



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:56 AM UTC

PDB ID : 7Q1Y / pdb_00007q1y
Title : X-ray structure of human A2ML1
Authors : Andersen, G.R.; Zarantonello, A.; Enghild, J.J.; Nielsen, N.S.
Deposited on : 2021-10-22
Resolution : 4.40 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

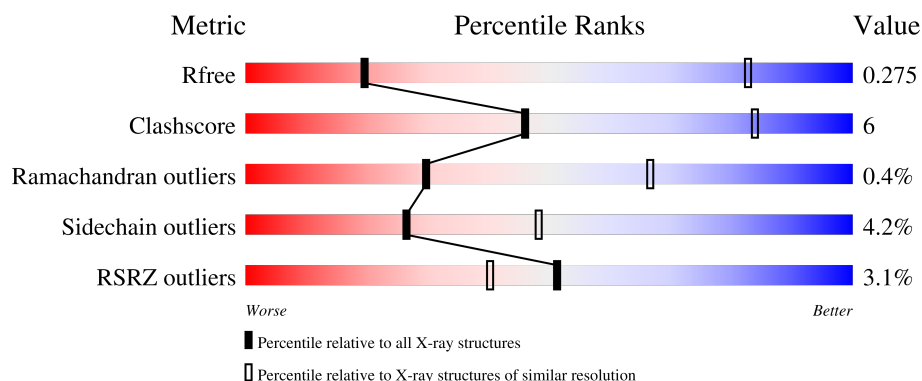
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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.



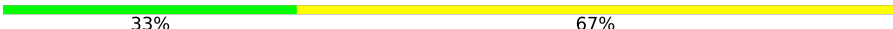
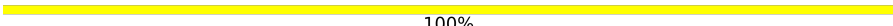
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	1436	 3% 77% 17% ..
1	B	1436	 3% 79% 15% ..
2	C	3	 100%
2	D	3	 67% 33%
2	E	3	 33% 33% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	 67% 33%
2	I	3	 33% 67%
3	G	2	 100%
3	H	2	 50% 50%

2 Entry composition [i](#)

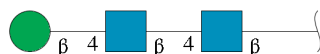
There are 4 unique types of molecules in this entry. The entry contains 21765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-2-macroglobulin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1374	Total	C	N	O	S	0	0	0
			10729	6858	1761	2058	52			
1	B	1374	Total	C	N	O	S	0	0	0
			10729	6858	1761	2058	52			

- 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.



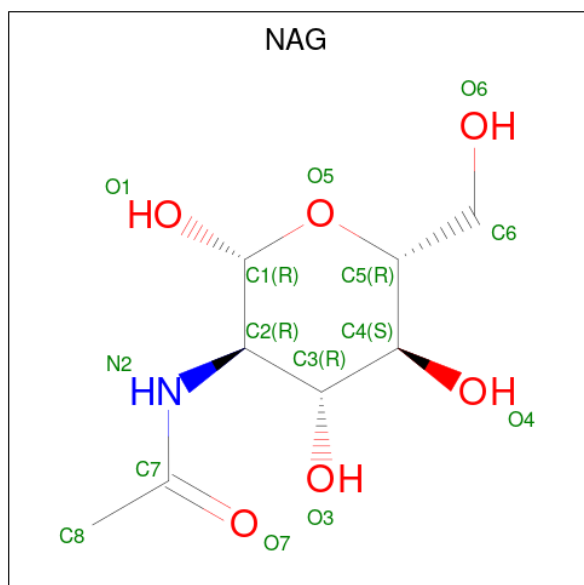
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

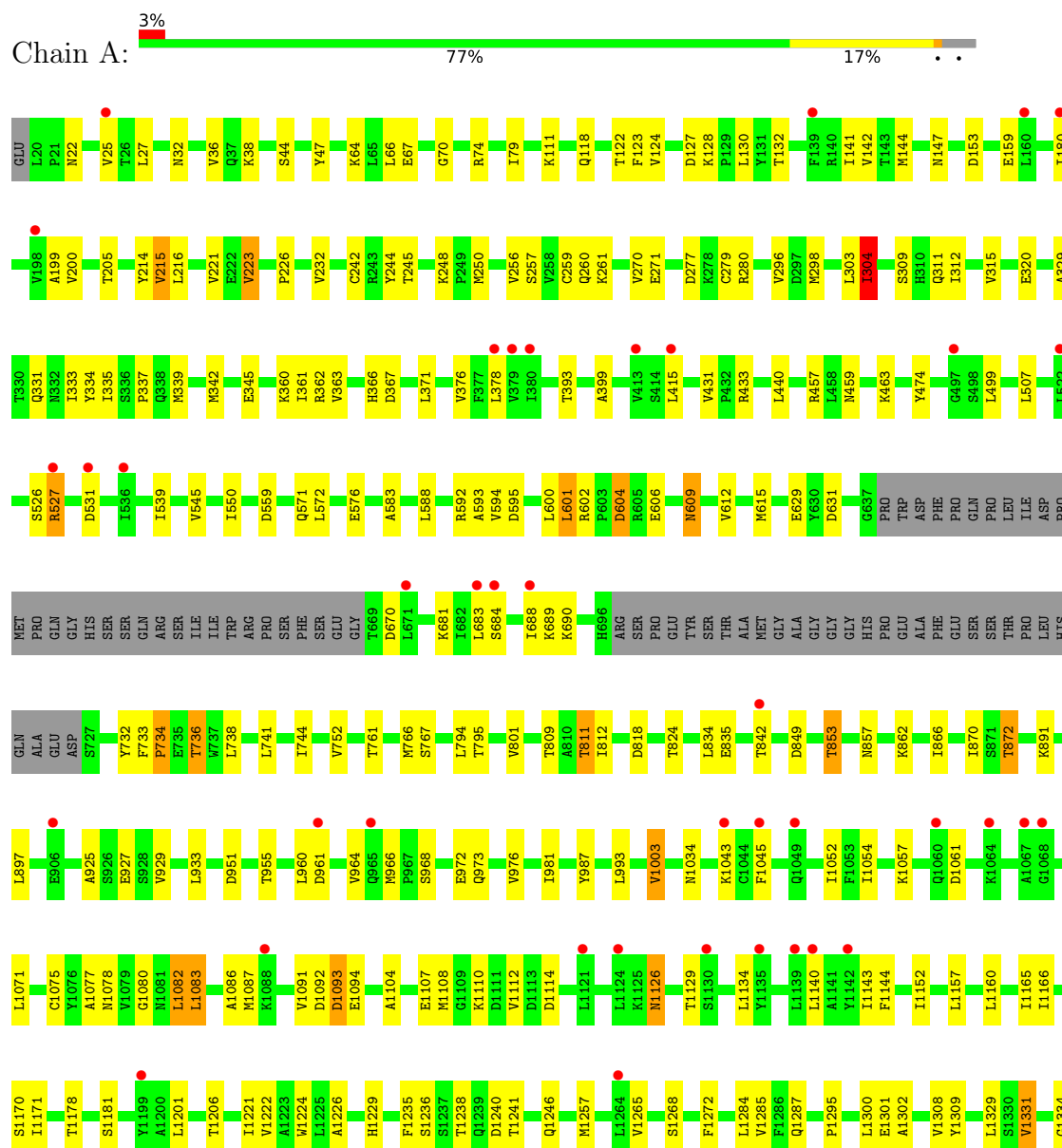


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

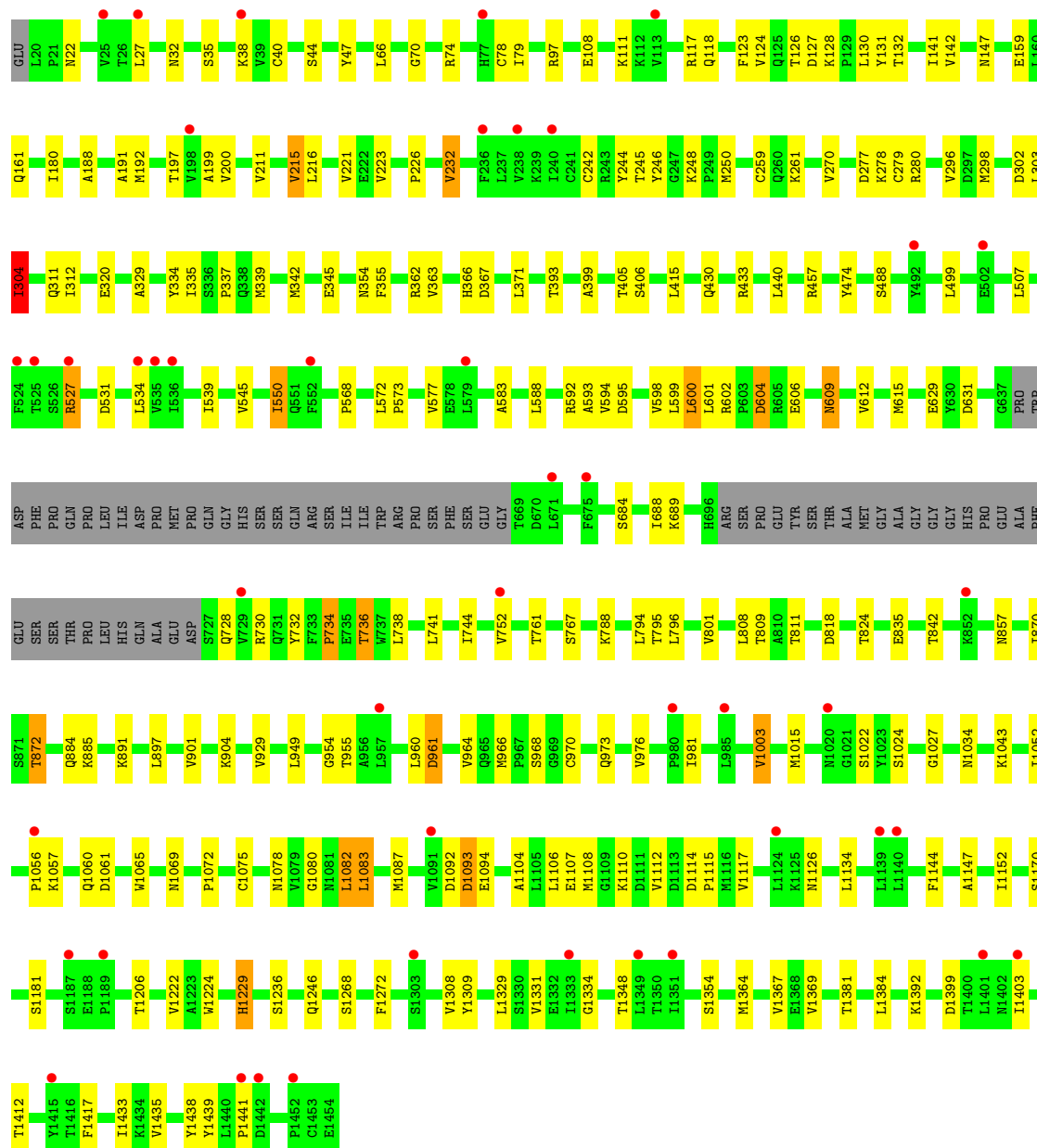
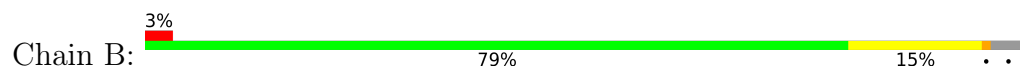
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-2-macroglobulin-like protein 1





