



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 02:38 PM EDT

PDB ID : 6B9O
Title : Structure of GH 38 Jack Bean alpha-mannosidase
Authors : Howard, E.; Cousido-Siah, A.; Lepage, M.; Bodlenner, A.; Mitschler, A.; Meli, A.; De Riccardis, F.; Izzo, I.; Podjarny, A.; Compain, P.
Deposited on : 2017-10-11
Resolution : 1.84 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

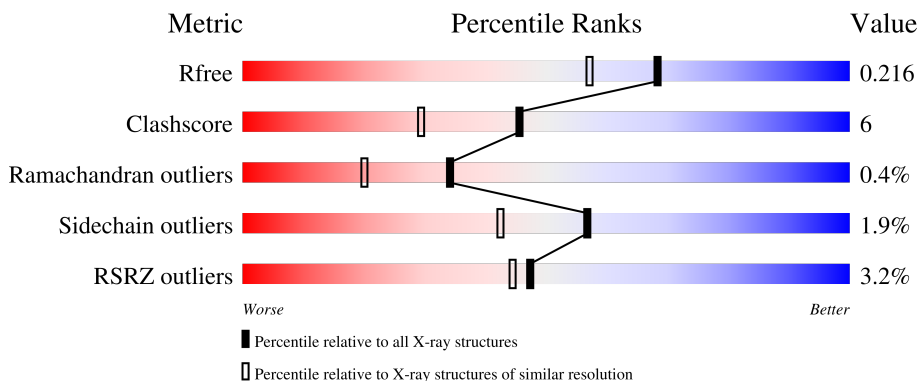
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	981	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 83% 12% • 5%</p>
1	B	981	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4% 83% 12% • •</p>
2	C	12	<div style="display: flex; align-items: center;"> <div style="width: 17%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></div> </div> <p style="margin-left: 20px;">17% 50% 33%</p>
2	E	12	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange;"></div> </div> <p style="margin-left: 20px;">8% 75% 17%</p>
3	D	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 20px;">50% 50%</p>

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Mol	Chain	Length	Quality of chain
3	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	2	-	-	-	X
3	NAG	F	1	-	-	-	X
3	NAG	F	2	-	-	-	X

2 Entry composition [i](#)

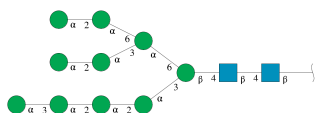
There are 5 unique types of molecules in this entry. The entry contains 17299 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-mannosidase from *Canavalia ensiformis* (jack bean).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	935	Total	C	N	O	S	0	10	0
			7561	4807	1288	1435	31			
1	B	937	Total	C	N	O	S	0	6	0
			7561	4805	1288	1437	31			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	12	Total	C	N	O	0	1	0
			149	82	2	65			
2	E	12	Total	C	N	O	0	0	0
			138	76	2	60			

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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

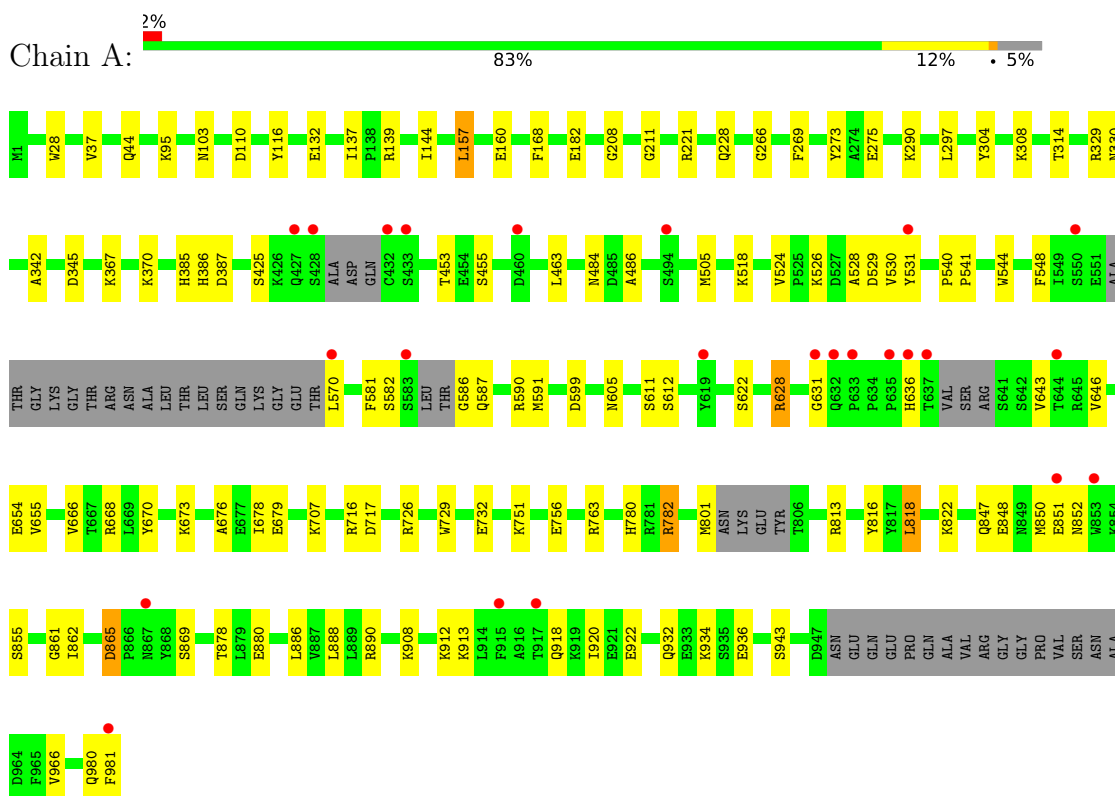
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	930	Total	O	0	3
			933	933		
5	B	898	Total	O	0	1
			899	899		

