	273	PHE	2.6
1	A	185	SER	2.6
1	D	80	LEU	2.6
1	D	571	SER	2.5
1	A	596	HIS	2.5
1	D	298	SER	2.4
1	A	514	THR	2.4
1	A	282	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	581	LEU	2.4
1	A	242	GLN	2.4
1	A	236	LEU	2.4
1	D	122	ALA	2.4
1	D	578	THR	2.3
1	A	393	LEU	2.3
1	D	455	PHE	2.3
1	A	328	THR	2.2
1	A	310	LEU	2.2
1	D	389	MET	2.2
1	D	376	GLY	2.2
1	A	367	ILE	2.2
1	D	575	LEU	2.2
1	A	101	TYR	2.1
1	A	186	ILE	2.1
1	D	544	ALA	2.1
1	D	225	VAL	2.1
1	A	82	THR	2.1
1	D	133	GLU	2.1
1	D	556	GLY	2.1
1	A	233	SER	2.1
1	D	308	ASN	2.1
1	D	469	VAL	2.1
1	D	186	ILE	2.1
1	D	117	PHE	2.1
1	D	329	ILE	2.0
1	A	297	ASN	2.0
1	D	388	ASP	2.0
1	A	121	GLY	2.0
1	D	504	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

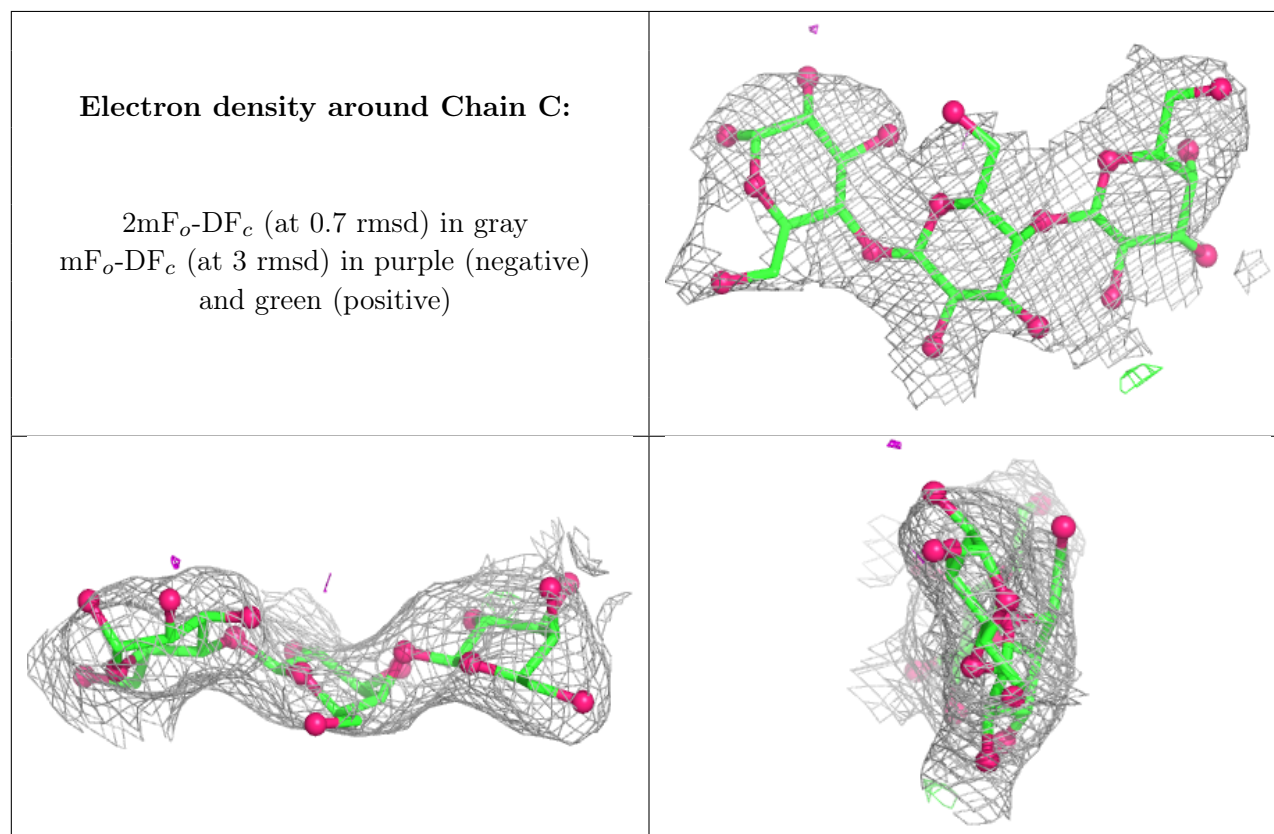
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