- Molecule 1: Alpha-2-macroglobulin-like protein 1



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





- 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: 67% 33%



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

Chain E: 33% 33% 33%



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

Chain F: 67% 33%



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

Chain I: 33% 67%



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

Chain G: 100%



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

Chain H: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	320.15Å 320.15Å 321.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 – 4.40 49.37 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.37-4.40) 99.9 (49.37-4.40)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.238 , 0.276 0.238 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	294.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 370.5	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	0.90	EDS
Total number of atoms	21765	wwPDB-VP
Average B, all atoms (Å ²)	342.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	0.30	0/10975	0.50	2/14922 (0.0%)
1	B	0.29	0/10975	0.50	1/14922 (0.0%)
All	All	0.30	0/21950	0.50	3/29844 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	TYR	CA-C-N	5.78	132.37	121.97
1	A	214	TYR	C-N-CA	5.78	132.37	121.97
1	B	970	CYS	CA-CB-SG	-5.35	102.09	114.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	10729	0	10606	135	0
1	B	10729	0	10607	119	0
2	C	39	0	34	1	0
2	D	39	0	34	0	0
2	E	39	0	34	2	0
2	F	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	39	0	34	0	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
All	All	21765	0	21485	252	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 6.

All (252) 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:B:128:LYS:NZ	1:B:734:PRO:O	2.01	0.93
1:A:128:LYS:NZ	1:A:734:PRO:O	2.02	0.92
1:A:147:ASN:O	1:A:527:ARG:NH1	2.10	0.85
1:B:904:LYS:NZ	1:B:1399:ASP:OD2	2.12	0.83
1:A:360:LYS:NZ	1:A:459:ASN:OD1	2.11	0.83
1:A:670:ASP:OD2	1:A:690:LYS:N	2.14	0.79
1:B:631:ASP:OD1	1:B:689:LYS:NZ	2.18	0.74
1:B:572:LEU:HD11	1:B:891:LYS:HB3	1.67	0.74
1:B:1107:GLU:OE2	1:B:1246:GLN:NE2	2.21	0.73
1:A:612:VAL:HA	1:A:615:MET:HE3	1.71	0.72
1:B:612:VAL:HA	1:B:615:MET:HE3	1.74	0.70
1:A:244:TYR:OH	1:A:320:GLU:OE2	2.11	0.67
1:A:960:LEU:HD22	1:A:981:ILE:HG12	1.76	0.66
1:A:1107:GLU:OE2	1:A:1246:GLN:NE2	2.29	0.66
1:A:22:ASN:H	1:A:44:SER:HB2	1.62	0.65
1:B:960:LEU:HD22	1:B:981:ILE:HG12	1.79	0.64
1:A:951:ASP:OD2	1:A:987:TYR:OH	2.11	0.64
1:A:1086:ALA:HB3	1:A:1363:ASN:HD21	1.64	0.62
1:B:298:MET:HB3	1:B:303:LEU:HD11	1.81	0.62
1:B:1229:HIS:ND1	1:B:1309:TYR:OH	2.20	0.62
1:B:835:GLU:HB2	1:B:857:ASN:HB3	1.81	0.62
1:A:74:ARG:HH22	1:A:539:ILE:HB	1.64	0.62
1:A:794:LEU:HD21	1:A:870:ILE:HD12	1.81	0.62
1:A:609:ASN:OD1	1:A:609:ASN:N	2.33	0.62
1:A:1126:ASN:OD1	1:A:1126:ASN:N	2.32	0.62
1:B:1110:LYS:HD2	1:B:1114:ASP:OD2	2.00	0.61
1:B:124:VAL:HG22	1:B:141:ILE:HG12	1.82	0.61
1:B:808:LEU:HD21	1:B:870:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ASP:OD1	1:A:689:LYS:NZ	2.32	0.60
1:B:593:ALA:HB3	1:B:738:LEU:H	1.66	0.60
1:A:572:LEU:HD11	1:A:891:LYS:HB3	1.83	0.60
1:B:1170:SER:HB3	1:B:1224:TRP:HB2	1.84	0.59
1:A:527:ARG:NH2	1:A:559:ASP:OD1	2.36	0.59
1:A:972:GLU:HG2	1:A:1087:MET:HE1	1.84	0.59
1:A:367:ASP:OD1	1:A:367:ASP:N	2.36	0.59
1:A:972:GLU:HG3	1:A:1238:THR:HG21	1.85	0.59
1:B:1329:LEU:HD22	1:B:1435:VAL:HG12	1.85	0.58
1:B:794:LEU:HD21	1:B:870:ILE:HD12	1.85	0.58
1:A:122:THR:HB	1:A:205:THR:HG21	1.83	0.58
1:A:795:THR:HB	1:A:809:THR:HB	1.84	0.58
1:A:592:ARG:HE	1:A:594:VAL:HG21	1.69	0.58
1:B:602:ARG:HG2	1:B:604:ASP:HB2	1.86	0.57
1:B:1043:LYS:HB2	1:B:1104:ALA:HB1	1.86	0.57
1:A:127:ASP:HB2	1:A:736:THR:HG21	1.87	0.57
1:A:629:GLU:OE2	1:A:681:LYS:HD2	2.05	0.57
1:A:463:LYS:NZ	2:E:3:BMA:H61	2.19	0.57
1:A:36:VAL:HG11	1:B:1115:PRO:HB3	1.86	0.57
1:B:588:LEU:HD11	1:B:741:LEU:HB3	1.87	0.57
1:B:127:ASP:HB2	1:B:736:THR:HG21	1.87	0.56
1:B:795:THR:HB	1:B:809:THR:HB	1.87	0.56
1:B:38:LYS:HB2	1:B:499:LEU:HD23	1.86	0.56
1:B:609:ASN:N	1:B:609:ASN:OD1	2.37	0.56
1:A:259:CYS:HA	1:A:279:CYS:HA	1.87	0.56
1:B:32:ASN:HB3	1:B:118:GLN:HG3	1.88	0.56
1:B:337:PRO:HB2	1:B:433:ARG:HA	1.87	0.56
1:B:1236:SER:HB2	1:B:1441:PRO:HG2	1.87	0.55
1:B:311:GLN:HG2	1:B:334:TYR:HA	1.88	0.55
1:A:363:VAL:HG21	1:A:376:VAL:HG11	1.87	0.55
1:B:22:ASN:H	1:B:44:SER:HB2	1.69	0.55
1:A:32:ASN:HB3	1:A:118:GLN:HG3	1.89	0.55
1:B:131:TYR:HB2	1:B:211:VAL:HG22	1.89	0.55
1:A:124:VAL:HG22	1:A:141:ILE:HG12	1.87	0.55
1:B:527:ARG:HA	1:B:527:ARG:HH11	1.71	0.54
1:A:1034:ASN:ND2	1:A:1080:GLY:O	2.40	0.54
1:B:964:VAL:HG12	1:B:966:MET:HG3	1.90	0.54
1:A:526:SER:HB2	1:A:527:ARG:HH21	1.73	0.54
1:A:1071:LEU:HD21	1:A:1077:ALA:HB2	1.90	0.54
1:B:312:ILE:HG13	1:B:335:ILE:HD11	1.90	0.54
1:A:123:PHE:CE1	1:A:142:VAL:HB	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG22	1:A:180:ILE:HA	1.90	0.53
1:B:961:ASP:OD1	1:B:961:ASP:N	2.34	0.53
1:A:1043:LYS:HB2	1:A:1104:ALA:HB1	1.90	0.53
1:A:1083:LEU:HD12	1:A:1087:MET:HG2	1.89	0.53
1:A:1057:LYS:HG2	1:A:1061:ASP:OD2	2.09	0.53
1:A:1268:SER:HB3	1:A:1272:PHE:HB3	1.89	0.53
1:A:1329:LEU:HD22	1:A:1435:VAL:HG12	1.91	0.53
1:B:592:ARG:HH12	1:B:606:GLU:HG3	1.73	0.53
1:B:1369:VAL:HG13	1:B:1433:ILE:HG12	1.90	0.53
1:A:280:ARG:HD3	1:A:296:VAL:HG13	1.92	0.52
1:B:74:ARG:HD3	1:B:488:SER:HB2	1.90	0.52
1:A:153:ASP:OD2	2:C:1:NAG:O6	2.09	0.52
1:B:188:ALA:HB3	1:B:191:ALA:HB2	1.90	0.52
1:A:248:LYS:HZ2	1:A:849:ASP:HA	1.74	0.52
1:B:159:GLU:HG2	1:B:199:ALA:HB3	1.91	0.52
1:A:794:LEU:HG	1:A:897:LEU:HD23	1.91	0.52
1:A:1110:LYS:HD2	1:A:1114:ASP:OD2	2.10	0.51
1:B:1078:ASN:HD22	1:B:1082:LEU:HD23	1.75	0.51
1:A:1229:HIS:ND1	1:A:1309:TYR:OH	2.35	0.51
1:A:463:LYS:HZ3	2:E:3:BMA:H61	1.75	0.51
1:A:1045:PHE:HB3	1:A:1054:ILE:HG21	1.93	0.51
1:A:1082:LEU:HD11	1:A:1091:VAL:HG23	1.92	0.51
1:B:123:PHE:CE1	1:B:142:VAL:HB	2.46	0.51
1:A:393:THR:HG22	1:A:399:ALA:HB2	1.92	0.51
1:A:684:SER:HB3	1:A:688:ILE:HD13	1.93	0.51
1:A:1166:ILE:HG12	1:A:1171:ILE:HG12	1.91	0.51
1:A:527:ARG:HG2	1:B:1072:PRO:HG3	1.92	0.51
1:B:147:ASN:O	1:B:527:ARG:NH2	2.38	0.50
1:A:248:LYS:NZ	1:A:849:ASP:HA	2.26	0.50
1:A:337:PRO:HB2	1:A:433:ARG:HA	1.94	0.50
1:A:824:THR:HG23	1:A:872:THR:HB	1.92	0.50
1:B:1367:VAL:HB	1:B:1403:ILE:HB	1.92	0.50
1:A:595:ASP:OD2	1:A:761:THR:HG21	2.12	0.50
1:B:393:THR:HG22	1:B:399:ALA:HB2	1.94	0.50
1:B:1106:LEU:HD21	1:B:1117:VAL:HG11	1.94	0.50
1:A:1363:ASN:HD22	1:A:1439:TYR:HB2	1.76	0.49
1:B:732:TYR:HD1	1:B:734:PRO:HD3	1.77	0.49