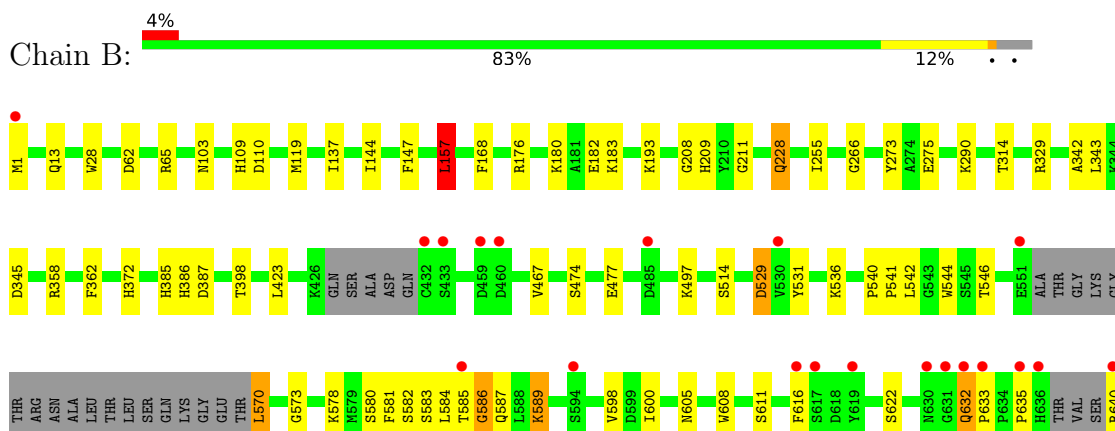
3 Residue-property plots [i](#)

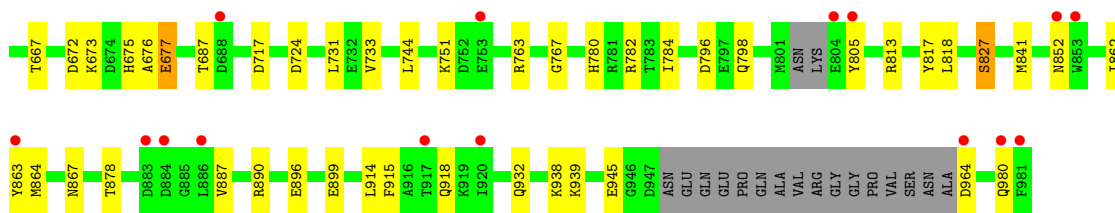
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-mannosidase from *Canavalia ensiformis* (jack bean)



- Molecule 1: Alpha-mannosidase from *Canavalia ensiformis* (jack bean)





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

Chain C: 17% 50% 33%



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

Chain E: 8% 75% 17%



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

Chain D: 50% 50%



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

Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.31Å 119.67Å 277.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 1.84 49.55 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.55-1.84) 99.4 (49.55-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.84Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.175 , 0.216 0.175 , 0.216	Depositor DCC
R_{free} test set	9670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17299	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, MAN, ZN

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	0.43	0/7777	0.60	1/10540 (0.0%)
1	B	0.43	1/7767 (0.0%)	0.59	4/10528 (0.0%)
All	All	0.43	1/15544 (0.0%)	0.60	5/21068 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	677	GLU	CD-OE2	6.45	1.32	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	677	GLU	OE1-CD-OE2	8.62	133.65	123.30
1	B	157	LEU	CA-CB-CG	-8.53	95.69	115.30
1	A	157	LEU	CA-CB-CG	-8.16	96.53	115.30
1	B	677	GLU	CG-CD-OE2	-5.49	107.32	118.30
1	B	570	LEU	CA-CB-CG	5.49	127.92	115.30

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	7561	0	7318	92	0
1	B	7561	0	7298	96	0
2	C	149	0	125	8	0
2	E	138	0	115	5	0
3	D	28	0	25	0	0
3	F	28	0	25	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	933	0	0	38	2
5	B	899	0	0	50	2
All	All	17299	0	14906	195	2