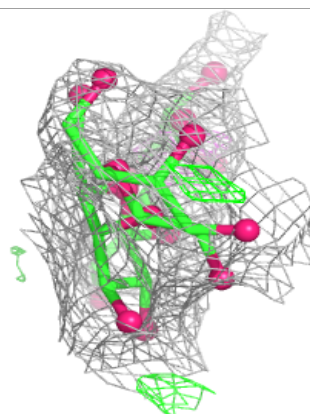
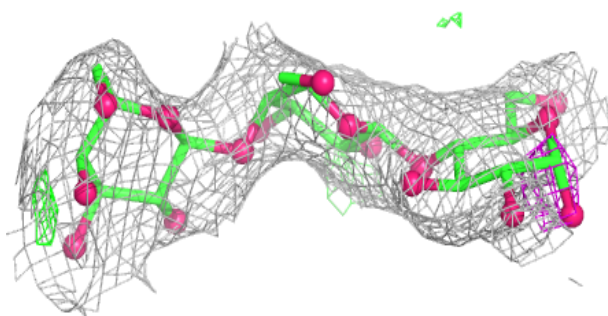
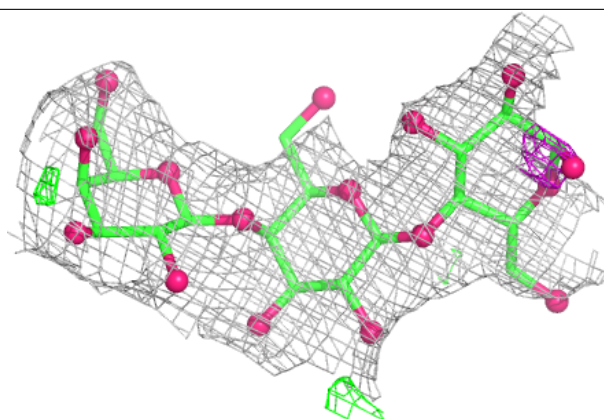
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	1	12/12	0.57	0.16	56,56,56,56	0
3	NAG	E	2	14/15	0.59	0.14	56,56,56,56	0
3	NAG	E	1	14/15	0.67	0.12	56,56,56,56	0
2	GLC	F	1	12/12	-	-	55,55,55,55	0
2	GAL	F	2	11/12	-	-	55,55,55,55	0
2	GAL	F	3	11/12	-	-	54,54,54,54	0
3	NAG	B	1	14/15	-	-	56,56,56,56	0
3	NAG	B	2	14/15	-	-	57,57,57,57	0
2	GAL	C	3	11/12	0.70	0.17	55,55,55,55	0
2	GAL	C	2	11/12	0.82	0.11	55,55,55,55	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.

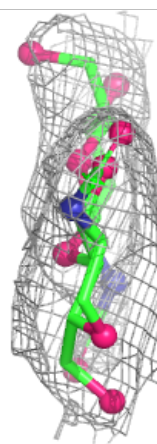
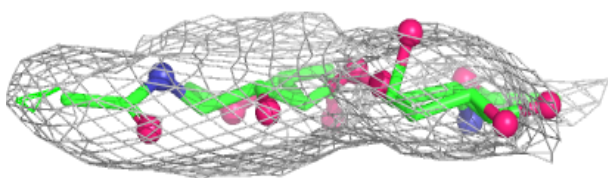
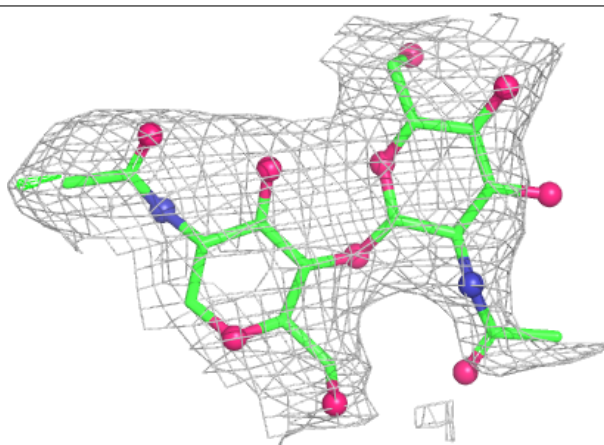