1:B:592:ARG:HE	1:B:594:VAL:HG21	1.77	0.49
1:A:223:VAL:HG21	1:A:331:GLN:HB2	1.94	0.49
1:A:732:TYR:HD1	1:A:734:PRO:HD3	1.76	0.49
1:A:811:THR:HG23	1:A:853:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TYR:HB2	1:B:70:GLY:HA3	1.95	0.49
1:B:531:ASP:OD1	1:B:531:ASP:N	2.46	0.49
1:B:1334:GLY:HA3	1:B:1348:THR:HB	1.95	0.49
1:A:1365:ALA:HB3	1:A:1405:LEU:HB2	1.94	0.48
1:A:221:VAL:HB	1:A:329:ALA:HB2	1.94	0.48
1:A:602:ARG:HG2	1:A:604:ASP:HB2	1.94	0.48
1:A:1226:ALA:HB1	1:A:1309:TYR:HE1	1.78	0.48
1:A:345:GLU:OE2	1:A:362:ARG:HD2	2.13	0.48
1:A:1354:SER:HB3	1:A:1412:THR:HA	1.94	0.48
1:A:361:ILE:HD11	1:A:378:LEU:HD13	1.95	0.48
1:A:1157:LEU:HD23	1:A:1160:LEU:HD12	1.96	0.48
1:A:159:GLU:HG2	1:A:199:ALA:HB3	1.95	0.48
1:A:539:ILE:HG12	1:A:545:VAL:HG12	1.95	0.48
1:B:527:ARG:HA	1:B:527:ARG:HD3	1.48	0.48
1:A:123:PHE:HE1	1:A:142:VAL:HB	1.78	0.48
1:A:583:ALA:HB3	1:A:744:ILE:HG13	1.96	0.48
1:A:588:LEU:HD11	1:A:741:LEU:HB3	1.96	0.48
1:A:1331:VAL:HG12	1:A:1447:ILE:HD13	1.94	0.48
1:B:824:THR:HG23	1:B:872:THR:HB	1.94	0.48
1:A:593:ALA:HB3	1:A:738:LEU:H	1.79	0.47
1:B:244:TYR:OH	1:B:320:GLU:OE2	2.23	0.47
1:A:339:MET:HA	1:A:366:HIS:HB3	1.96	0.47
1:B:1369:VAL:HG22	1:B:1433:ILE:HG23	1.95	0.47
1:A:1257:MET:HE3	1:A:1257:MET:HB2	1.83	0.47
1:A:1285:VAL:HG12	1:A:1287:GLN:HG3	1.95	0.47
1:B:1381:THR:HA	1:B:1384:LEU:HD12	1.97	0.47
1:A:64:LYS:HD3	1:A:67:GLU:OE2	2.15	0.47
1:A:993:LEU:HD13	1:A:1284:LEU:HD21	1.96	0.47
1:B:1034:ASN:ND2	1:B:1080:GLY:O	2.48	0.47
1:B:1354:SER:HB3	1:B:1412:THR:HA	1.97	0.47
1:A:531:ASP:N	1:A:531:ASP:OD1	2.45	0.46
1:A:1003:VAL:HG13	1:A:1052:ILE:HG22	1.96	0.46
1:B:884:GLN:HG2	1:B:885:LYS:H	1.80	0.46
1:B:74:ARG:HH22	1:B:539:ILE:HB	1.81	0.46
1:B:66:LEU:HD12	1:B:79:ILE:HG12	1.96	0.46
1:B:1022:SER:HB3	1:B:1065:TRP:CD2	2.51	0.46
1:B:354:ASN:HA	1:B:406:SER:HA	1.97	0.46
1:A:226:PRO:HB3	1:A:333:ILE:HD11	1.98	0.46
1:A:298:MET:HB3	1:A:303:LEU:HD11	1.98	0.46
1:B:684:SER:HB3	1:B:688:ILE:HD13	1.96	0.46
1:A:1235:PHE:HD2	1:A:1241:THR:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:MET:HE3	1:B:1015:MET:HG2	1.98	0.46
1:B:1087:MET:HB2	1:B:1439:TYR:CD2	2.51	0.46
1:A:1265:VAL:HB	1:A:1301:GLU:HB2	1.97	0.46
1:A:1140:LEU:HA	1:A:1143:ILE:HD12	1.97	0.46
1:A:38:LYS:HB2	1:A:499:LEU:HD23	1.96	0.45
1:A:111:LYS:HD2	1:A:629:GLU:OE2	2.16	0.45
1:B:600:LEU:HD22	1:B:730:ARG:HH11	1.81	0.45
1:B:1024:SER:OG	1:B:1027:GLY:N	2.49	0.45
1:B:1093:ASP:HB2	1:B:1094:GLU:H	1.63	0.45
1:A:66:LEU:HD12	1:A:79:ILE:HG12	1.98	0.45
1:A:670:ASP:OD1	1:A:670:ASP:N	2.49	0.45
1:A:933:LEU:HD11	1:A:1295:PRO:HG2	1.98	0.45
1:B:949:LEU:HD22	1:B:954:GLY:HA3	1.98	0.45
1:A:261:LYS:HG2	1:A:277:ASP:OD2	2.17	0.45
1:B:1003:VAL:HG13	1:B:1052:ILE:HG22	1.99	0.45
1:B:345:GLU:OE2	1:B:362:ARG:HD2	2.16	0.45
1:B:1083:LEU:HD13	1:B:1083:LEU:HA	1.85	0.45
1:B:583:ALA:HB3	1:B:744:ILE:HG13	1.98	0.45
1:B:592:ARG:NH2	1:B:599:LEU:HD21	2.32	0.45
1:A:927:GLU:HB3	1:A:1300:LEU:HD12	1.98	0.45
1:B:304:ILE:HG23	1:B:430:GLN:HA	1.98	0.45
1:B:1057:LYS:HE2	1:B:1061:ASP:OD2	2.16	0.45
1:A:925:ALA:HB3	1:A:1302:ALA:HB3	1.99	0.45
1:B:796:LEU:HD22	1:B:901:VAL:HG21	1.99	0.45
1:B:1065:TRP:O	1:B:1069:ASN:ND2	2.49	0.45
1:A:1078:ASN:HD22	1:A:1082:LEU:HD23	1.82	0.44
1:A:1140:LEU:HD22	1:A:1144:PHE:HE2	1.82	0.44
1:B:232:VAL:HG22	1:B:433:ARG:HD3	1.98	0.44
1:B:573:PRO:HD2	1:B:788:LYS:HB2	2.00	0.44
1:B:794:LEU:HG	1:B:897:LEU:HD23	1.98	0.44
1:A:1236:SER:OG	1:A:1240:ASP:OD2	2.27	0.44
1:B:534:LEU:HB3	1:B:550:ILE:HG23	1.99	0.44
1:B:246:TYR:HE1	1:B:248:LYS:HB2	1.83	0.44
1:B:474:TYR:CZ	1:B:507:LEU:HD13	2.52	0.44
1:A:527:ARG:HD3	1:A:527:ARG:HA	1.74	0.44
1:B:355:PHE:O	1:B:405:THR:OG1	2.34	0.44
1:B:221:VAL:HB	1:B:329:ALA:HB2	1.99	0.44
1:A:571:GLN:NE2	1:A:576:GLU:O	2.51	0.43
1:B:259:CYS:HA	1:B:279:CYS:HA	1.99	0.43
1:B:1268:SER:HB3	1:B:1272:PHE:HB3	1.99	0.43
1:A:47:TYR:HB2	1:A:70:GLY:HA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:MET:HE1	1:A:1419:ILE:HG21	2.00	0.43
1:A:1385:LEU:HB2	1:A:1394:VAL:HG21	2.01	0.43
1:A:311:GLN:HG2	1:A:334:TYR:HA	2.01	0.43
1:B:278:LYS:NZ	1:B:302:ASP:HB2	2.33	0.43
1:B:161:GLN:HB2	1:B:197:THR:HB	2.01	0.43
1:B:342:MET:HE2	1:B:363:VAL:HG22	1.99	0.43
1:B:794:LEU:HD22	1:B:808:LEU:HD11	1.99	0.43
1:A:1370:LYS:HA	1:A:1400:THR:HG22	2.00	0.43
1:B:1056:PRO:O	1:B:1060:GLN:HG2	2.19	0.43
1:B:111:LYS:HZ2	1:B:629:GLU:CD	2.27	0.42
1:A:257:SER:HB3	1:A:315:VAL:HB	2.02	0.42
1:B:126:THR:OG1	1:B:128:LYS:O	2.26	0.42
1:B:339:MET:HA	1:B:366:HIS:HB3	2.01	0.42
1:A:474:TYR:CZ	1:A:507:LEU:HD13	2.54	0.42
1:A:964:VAL:HG12	1:A:966:MET:HG3	2.01	0.42
1:A:1170:SER:HB3	1:A:1224:TRP:HB2	2.00	0.42
1:B:280:ARG:HD3	1:B:296:VAL:HG13	2.00	0.42
1:B:1083:LEU:HG	1:B:1087:MET:HE2	2.02	0.42
1:A:312:ILE:HG13	1:A:335:ILE:HD11	2.01	0.42
1:A:601:LEU:HD12	1:A:733:PHE:HE1	1.84	0.42
1:A:862:LYS:HB3	1:A:866:ILE:HD11	2.01	0.42
1:B:128:LYS:HB3	1:B:598:VAL:HG11	2.01	0.42
1:A:415:LEU:HD12	1:A:440:LEU:HD23	2.02	0.42
1:B:117:ARG:HH11	3:G:1:NAG:H3	1.85	0.42
1:B:261:LYS:HG2	1:B:277:ASP:OD2	2.19	0.42
1:B:1364:MET:HE2	1:B:1364:MET:HB3	1.88	0.42
1:B:367:ASP:OD1	1:B:367:ASP:N	2.47	0.41
1:B:415:LEU:HD12	1:B:440:LEU:HD23	2.02	0.41
1:B:1144:PHE:HA	1:B:1147:ALA:HB3	2.02	0.41
1:A:342:MET:HE2	1:A:363:VAL:HG22	2.01	0.41
1:A:361:ILE:HB	1:A:399:ALA:HB3	2.03	0.41
1:A:1165:ILE:HD13	1:A:1178:THR:HG23	2.03	0.41
1:B:539:ILE:HG12	1:B:545:VAL:HG12	2.03	0.41
1:A:270:VAL:HG12	1:A:271:GLU:HG3	2.02	0.41
1:A:363:VAL:HG12	1:A:371:LEU:HD12	2.03	0.41
1:A:1334:GLY:N	1:A:1348:THR:O	2.41	0.41
1:B:568:PRO:HD2	1:B:577:VAL:HG23	2.01	0.41
1:B:964:VAL:HG11	1:B:966:MET:HE2	2.03	0.41
1:A:1093:ASP:HB2	1:A:1094:GLU:H	1.65	0.41
1:A:1236:SER:HB2	1:A:1441:PRO:HG2	2.01	0.41
1:B:527:ARG:HH11	1:B:527:ARG:CA	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:ASP:N	1:A:1399:ASP:OD1	2.54	0.41
1:B:595:ASP:OD2	1:B:761:THR:HG21	2.20	0.41
1:A:74:ARG:HH12	1:A:539:ILE:HB	1.86	0.41
1:B:363:VAL:HG12	1:B:371:LEU:HD12	2.01	0.41
1:A:260:GLN:NE2	1:A:309:SER:O	2.45	0.41
1:A:1126:ASN:O	1:A:1129:THR:OG1	2.27	0.41
1:A:304:ILE:HG13	1:A:431:VAL:H	1.86	0.40
1:A:604:ASP:N	1:A:606:GLU:OE1	2.53	0.40
1:A:834:LEU:HA	1:A:834:LEU:HD23	1.89	0.40
1:B:1381:THR:HG23	1:B:1417:PHE:HB2	2.03	0.40
1:A:144:MET:HE2	1:A:144:MET:HB3	1.90	0.40
1:B:40:CYS:HA	1:B:78:CYS:HA	2.03	0.40
1:B:97:ARG:NH2	1:B:108:GLU:OE2	2.34	0.40
1:A:25:VAL:HB	1:A:683:LEU:HB2	2.04	0.40
1:A:835:GLU:HB2	1:A:857:ASN:HB3	2.03	0.40
1:A:1201:LEU:HB2	1:A:1221:ILE:HG21	2.03	0.40
1:B:142:VAL:HG22	1:B:180:ILE:HA	2.02	0.40
1:B:966:MET:HE3	1:B:1438:TYR:CZ	2.57	0.40
1:B:1392:LYS:HD3	1:B:1392:LYS:HA	1.95	0.40

There are no symmetry-related clashes.