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 (195) 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:541:PRO:O	1:B:862:ILE:CD1	2.06	1.03
1:B:541:PRO:O	1:B:862:ILE:HD13	1.64	0.97
1:B:813:ARG:H	2:E:1:NAG:H81	1.40	0.84
1:B:632:GLN:NE2	1:B:633:PRO:O	2.13	0.81
1:B:329:ARG:NH2	5:B:1102:HOH:O	2.15	0.80
1:B:585:THR:O	1:B:587:GLN:N	2.18	0.77
1:A:813:ARG:H	2:C:1:NAG:H81	1.52	0.73
1:B:314:THR:HB	5:B:1146:HOH:O	1.90	0.70
1:B:640:ARG:N	5:B:1112:HOH:O	2.26	0.69
1:B:632:GLN:HE22	1:B:635:PRO:HD3	1.58	0.69
1:B:183:LYS:NZ	5:B:1114:HOH:O	2.26	0.69
1:B:541:PRO:O	1:B:862:ILE:HD11	1.91	0.68
1:A:505:MET:SD	5:A:1917:HOH:O	2.52	0.67
1:A:850:MET:SD	5:A:1951:HOH:O	2.53	0.66
1:B:540:PRO:HA	5:B:1103:HOH:O	1.96	0.66
1:B:546:THR:HG22	5:B:1115:HOH:O	1.96	0.65
1:B:675:HIS:NE2	5:B:1101:HOH:O	2.08	0.63
1:A:678:ILE:HG13	5:A:1341:HOH:O	1.98	0.63
1:B:13:GLN:NE2	5:B:1127:HOH:O	2.33	0.61
1:B:183:LYS:N	1:B:183:LYS:HD3	2.16	0.61
1:B:573:GLY:O	1:B:578:LYS:NZ	2.33	0.61
1:A:529:ASP:OD1	1:A:529:ASP:N	2.30	0.60
1:B:290:LYS:NZ	5:B:1125:HOH:O	2.32	0.60
1:B:474:SER:OG	5:B:1103:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LEU:HD21	5:A:1971:HOH:O	2.00	0.60
1:B:582:SER:O	1:B:586:GLY:HA2	2.02	0.59
1:A:182:GLU:OE2	5:A:1101:HOH:O	2.16	0.59
1:A:880:GLU:HB3	5:A:1166:HOH:O	2.02	0.59
1:B:193:LYS:NZ	1:B:896:GLU:OE1	2.36	0.59
1:B:852:ASN:ND2	5:B:1136:HOH:O	2.36	0.59
1:A:330:ASN:HB3	1:A:628:ARG:HD3	1.84	0.58
1:B:183:LYS:HE2	5:B:1731:HOH:O	2.04	0.58
1:A:590:ARG:HD2	1:A:599:ASP:OD1	2.04	0.57
1:A:668:ARG:NH2	1:A:679:GLU:OE2	2.37	0.57
1:B:119:MET:HE2	5:B:1260:HOH:O	2.05	0.57
1:A:548:PHE:CD1	1:A:850:MET:HG3	2.40	0.56
1:B:183:LYS:HD2	1:B:255:ILE:HA	1.87	0.56
1:B:731:LEU:HD23	5:B:1105:HOH:O	2.05	0.56
1:B:733:VAL:HG22	5:B:1105:HOH:O	2.05	0.56
1:B:570:LEU:HB2	1:B:581:PHE:O	2.06	0.56
1:A:934:LYS:HE3	5:A:1116:HOH:O	2.07	0.55
5:A:1775:HOH:O	2:C:2:NAG:H83	2.06	0.54
1:B:945:GLU:N	5:B:1146:HOH:O	2.40	0.54
5:A:1937:HOH:O	2:C:2:NAG:H81	2.07	0.54
1:A:886:LEU:HB3	5:A:1906:HOH:O	2.08	0.54
1:B:724:ASP:O	5:B:1105:HOH:O	2.18	0.54
1:A:95:LYS:HE2	5:A:1943:HOH:O	2.08	0.54
1:A:888:LEU:HB3	5:A:1166:HOH:O	2.07	0.54
1:A:518:LYS:HE3	1:A:801:MET:HG2	1.89	0.54
1:A:612:SER:HB3	1:A:628:ARG:HG2	1.90	0.54
1:A:44:GLN:NE2	5:A:1113:HOH:O	2.41	0.54
1:A:139:ARG:HD2	5:A:1321:HOH:O	2.08	0.53
2:C:6[B]:MAN:H3	2:C:7:MAN:C1	2.37	0.53
1:A:524:VAL:HG12	5:A:1223:HOH:O	2.07	0.53
1:A:540:PRO:HB2	1:A:862:ILE:HD12	1.91	0.53
5:A:1574:HOH:O	2:C:1:NAG:H83	2.08	0.53
1:A:484:ASN:HA	1:A:530:VAL:HG22	1.90	0.53
1:A:345:ASP:HB2	1:A:763:ARG:CZ	2.40	0.52
5:B:1106:HOH:O	3:F:1:NAG:O7	2.19	0.52
1:A:570:LEU:HD22	1:A:581:PHE:HB2	1.91	0.52
1:A:342:ALA:HB1	2:C:2:NAG:H82	1.91	0.52
1:A:586:GLY:CA	1:A:643:VAL:HG23	2.40	0.52
1:A:888:LEU:HD23	5:A:1166:HOH:O	2.10	0.52
1:B:813:ARG:N	2:E:1:NAG:H81	2.17	0.51
1:A:676:ALA:HB3	1:A:818[A]:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:GLN:HG2	1:B:633:PRO:HD2	1.91	0.51
1:A:920:ILE:HD13	1:A:981:PHE:CE1	2.45	0.51
1:A:586:GLY:HA3	1:A:643:VAL:HG23	1.91	0.51
1:A:852:ASN:HB2	5:A:1640:HOH:O	2.11	0.51
1:A:160:GLU:OE1	5:A:1102:HOH:O	2.18	0.50
1:A:847:GLN:O	1:A:848:GLU:HG2	2.10	0.50
1:B:497:LYS:HE3	5:B:1943:HOH:O	2.11	0.50
1:B:109:HIS:CE1	5:B:1260:HOH:O	2.63	0.50
1:A:908:LYS:HE2	1:A:966:VAL:HG11	1.93	0.50
1:B:667:THR:HG22	5:B:1685:HOH:O	2.12	0.50
1:B:157:LEU:HD13	5:B:1260:HOH:O	2.11	0.49
1:B:342:ALA:HB1	2:E:2:NAG:H82	1.94	0.49
1:B:600:ILE:HG12	5:B:1893:HOH:O	2.11	0.49
1:A:587:GLN:NE2	5:A:1147:HOH:O	2.45	0.49
1:A:144:ILE:HA	1:A:168:PHE:HA	1.95	0.49
1:A:726[B]:ARG:HD3	1:A:729:TRP:CH2	2.48	0.49
1:B:529:ASP:OD1	1:B:529:ASP:N	2.38	0.49
1:B:673:LYS:HD2	5:B:1101:HOH:O	2.12	0.49
1:A:544:TRP:CH2	1:A:861:GLY:HA3	2.48	0.48
1:B:945:GLU:HG3	5:B:1146:HOH:O	2.13	0.48
1:A:850:MET:HE2	5:A:1119:HOH:O	2.11	0.48
1:B:110:ASP:HB2	1:B:386:HIS:HA	1.96	0.48
1:A:290:LYS:HE2	1:A:290:LYS:HB3	1.68	0.48
1:B:585:THR:O	1:B:585:THR:OG1	2.29	0.48
1:B:964:ASP:N	5:B:1158:HOH:O	2.45	0.48
1:B:273:TYR:CZ	1:B:275:GLU:HB3	2.49	0.48
1:B:542:LEU:O	1:B:862:ILE:HD12	2.14	0.47
1:B:640:ARG:CZ	1:B:640:ARG:HB2	2.44	0.47
1:B:827:SER:OG	1:B:899:GLU:HB3	2.14	0.47
1:A:548:PHE:CG	1:A:850:MET:HG3	2.49	0.47
1:A:813:ARG:N	2:C:1:NAG:H81	2.25	0.47
1:A:221:ARG:HA	5:B:1388:HOH:O	2.13	0.47
5:B:1223:HOH:O	2:E:1:NAG:H83	2.14	0.47
1:A:530:VAL:HG23	1:A:531:TYR:CD2	2.50	0.47