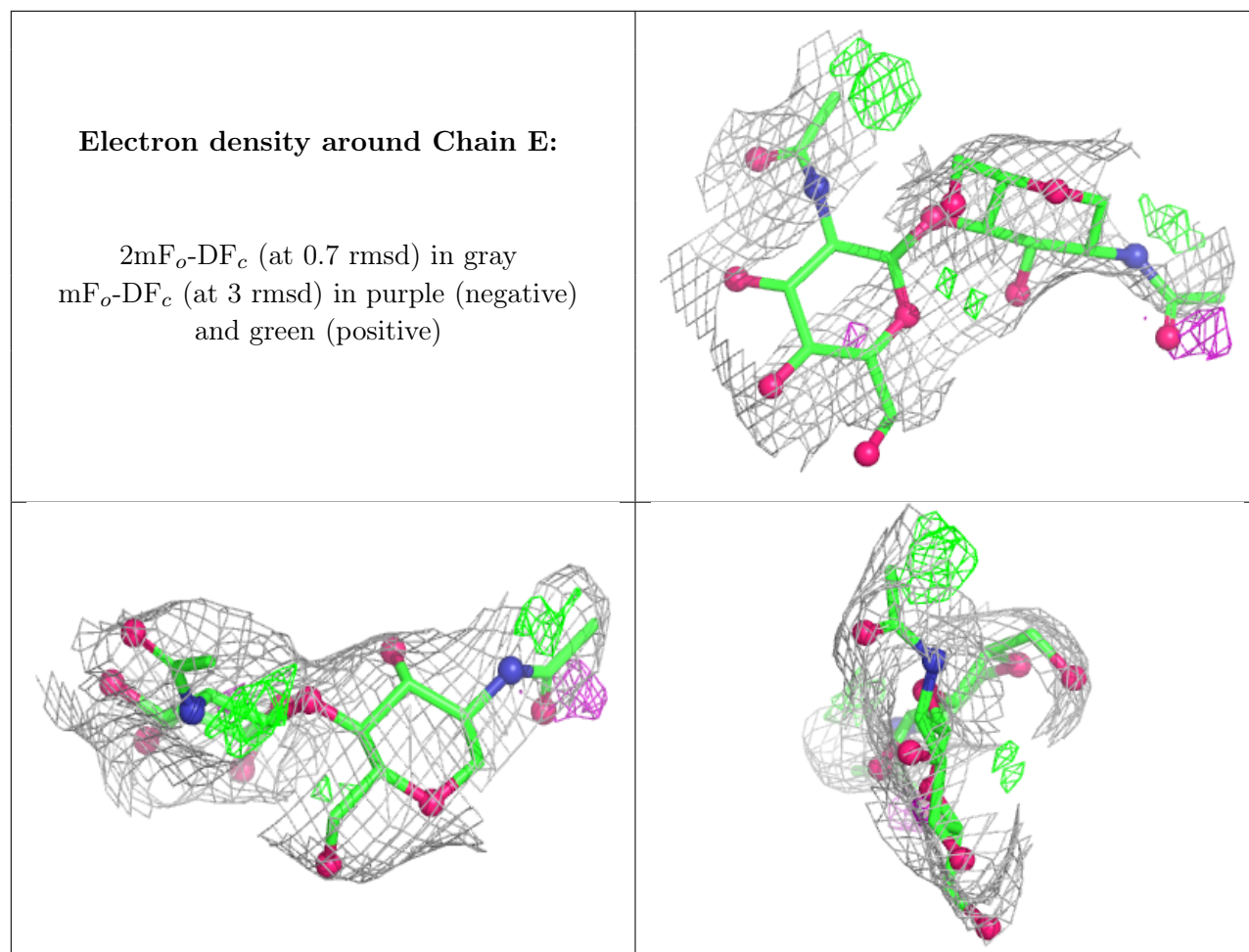
Electron density around Chain F:

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

**Electron density around Chain B:**

$2mF_o-DF_c$ (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	NAG	D	604	14/15	0.53	0.15	57,57,57,57	0
4	MAN	A	601	11/12	0.58	0.19	20,20,20,20	0
4	MAN	D	601	11/12	0.61	0.31	20,20,20,20	0
5	NAG	D	602	14/15	0.62	0.14	55,55,55,55	0
5	NAG	D	605	14/15	0.64	0.16	54,54,54,54	0
5	NAG	D	603	14/15	0.65	0.13	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.