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	1368/1436 (95%)	1304 (95%)	58 (4%)	6 (0%)	30	66
1	B	1368/1436 (95%)	1304 (95%)	58 (4%)	6 (0%)	30	66
All	All	2736/2872 (95%)	2608 (95%)	116 (4%)	12 (0%)	30	66

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	VAL
1	A	1181	SER
1	B	215	VAL
1	B	1092	ASP
1	B	1181	SER
1	A	1092	ASP
1	A	604	ASP
1	B	604	ASP
1	A	734	PRO
1	B	734	PRO
1	A	304	ILE
1	B	304	ILE

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	1201/1253 (96%)	1151 (96%)	50 (4%)	26	48
1	B	1201/1253 (96%)	1150 (96%)	51 (4%)	26	48
All	All	2402/2506 (96%)	2301 (96%)	101 (4%)	26	48

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	130	LEU
1	A	132	THR
1	A	200	VAL
1	A	215	VAL
1	A	216	LEU
1	A	223	VAL
1	A	232	VAL
1	A	242	CYS
1	A	245	THR
1	A	250	MET
1	A	256	VAL

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Mol	Chain	Res	Type
1	A	304	ILE
1	A	457	ARG
1	A	527	ARG
1	A	550	ILE
1	A	600	LEU
1	A	601	LEU
1	A	609	ASN
1	A	736	THR
1	A	752	VAL
1	A	766	MET
1	A	767	SER
1	A	801	VAL
1	A	811	THR
1	A	812	ILE
1	A	818	ASP
1	A	842	THR
1	A	853	THR
1	A	872	THR
1	A	929	VAL
1	A	955	THR
1	A	961	ASP
1	A	968	SER
1	A	973	GLN
1	A	976	VAL
1	A	1003	VAL
1	A	1075	CYS
1	A	1082	LEU
1	A	1083	LEU
1	A	1093	ASP
1	A	1108	MET
1	A	1112	VAL
1	A	1126	ASN
1	A	1134	LEU
1	A	1152	ILE
1	A	1206	THR
1	A	1222	VAL
1	A	1308	VAL
1	A	1331	VAL
1	B	27	LEU
1	B	35	SER
1	B	130	LEU
1	B	132	THR

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Mol	Chain	Res	Type
1	B	200	VAL
1	B	215	VAL
1	B	216	LEU
1	B	223	VAL
1	B	226	PRO
1	B	232	VAL
1	B	242	CYS
1	B	245	THR
1	B	250	MET
1	B	270	VAL
1	B	304	ILE
1	B	457	ARG
1	B	527	ARG
1	B	550	ILE
1	B	600	LEU
1	B	601	LEU
1	B	609	ASN
1	B	728	GLN
1	B	736	THR
1	B	752	VAL
1	B	767	SER
1	B	801	VAL
1	B	811	THR
1	B	818	ASP
1	B	842	THR
1	B	872	THR
1	B	929	VAL
1	B	955	THR
1	B	961	ASP
1	B	968	SER
1	B	973	GLN
1	B	976	VAL
1	B	1003	VAL
1	B	1075	CYS
1	B	1082	LEU
1	B	1083	LEU
1	B	1093	ASP
1	B	1108	MET
1	B	1112	VAL
1	B	1126	ASN
1	B	1134	LEU
1	B	1152	ILE

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Mol	Chain	Res	Type
1	B	1206	THR
1	B	1222	VAL
1	B	1229	HIS
1	B	1308	VAL
1	B	1331	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	186	GLN
1	A	855	HIS
1	A	1317	ASN
1	A	1402	ASN
1	B	22	ASN
1	B	135	GLN
1	B	152	ASN
1	B	166	ASN
1	B	170	GLN
1	B	178	GLN
1	B	441	HIS
1	B	504	GLN
1	B	772	GLN
1	B	855	HIS
1	B	865	HIS
1	B	878	ASN
1	B	1011	GLN
1	B	1049	GLN
1	B	1137	GLN
1	B	1163	GLN
1	B	1175	GLN
1	B	1228	GLN
1	B	1317	ASN
1	B	1388	GLN
1	B	1402	ASN
1	B	1421	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 ⓘ

19 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	C	1	1,2	14,14,15	0.51	0	17,19,21	0.49	0
2	NAG	C	2	2	14,14,15	0.80	1 (7%)	17,19,21	0.69	0
2	BMA	C	3	2	11,11,12	1.70	4 (36%)	15,15,17	0.90	0
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	0.63	0
2	NAG	D	2	2	14,14,15	0.69	0	17,19,21	0.53	0
2	BMA	D	3	2	11,11,12	1.56	3 (27%)	15,15,17	0.95	0
2	NAG	E	1	1,2	14,14,15	0.55	0	17,19,21	0.74	0
2	NAG	E	2	2	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
2	BMA	E	3	2	11,11,12	1.02	1 (9%)	15,15,17	1.06	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.44	0	17,19,21	0.71	0
2	NAG	F	2	2	14,14,15	0.57	0	17,19,21	0.58	0
2	BMA	F	3	2	11,11,12	1.78	4 (36%)	15,15,17	1.00	0
3	NAG	G	1	1,3	14,14,15	0.31	0	17,19,21	0.45	0
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	0.67	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	0.71	0
3	NAG	H	2	3	14,14,15	0.89	2 (14%)	17,19,21	0.58	0
2	NAG	I	1	1,2	14,14,15	0.31	0	17,19,21	0.54	0
2	NAG	I	2	2	14,14,15	0.84	1 (7%)	17,19,21	0.65	0
2	BMA	I	3	2	11,11,12	1.26	2 (18%)	15,15,17	0.79	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	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	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	C1-C2	3.13	1.59	1.52
2	C	3	BMA	C1-C2	3.00	1.59	1.52
2	F	3	BMA	C1-C2	2.92	1.59	1.52
2	F	3	BMA	C4-C3	2.88	1.59	1.52
2	I	2	NAG	C1-C2	2.57	1.55	1.52
3	H	2	NAG	O5-C1	2.48	1.47	1.43
2	C	3	BMA	C2-C3	2.44	1.56	1.52
2	F	3	BMA	O5-C1	2.33	1.47	1.43
2	I	3	BMA	O5-C5	2.30	1.47	1.43
2	C	3	BMA	C4-C3	2.29	1.58	1.52
2	I	3	BMA	C1-C2	2.17	1.57	1.52
2	D	3	BMA	O5-C5	2.12	1.47	1.43
2	E	3	BMA	O5-C5	2.10	1.47	1.43
2	D	3	BMA	C4-C5	2.09	1.57	1.53
2	F	3	BMA	C2-C3	2.08	1.55	1.52
2	C	2	NAG	O5-C1	2.08	1.47	1.43
2	C	3	BMA	C4-C5	2.05	1.57	1.53
3	H	2	NAG	C1-C2	2.04	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C1-O5-C5	3.21	116.48	112.19
2	E	2	NAG	C2-N2-C7	2.88	126.76	122.90
2	E	2	NAG	C3-C4-C5	2.84	115.37	110.23
3	G	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