1:B:536:LYS:HE2	1:B:672:ASP:OD2	2.15	0.47
1:B:193:LYS:HG3	5:B:1542:HOH:O	2.15	0.47
1:B:611:SER:HB3	1:B:622:SER:HB3	1.97	0.47
1:A:936:GLU:HG2	5:A:1934:HOH:O	2.15	0.47
1:B:514:SER:HB2	5:B:1234:HOH:O	2.15	0.47
5:B:1860:HOH:O	2:E:2:NAG:H83	2.15	0.47
1:A:137:ILE:HD13	1:A:932:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:LEU:HB3	5:B:1876:HOH:O	2.15	0.46
1:B:589:LYS:O	5:B:1108:HOH:O	2.21	0.46
1:B:798:GLN:NE2	5:B:1130:HOH:O	2.34	0.46
1:A:528:ALA:HB1	5:A:1917:HOH:O	2.14	0.46
1:A:605:ASN:ND2	1:A:636:HIS:CE1	2.84	0.46
1:A:385:HIS:CD2	1:A:387:ASP:H	2.33	0.46
1:B:137:ILE:HD13	1:B:932:GLN:HG2	1.98	0.46
1:B:497:LYS:HD2	5:B:1873:HOH:O	2.15	0.46
1:B:980:GLN:HB2	5:B:1795:HOH:O	2.14	0.46
1:A:878:THR:HB	1:A:890:ARG:HB2	1.97	0.46
1:B:782:ARG:HD2	1:B:796:ASP:OD1	2.16	0.46
1:A:922:GLU:CD	1:A:980:GLN:HE21	2.18	0.46
1:A:678:ILE:HG21	1:A:816:TYR:CZ	2.51	0.45
1:B:676:ALA:HB3	1:B:818:LEU:CD2	2.46	0.45
1:B:864:MET:SD	1:B:914:LEU:HD12	2.56	0.45
1:A:110:ASP:HB2	1:A:386:HIS:HA	1.97	0.45
1:A:273:TYR:CZ	1:A:275:GLU:HB3	2.52	0.45
1:A:329:ARG:NH2	1:A:732:GLU:OE2	2.43	0.45
1:A:912:LYS:HE3	5:A:1192:HOH:O	2.17	0.45
1:A:851:GLU:CD	1:A:851:GLU:H	2.20	0.45
1:A:782:ARG:HD3	5:A:1442:HOH:O	2.18	0.44
1:B:580:SER:HB2	1:B:589:LYS:HG2	1.98	0.44
1:A:611:SER:HB3	1:A:622:SER:HB3	2.00	0.44
1:A:707:LYS:NZ	5:A:1154:HOH:O	2.46	0.44
1:B:144:ILE:HA	1:B:168:PHE:HA	1.99	0.44
1:A:570:LEU:HB3	1:A:581:PHE:O	2.17	0.44
1:A:655:VAL:HG22	5:A:1971:HOH:O	2.17	0.44
1:B:751:LYS:NZ	5:B:1159:HOH:O	2.46	0.44
1:A:912:LYS:HE2	5:A:1914:HOH:O	2.16	0.44
1:B:345:ASP:HB2	1:B:763:ARG:CZ	2.47	0.44
1:B:477:GLU:HG3	5:B:1749:HOH:O	2.16	0.44
1:A:646:VAL:HG13	5:A:1971:HOH:O	2.18	0.44
1:A:670:TYR:HB2	1:A:673:LYS:HG3	2.00	0.44
1:A:922:GLU:OE2	1:A:980:GLN:NE2	2.48	0.44
1:A:570:LEU:C	1:A:570:LEU:HD23	2.38	0.44
1:A:591:MET:HB3	5:A:1410:HOH:O	2.18	0.44
1:A:631:GLY:N	5:A:1126:HOH:O	2.51	0.44
1:B:211:GLY:HA2	1:B:266:GLY:O	2.18	0.44
1:A:269:PHE:HE2	5:A:1113:HOH:O	2.01	0.43
1:A:654:GLU:OE2	1:A:668:ARG:HD3	2.18	0.43
1:B:586:GLY:N	5:B:1184:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:PRO:HG2	1:A:862:ILE:HD11	2.00	0.43
1:B:343:LEU:HD22	1:B:398:THR:HG23	1.99	0.43
1:A:330:ASN:HB3	1:A:628:ARG:CD	2.46	0.43
1:A:922:GLU:HB3	1:A:980:GLN:HG3	2.00	0.43
1:A:211:GLY:HA2	1:A:266:GLY:O	2.19	0.43
1:B:1:MET:SD	5:B:1872:HOH:O	2.62	0.43
1:B:385:HIS:CD2	1:B:387:ASP:H	2.37	0.43
5:A:1202:HOH:O	2:C:6[A]:MAN:H61	2.18	0.43
1:A:486:ALA:HB2	1:A:531:TYR:CE2	2.54	0.43
1:A:751:LYS:HB3	1:A:756:GLU:HG3	2.00	0.43
1:A:886:LEU:HD12	5:A:1416:HOH:O	2.17	0.42
1:A:37:VAL:HG11	1:B:228:GLN:HG2	2.01	0.42
1:A:666:VAL:HG12	1:A:668:ARG:HG3	2.01	0.42
1:B:62:ASP:HB3	1:B:65:ARG:HD2	2.01	0.42
1:B:209:HIS:HB3	5:B:1821:HOH:O	2.19	0.42
1:B:862:ILE:HG23	1:B:864:MET:O	2.20	0.42
1:A:922:GLU:HG2	5:A:1187:HOH:O	2.18	0.42
1:B:358:ARG:NH2	5:B:1194:HOH:O	2.52	0.42
1:B:467:VAL:O	1:B:544:TRP:HA	2.20	0.42
1:B:598:VAL:HG12	5:B:1893:HOH:O	2.18	0.42
1:A:582:SER:O	1:A:586:GLY:HA2	2.20	0.42
1:B:939:LYS:HE2	5:B:1890:HOH:O	2.20	0.42
1:A:132:GLU:HG3	5:A:1779:HOH:O	2.20	0.42
1:B:176:ARG:HG2	1:B:180:LYS:HE3	2.01	0.42
1:B:744:LEU:HD11	1:B:767:GLY:HA3	2.01	0.42
1:B:687:THR:HG21	1:B:782:ARG:HG2	2.01	0.41
1:B:583:SER:O	5:B:1109:HOH:O	2.21	0.41
1:A:865:ASP:OD2	1:A:913:LYS:HA	2.21	0.41
1:B:477:GLU:HB3	1:B:841[A]:MET:SD	2.60	0.41
1:B:608:TRP:O	1:B:635:PRO:HD2	2.21	0.41
1:B:878:THR:HB	1:B:890:ARG:HB2	2.02	0.41
1:B:362:PHE:CE1	1:B:887:VAL:HG21	2.55	0.41
1:B:635:PRO:HG3	5:B:1822:HOH:O	2.19	0.41
1:B:938:LYS:NZ	5:B:1199:HOH:O	2.53	0.41
1:A:304:TYR:O	1:A:308:LYS:HG2	2.21	0.41
1:B:423:LEU:HD22	1:B:863:TYR:CE1	2.55	0.41
1:A:587:GLN:HG3	5:A:1135:HOH:O	2.21	0.41
1:A:116:TYR:CD1	1:A:716:ARG:HG3	2.56	0.41
1:B:183:LYS:HD3	1:B:183:LYS:H	1.83	0.41
1:B:915:PHE:HB3	5:B:1363:HOH:O	2.21	0.41
1:A:822:LYS:NZ	5:A:1186:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:GLN:HB2	5:B:1363:HOH:O	2.21	0.41
1:A:314:THR:HG22	1:A:943:SER:OG	2.21	0.40
1:A:370:LYS:HD2	1:A:880:GLU:OE2	2.21	0.40
1:A:453:THR:HG22	1:A:463:LEU:HD21	2.04	0.40
1:B:687:THR:HB	1:B:784:ILE:HD11	2.03	0.40
1:B:677:GLU:HG2	1:B:817:TYR:CD2	2.57	0.40
1:B:867:ASN:N	5:B:1129:HOH:O	2.34	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1365:HOH:O	5:B:1804:HOH:O[1_655]	1.93	0.27
5:A:1365:HOH:O	5:B:1133:HOH:O[1_655]	2.19	0.01