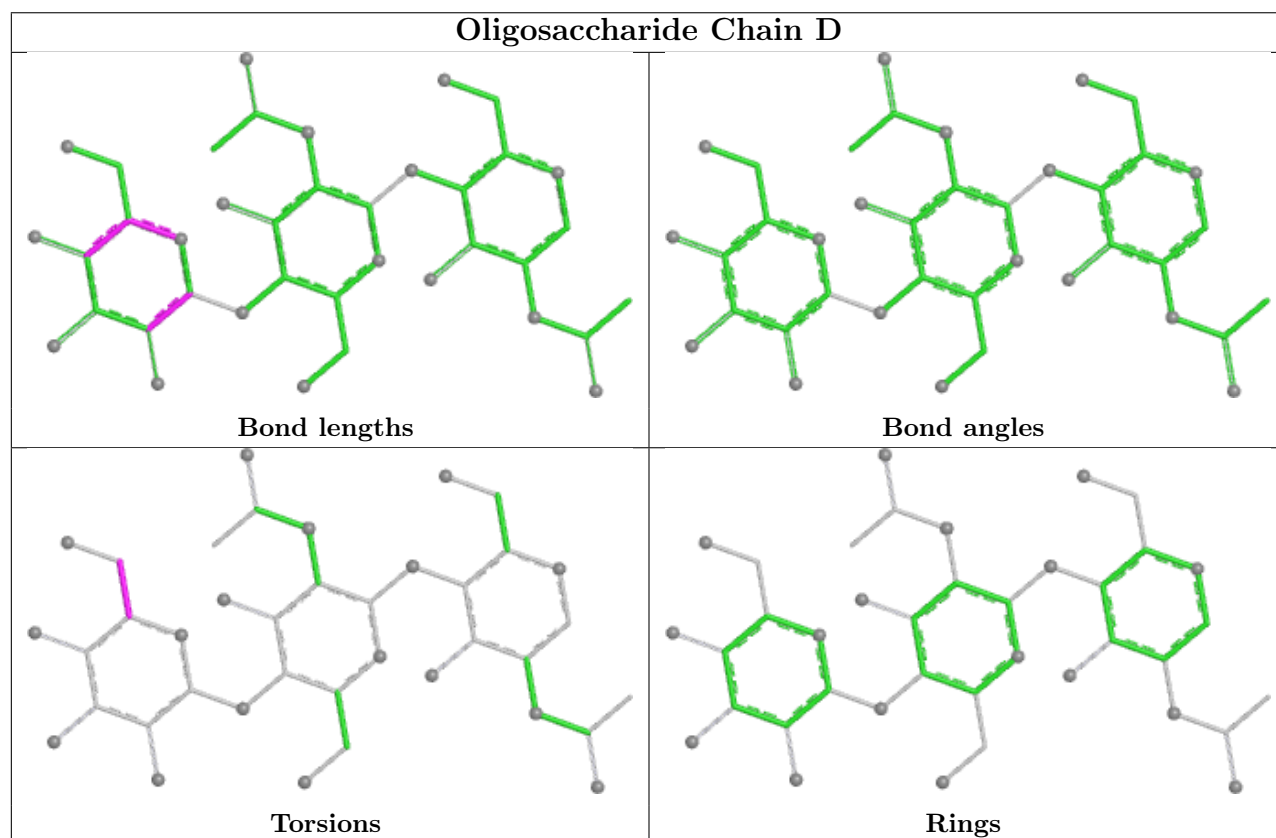
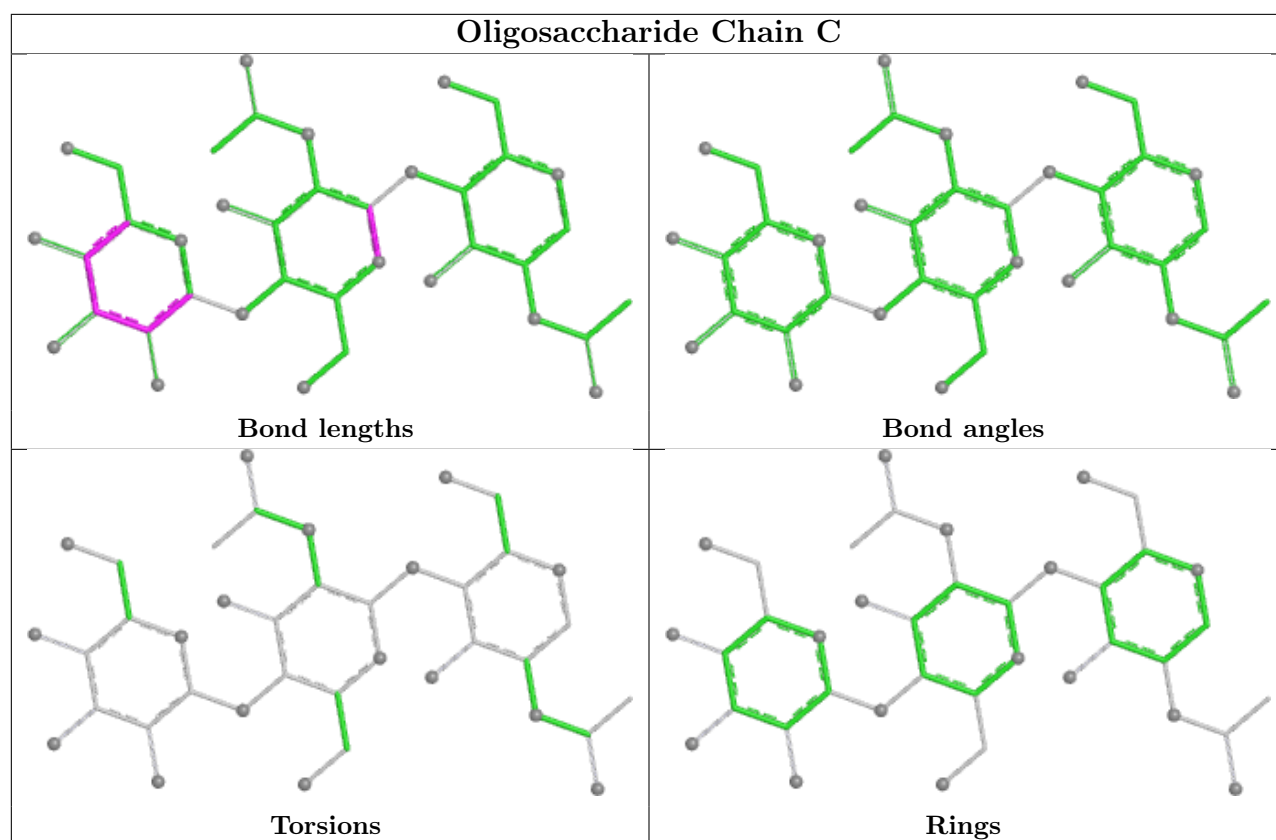
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
3	H	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	F	1	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6

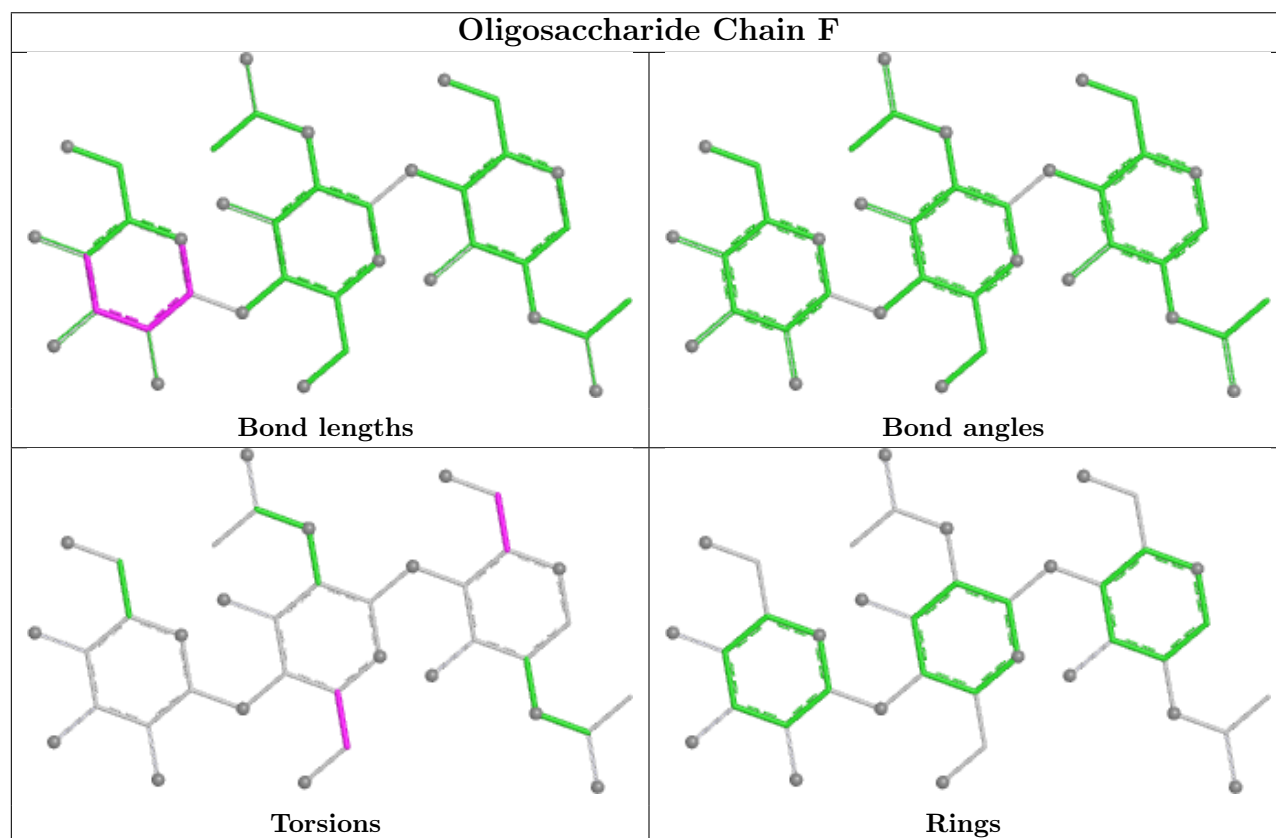
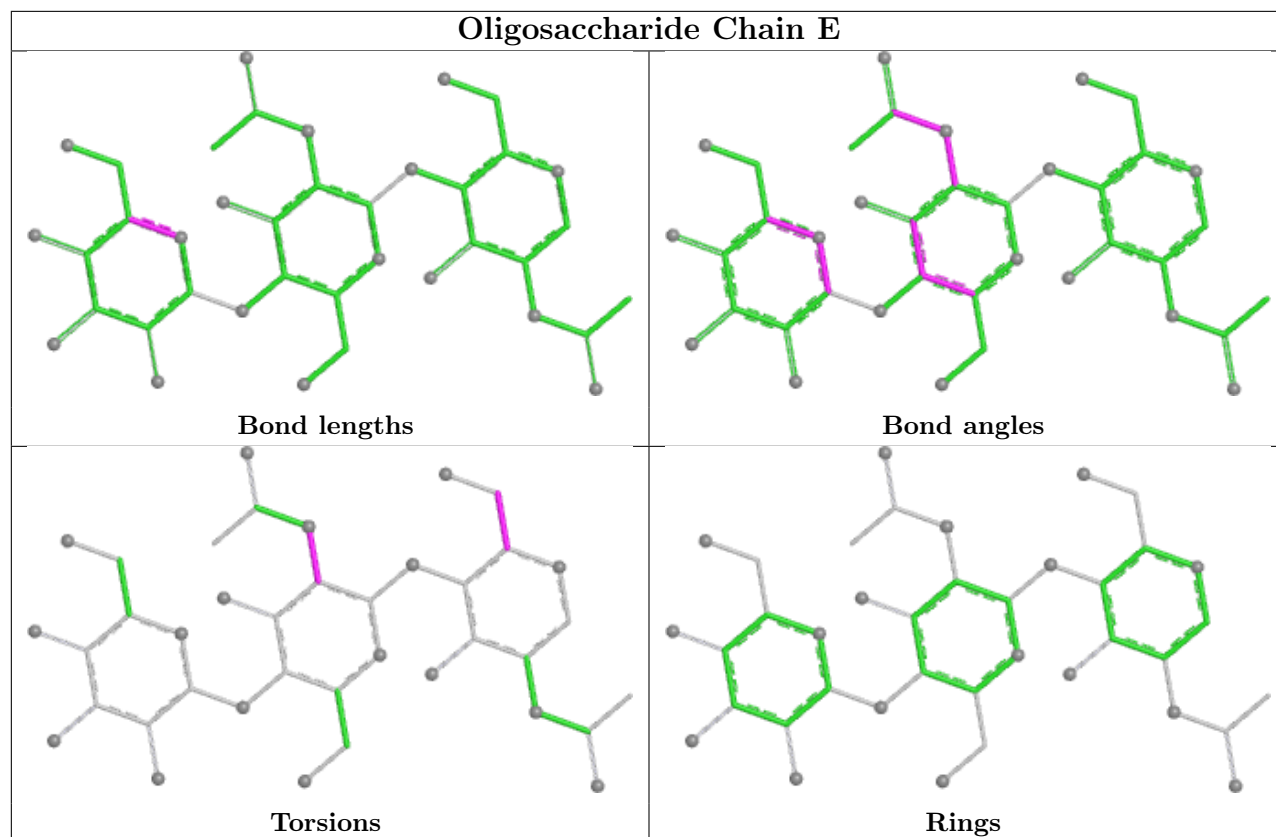
There are no ring outliers.