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	931/981 (95%)	894 (96%)	34 (4%)	3 (0%)	41 27
1	B	931/981 (95%)	893 (96%)	34 (4%)	4 (0%)	34 20
All	All	1862/1962 (95%)	1787 (96%)	68 (4%)	7 (0%)	34 20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	586	GLY
1	A	28	TRP
1	B	28	TRP
1	B	208	GLY
1	B	103	ASN

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Mol	Chain	Res	Type
1	A	103	ASN
1	A	208	GLY

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	823/849 (97%)	806 (98%)	17 (2%)	53	38
1	B	821/849 (97%)	806 (98%)	15 (2%)	59	44
All	All	1644/1698 (97%)	1612 (98%)	32 (2%)	57	42

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	LEU
1	A	228	GLN
1	A	297	LEU
1	A	367	LYS
1	A	425	SER
1	A	455	SER
1	A	526	LYS
1	A	628	ARG
1	A	717	ASP
1	A	780	HIS
1	A	782	ARG
1	A	818[A]	LEU
1	A	818[B]	LEU
1	A	855	SER
1	A	865	ASP
1	A	869	SER
1	A	918	GLN
1	B	147	PHE
1	B	157	LEU
1	B	182	GLU
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	372	HIS
1	B	529	ASP
1	B	531	TYR
1	B	589	LYS
1	B	605	ASN
1	B	616	PHE
1	B	632	GLN
1	B	717	ASP
1	B	780	HIS
1	B	805	TYR
1	B	827	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	636	HIS
1	A	980	GLN
1	B	587	GLN
1	B	605	ASN
1	B	632	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

29 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	2,1	14,14,15	0.82	1 (7%)	17,19,21	0.80	1 (5%)
2	MAN	C	10	2	11,11,12	0.78	0	15,15,17	1.10	1 (6%)
2	MAN	C	11	2	11,11,12	1.04	1 (9%)	15,15,17	1.35	2 (13%)
2	MAN	C	12	2	11,11,12	0.55	0	15,15,17	1.08	1 (6%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	0.80	1 (5%)
2	BMA	C	3	2	11,11,12	0.87	0	15,15,17	0.92	0
2	MAN	C	4	2	11,11,12	0.82	0	15,15,17	1.17	2 (13%)
2	MAN	C	5	2	11,11,12	0.79	0	15,15,17	1.10	0
2	MAN	C	6[A]	2	11,11,12	1.65	3 (27%)	15,15,17	1.87	4 (26%)
2	MAN	C	6[B]	2	11,11,12	2.00	3 (27%)	15,15,17	2.24	4 (26%)
2	MAN	C	7	2	11,11,12	1.96	3 (27%)	15,15,17	1.83	4 (26%)
2	MAN	C	8	2	11,11,12	0.73	0	15,15,17	1.30	2 (13%)
2	MAN	C	9	2	11,11,12	0.70	0	15,15,17	1.13	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.34	0	17,19,21	0.69	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	1.97	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.63	0	17,19,21	0.75	1 (5%)
2	MAN	E	10	2	11,11,12	0.99	1 (9%)	15,15,17	1.19	2 (13%)
2	MAN	E	11	2	11,11,12	0.87	0	15,15,17	1.18	2 (13%)
2	MAN	E	12	2	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
2	NAG	E	2	2	14,14,15	0.66	0	17,19,21	0.81	1 (5%)
2	BMA	E	3	2	11,11,12	0.65	0	15,15,17	1.01	0
2	MAN	E	4	2	11,11,12	0.79	0	15,15,17	1.10	1 (6%)
2	MAN	E	5	2	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
2	MAN	E	6	2	11,11,12	1.06	0	15,15,17	1.37	2 (13%)
2	MAN	E	7	2	11,11,12	1.64	1 (9%)	15,15,17	1.47	3 (20%)
2	MAN	E	8	2	11,11,12	0.80	0	15,15,17	1.17	2 (13%)
2	MAN	E	9	2	11,11,12	0.85	1 (9%)	15,15,17	1.31	2 (13%)
3	NAG	F	1	1,3	14,14,15	1.52	2 (14%)	17,19,21	1.36	1 (5%)
3	NAG	F	2	3	14,14,15	1.33	1 (7%)	17,19,21	1.40	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	C	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	10	2	-	0/2/19/22	0/1/1/1
2	MAN	C	11	2	-	0/2/19/22	0/1/1/1
2	MAN	C	12	2	-	0/2/19/22	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	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6[A]	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6[B]	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	MAN	E	10	2	-	2/2/19/22	0/1/1/1
2	MAN	E	11	2	-	0/2/19/22	0/1/1/1
2	MAN	E	12	2	-	0/2/19/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
2	MAN	E	7	2	-	0/2/19/22	0/1/1/1
2	MAN	E	8	2	-	0/2/19/22	0/1/1/1
2	MAN	E	9	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	MAN	C2-C3	5.48	1.60	1.52
2	E	7	MAN	C2-C3	4.81	1.59	1.52
3	F	1	NAG	O5-C1	4.79	1.51	1.43
3	F	2	NAG	O5-C1	4.57	1.51	1.43
2	C	6[B]	MAN	C2-C3	4.38	1.59	1.52
2	C	6[B]	MAN	O5-C5	3.85	1.51	1.43
2	C	6[A]	MAN	C2-C3	-3.14	1.47	1.52
3	F	1	NAG	C1-C2	2.95	1.56	1.52
2	C	6[A]	MAN	C1-C2	2.76	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	MAN	C4-C3	2.64	1.59	1.52
2	C	6[A]	MAN	C4-C5	2.56	1.58	1.53
2	C	11	MAN	O5-C5	2.43	1.48	1.43
2	E	10	MAN	C1-C2	2.19	1.57	1.52
2	C	7	MAN	O5-C1	-2.17	1.40	1.43
2	E	9	MAN	O5-C5	2.13	1.47	1.43
2	C	1	NAG	C1-C2	2.10	1.55	1.52
2	C	6[B]	MAN	O5-C1	-2.05	1.40	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	7.35	122.14	112.19
3	F	2	NAG	C1-O5-C5	5.50	119.65	112.19
2	C	6[B]	MAN	C2-C3-C4	5.50	120.41	110.89
3	F	1	NAG	C1-O5-C5	5.26	119.32	112.19
2	C	6[A]	MAN	C1-O5-C5	4.24	117.93	112.19
2	C	6[B]	MAN	C1-C2-C3	4.01	114.59	109.67
2	C	7	MAN	O5-C1-C2	3.98	116.92	110.77
2	E	6	MAN	C1-O5-C5	3.93	117.52	112.19
2	C	6[A]	MAN	O5-C1-C2	3.89	116.77	110.77
2	E	4	MAN	O2-C2-C3	-3.59	102.94	110.14
2	C	7	MAN	C1-C2-C3	3.57	114.05	109.67
2	C	11	MAN	O2-C2-C3	-3.44	103.25	110.14
2	E	9	MAN	O2-C2-C3	-3.26	103.61	110.14
2	C	6[B]	MAN	O2-C2-C3	-3.19	103.74	110.14
2	E	9	MAN	C1-O5-C5	3.16	116.47	112.19
2	E	7	MAN	C1-C2-C3	3.12	113.50	109.67
2	C	6[B]	MAN	O5-C5-C6	3.12	112.09	107.20
2	C	4	MAN	O2-C2-C3	-3.07	103.98	110.14
2	E	11	MAN	O2-C2-C3	-3.04	104.04	110.14
2	C	12	MAN	C1-O5-C5	3.00	116.26	112.19
2	E	10	MAN	C1-O5-C5	2.85	116.05	112.19
2	E	8	MAN	O2-C2-C3	-2.78	104.57	110.14
2	E	7	MAN	C2-C3-C4	2.73	115.62	110.89
2	C	8	MAN	O2-C2-C3	-2.67	104.78	110.14
2	C	9	MAN	O2-C2-C3	-2.67	104.80	110.14
2	C	9	MAN	C1-O5-C5	2.65	115.78	112.19
3	D	2	NAG	C3-C4-C5	2.63	114.92	110.24
2	C	11	MAN	C1-O5-C5	2.62	115.74	112.19
2	C	10	MAN	O2-C2-C3	-2.58	104.96	110.14
2	E	5	MAN	C1-O5-C5	2.58	115.68	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	MAN	C1-O5-C5	2.53	115.62	112.19
2	C	7	MAN	C2-C3-C4	2.53	115.27	110.89
2	E	5	MAN	O2-C2-C3	-2.46	105.22	110.14
2	E	2	NAG	C1-O5-C5	2.42	115.47	112.19
2	C	6[A]	MAN	C2-C3-C4	-2.40	106.74	110.89
2	E	7	MAN	O5-C1-C2	2.35	114.40	110.77
2	E	12	MAN	C1-O5-C5	2.34	115.37	112.19
2	C	8	MAN	C1-O5-C5	2.20	115.17	112.19
2	E	11	MAN	C1-C2-C3	-2.18	106.98	109.67
2	C	6[A]	MAN	O2-C2-C1	2.18	113.62	109.15
2	C	1	NAG	C1-O5-C5	2.18	115.14	112.19
2	E	1	NAG	C1-O5-C5	2.15	115.11	112.19
2	E	8	MAN	C1-O5-C5	2.13	115.08	112.19
2	C	2	NAG	C1-O5-C5	2.11	115.05	112.19
2	E	6	MAN	O2-C2-C3	-2.10	105.93	110.14
2	C	4	MAN	C1-C2-C3	-2.10	107.09	109.67
2	E	10	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