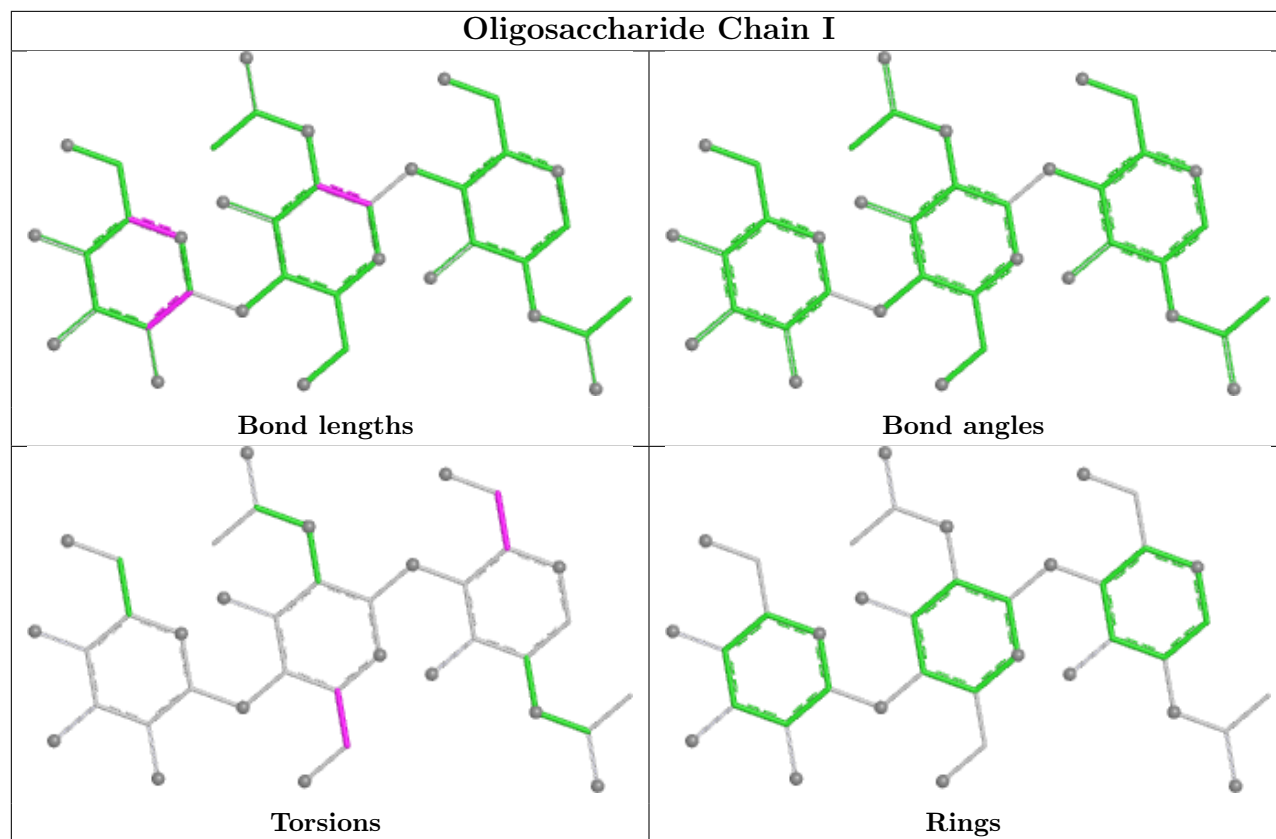
3 monomers are involved in 4 short contacts:

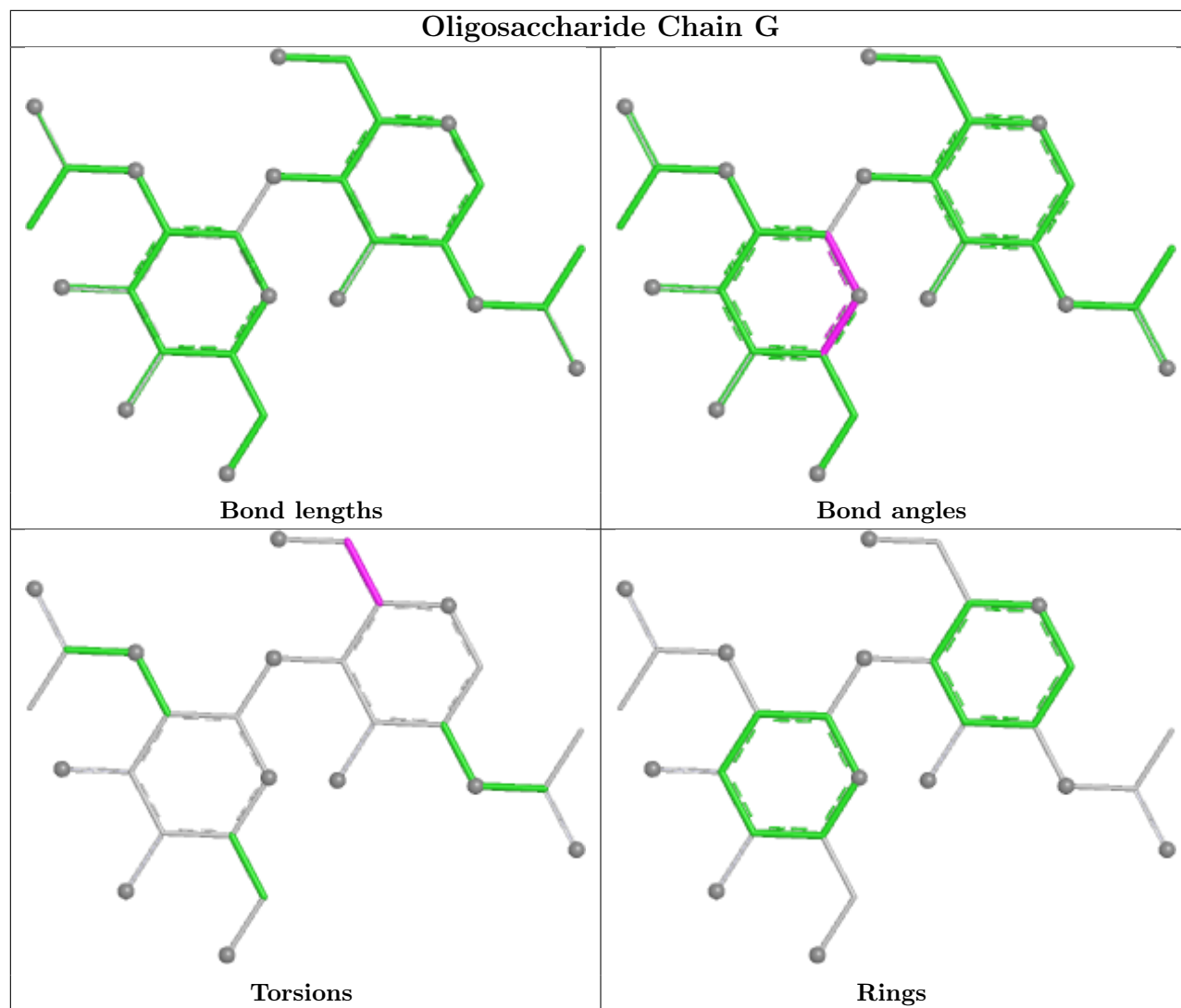
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
2	C	1	NAG	1	0
2	E	3	BMA	2	0

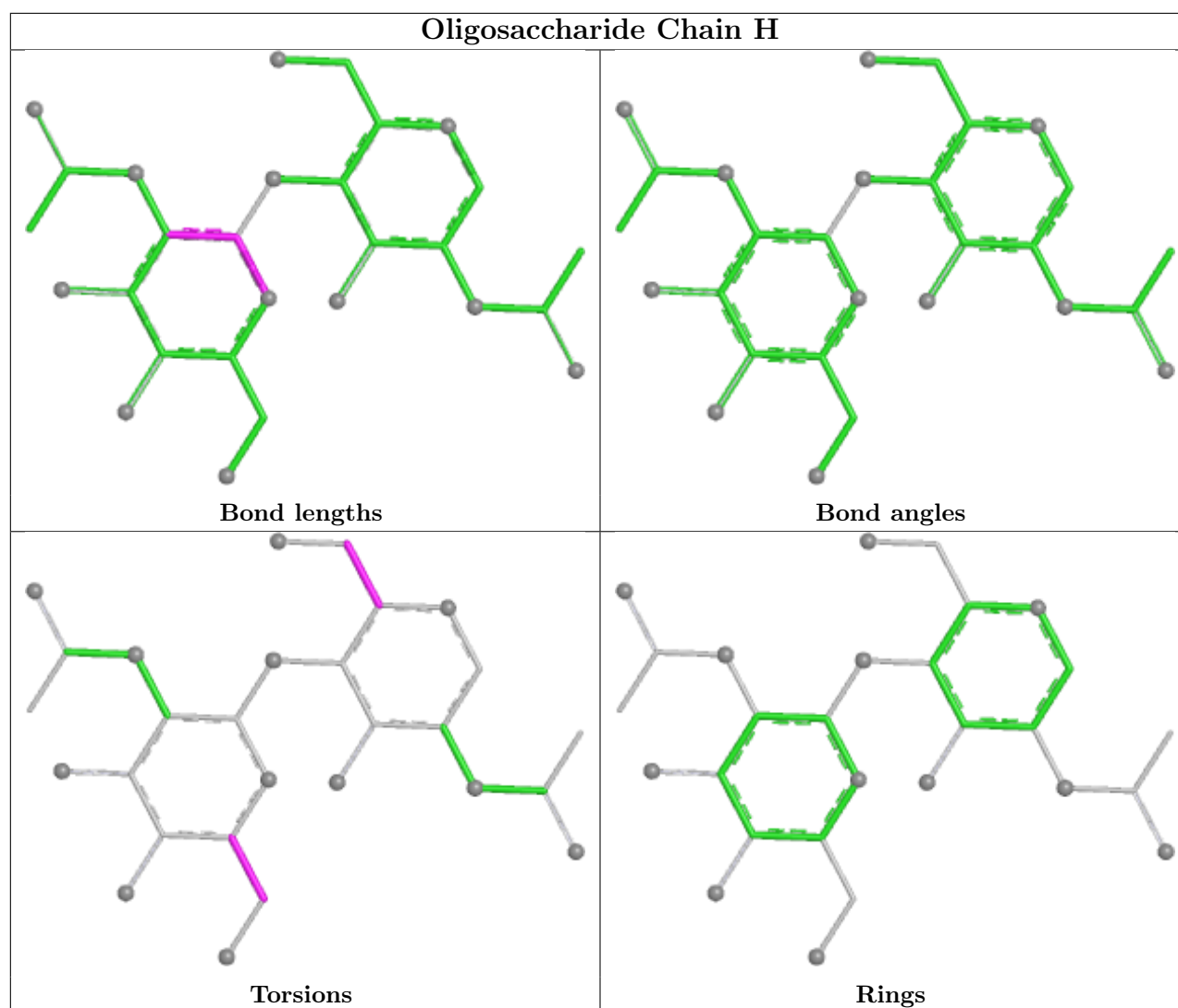
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

4 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	NAG	B	1501	1	14,14,15	0.45	0	17,19,21	0.56	0
4	NAG	A	1502	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	B	1502	1	14,14,15	0.90	1 (7%)	17,19,21	2.12	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1501	1	14,14,15	0.50	0	17,19,21	0.44	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
4	NAG	B	1501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1502	1	-	6/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1502	NAG	C1-C2	2.74	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1502	NAG	C2-N2-C7	7.60	133.08	122.90
4	B	1502	NAG	C1-C2-N2	2.97	115.11	110.43
4	B	1502	NAG	C8-C7-N2	2.03	119.49	116.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1502	NAG	C4-C5-C6-O6
4	B	1502	NAG	O5-C5-C6-O6
4	B	1502	NAG	C8-C7-N2-C2
4	B	1502	NAG	O7-C7-N2-C2
4	A	1501	NAG	O5-C5-C6-O6
4	B	1501	NAG	C1-C2-N2-C7
4	B	1502	NAG	C1-C2-N2-C7
4	B	1502	NAG	C3-C2-N2-C7

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	1374/1436 (95%)	0.07	41 (2%)	52 41	260, 325, 433, 464	0
1	B	1374/1436 (95%)	0.11	45 (3%)	49 39	253, 327, 464, 491	0
All	All	2748/2872 (95%)	0.09	86 (3%)	51 40	253, 326, 451, 491	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	524	PHE	5.8
1	B	238	VAL	5.6
1	B	535	VAL	5.5
1	A	1199	TYR	4.9
1	A	1064	LYS	4.5
1	A	1264	LEU	4.4
1	B	671	LEU	4.0
1	A	1139	LEU	3.9
1	B	534	LEU	3.9
1	A	415	LEU	3.7
1	A	1121	LEU	3.7
1	B	1140	LEU	3.7
1	B	236	PHE	3.6
1	B	1403	ILE	3.6
1	B	1415	TYR	3.6
1	A	413	VAL	3.4
1	A	671	LEU	3.4
1	A	160	LEU	3.3
1	A	180	ILE	3.3
1	B	1139	LEU	3.2
1	B	579	LEU	3.1
1	B	25	VAL	3.1
1	A	198	VAL	3.1
1	B	1124	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	502	GLU	3.0
1	A	1135	TYR	2.9
1	B	957	LEU	2.9
1	B	27	LEU	2.9
1	B	113	VAL	2.9
1	B	1442	ASP	2.8
1	B	675	PHE	2.8
1	A	965	GLN	2.8
1	A	1049	GLN	2.8
1	A	1130	SER	2.8
1	A	139	PHE	2.8
1	A	1045	PHE	2.8
1	A	1140	LEU	2.7
1	B	492	TYR	2.7
1	B	536	ILE	2.7
1	A	1408	LEU	2.7
1	A	1124	LEU	2.7
1	B	752	VAL	2.7
1	A	378	LEU	2.7
1	A	380	ILE	2.6
1	A	684	SER	2.6
1	B	1441	PRO	2.6
1	B	1333	ILE	2.5
1	A	842	THR	2.5
1	A	688	ILE	2.5
1	A	25	VAL	2.5
1	A	1067	ALA	2.5
1	A	1088	LYS	2.5
1	B	552	PHE	2.5
1	B	525	THR	2.4
1	B	198	VAL	2.4
1	A	527	ARG	2.4
1	A	497	GLY	2.4
1	B	1303	SER	2.4
1	B	1187	SER	2.3
1	B	38	LYS	2.3
1	A	906	GLU	2.3
1	B	1351	ILE	2.3
1	A	683	LEU	2.3
1	A	1043	LYS	2.2
1	A	522	LEU	2.2
1	B	1056	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	379	VAL	2.2
1	B	1189	PRO	2.2
1	A	1068	GLY	2.2
1	B	1020	ASN	2.2
1	B	240	ILE	2.2
1	A	531	ASP	2.2
1	B	527	ARG	2.2
1	B	1091	VAL	2.2
1	B	1452	PRO	2.1
1	B	77	HIS	2.1
1	A	536	ILE	2.1
1	B	1349	LEU	2.1
1	A	1142	TYR	2.1
1	A	961	ASP	2.1
1	B	985	LEU	2.1
1	B	729	VAL	2.0
1	B	1401	LEU	2.0
1	B	980	PRO	2.0
1	B	852	LYS	2.0
1	A	1060	GLN	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.

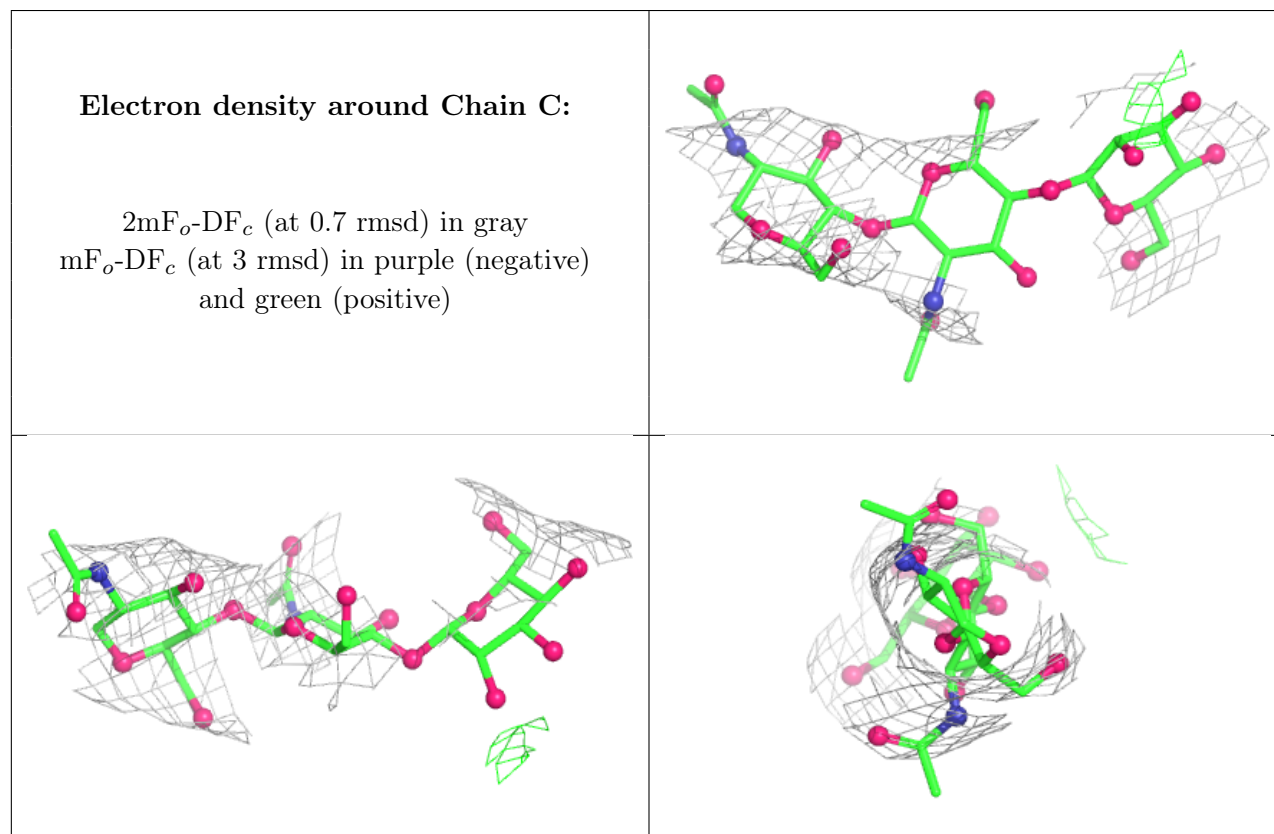
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	E	3	11/12	-0.37	0.19	371,374,379,380	0
2	BMA	C	3	11/12	-0.20	0.18	354,355,359,359	0
2	BMA	D	3	11/12	-0.17	0.12	374,378,380,381	0
2	BMA	I	3	11/12	0.10	0.16	376,378,383,385	0
2	BMA	F	3	11/12	0.12	0.10	352,353,354,354	0
2	NAG	I	2	14/15	0.55	0.11	372,377,381,382	0
3	NAG	G	2	14/15	0.68	0.16	372,374,377,380	0
2	NAG	D	2	14/15	0.69	0.12	368,374,380,381	0

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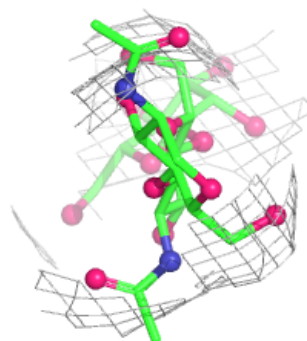
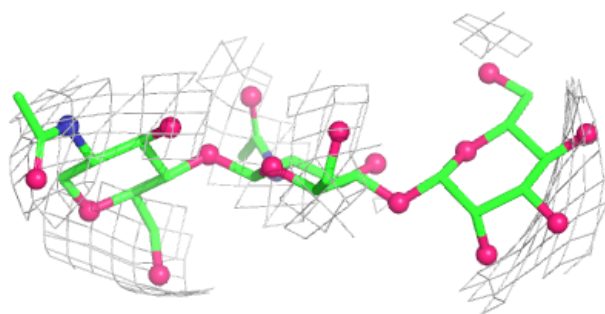
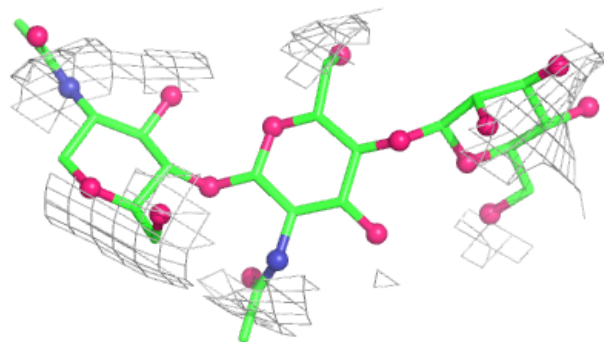
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	H	2	14/15	0.76	0.14	399,406,411,414	0
2	NAG	I	1	14/15	0.81	0.09	370,373,377,378	0
2	NAG	F	2	14/15	0.87	0.09	352,353,357,357	0
2	NAG	C	2	14/15	0.88	0.14	347,351,356,357	0
2	NAG	E	1	14/15	0.88	0.13	358,363,366,367	0
2	NAG	E	2	14/15	0.90	0.12	360,368,374,375	0
2	NAG	D	1	14/15	0.91	0.06	373,377,384,385	0
2	NAG	F	1	14/15	0.92	0.08	353,356,359,360	0
3	NAG	H	1	14/15	0.92	0.12	392,402,407,408	0
3	NAG	G	1	14/15	0.92	0.12	370,376,380,383	0
2	NAG	C	1	14/15	0.96	0.09	348,352,356,358	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.