All (20) torsion outliers are listed below:

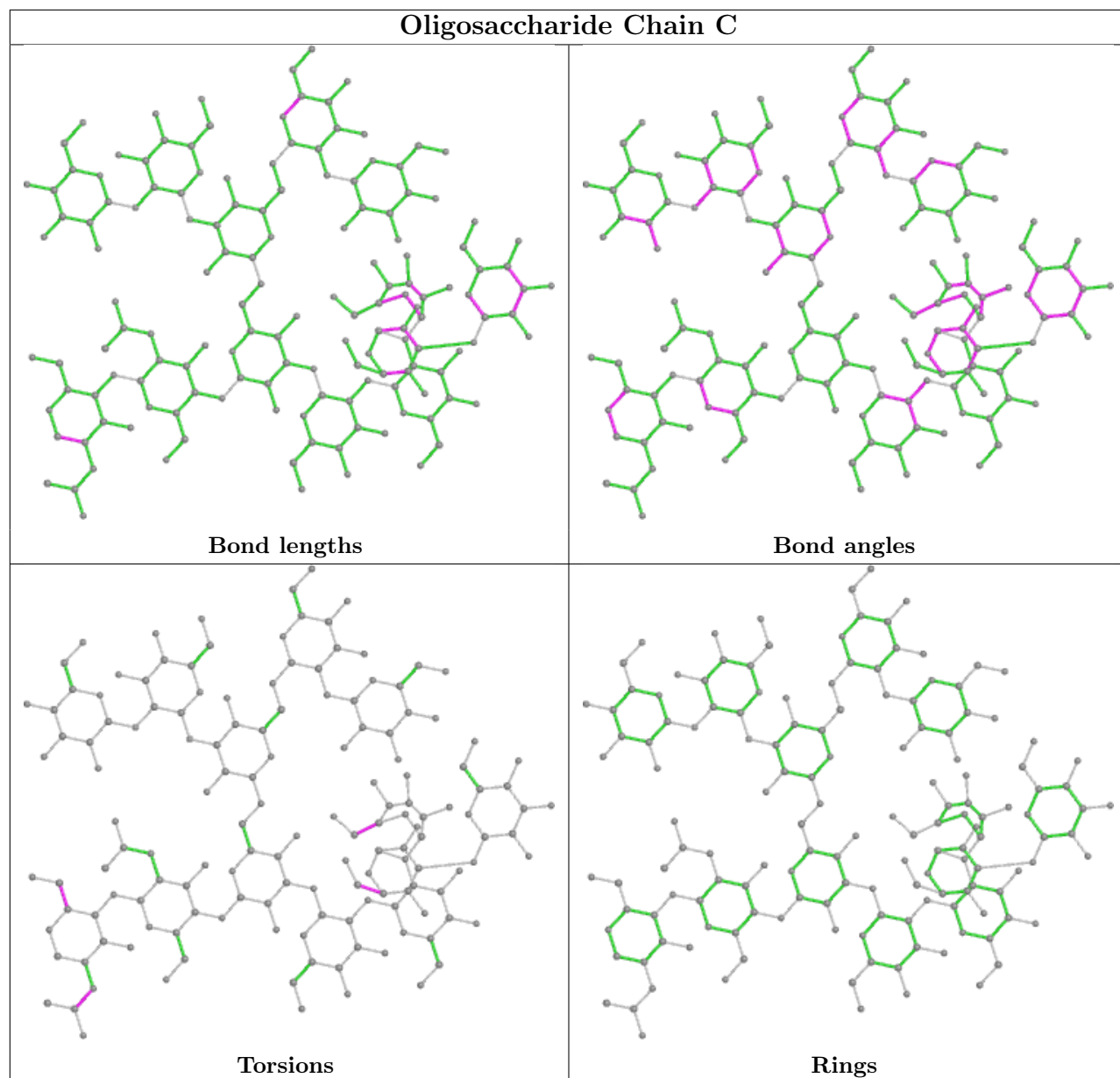
Mol	Chain	Res	Type	Atoms
2	C	6[A]	MAN	O5-C5-C6-O6
2	C	6[B]	MAN	C4-C5-C6-O6
2	C	6[B]	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	6[A]	MAN	C4-C5-C6-O6
2	E	6	MAN	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6
2	E	10	MAN	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	E	10	MAN	C4-C5-C6-O6
2	E	6	MAN	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6