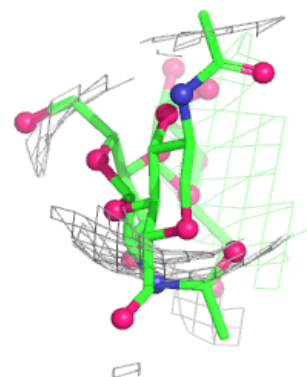
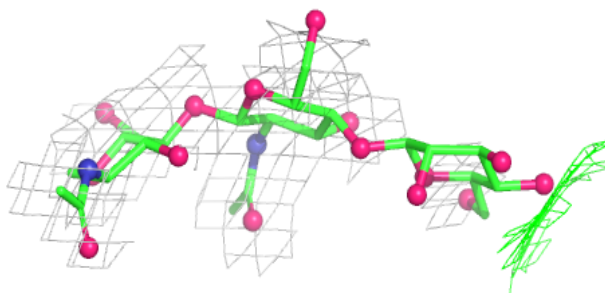
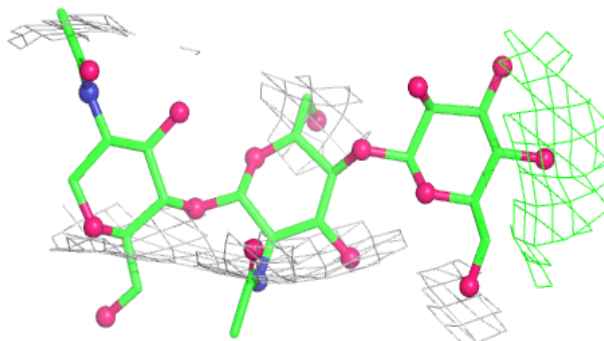


Electron density around Chain D:

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

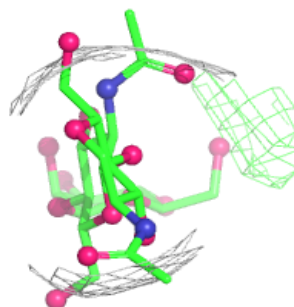
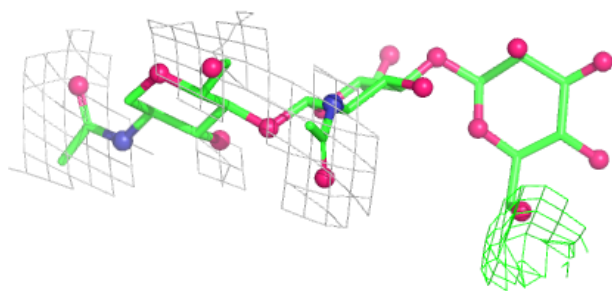
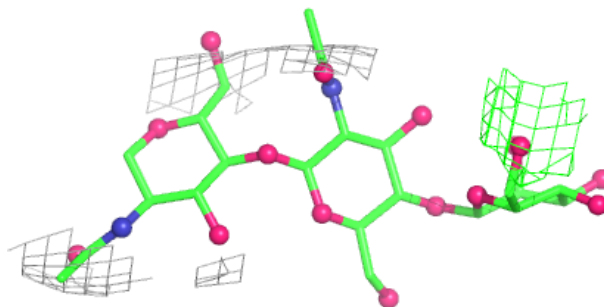
**Electron density around Chain E:**

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

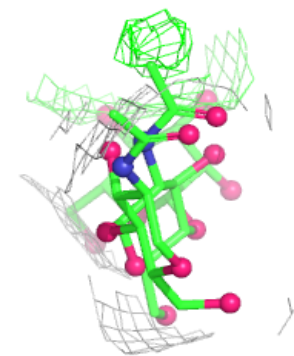
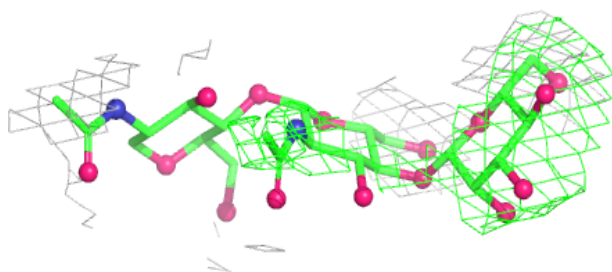
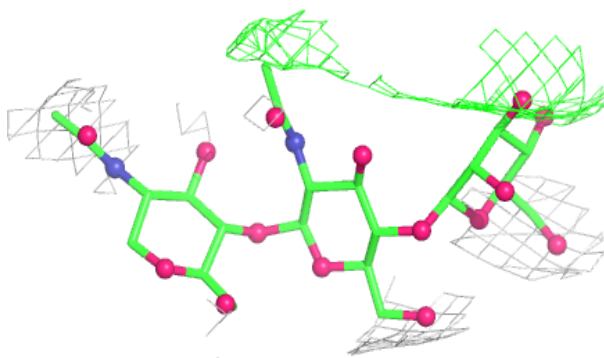


Electron density around Chain F:

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

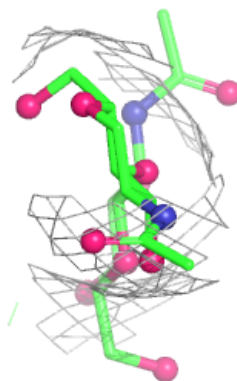
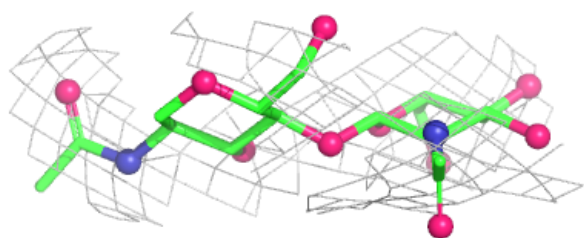
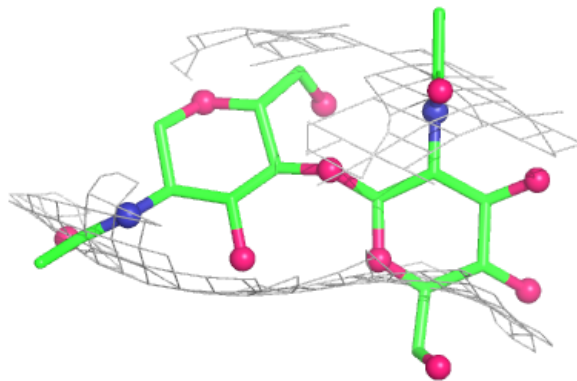
**Electron density around Chain I:**

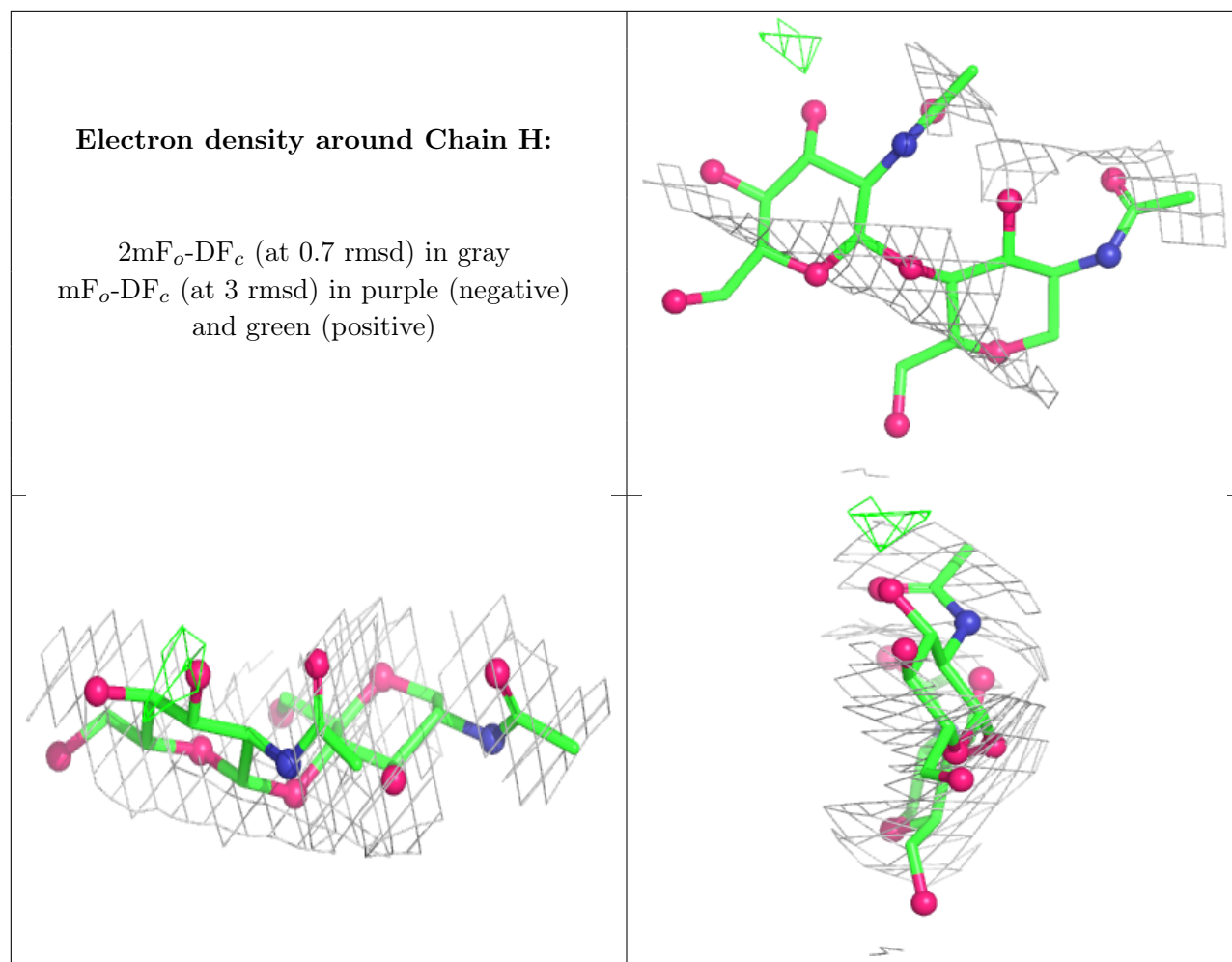
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o - DF_c$ (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
4	NAG	B	1501	14/15	0.42	0.08	381,386,396,396	0
4	NAG	B	1502	14/15	0.71	0.12	334,338,340,340	0
4	NAG	A	1502	14/15	0.86	0.21	384,391,395,396	0
4	NAG	A	1501	14/15	0.88	0.09	367,368,370,370	0

6.5 Other polymers [i](#)

There are no such residues in this entry.