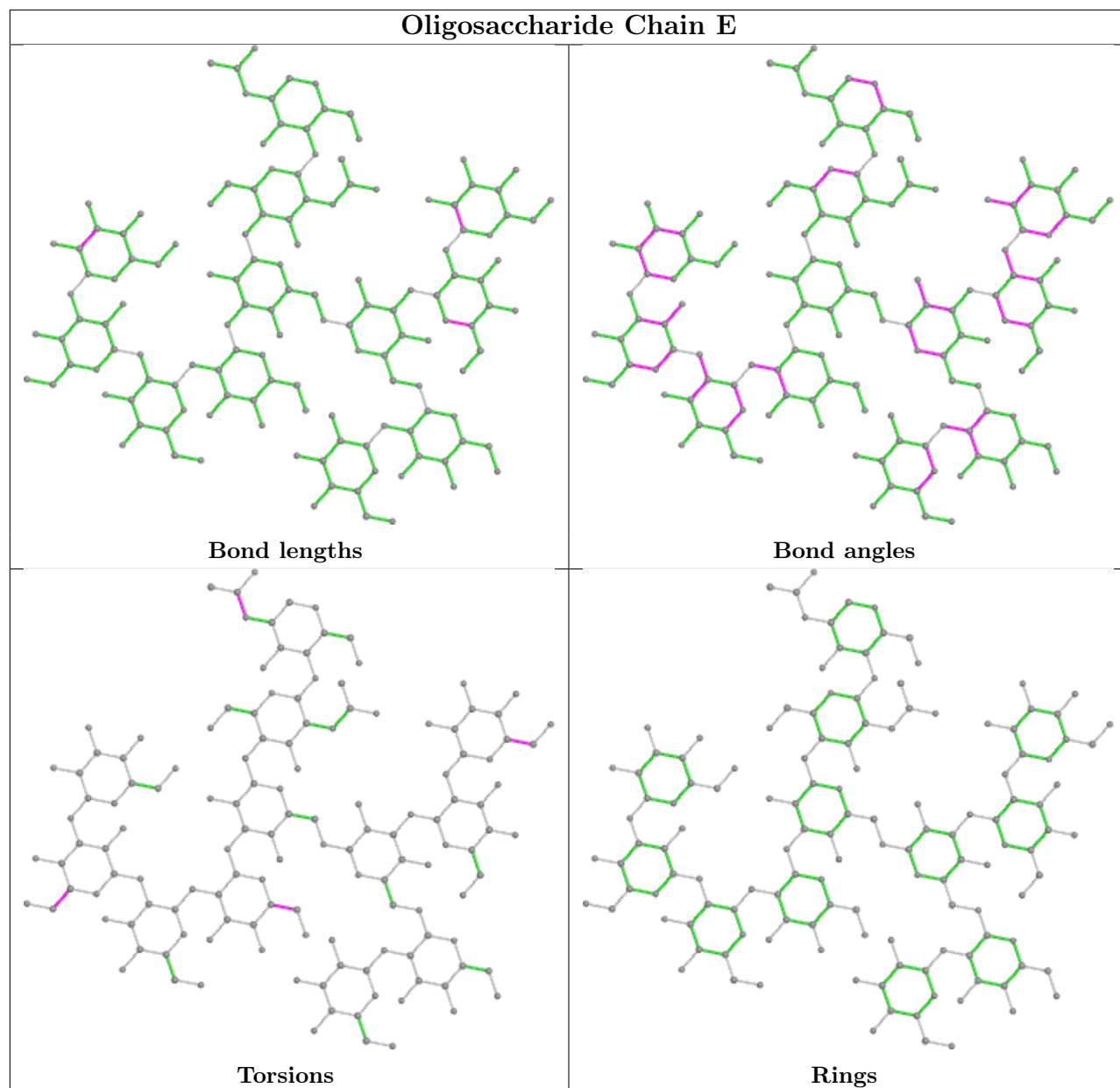
There are no ring outliers.

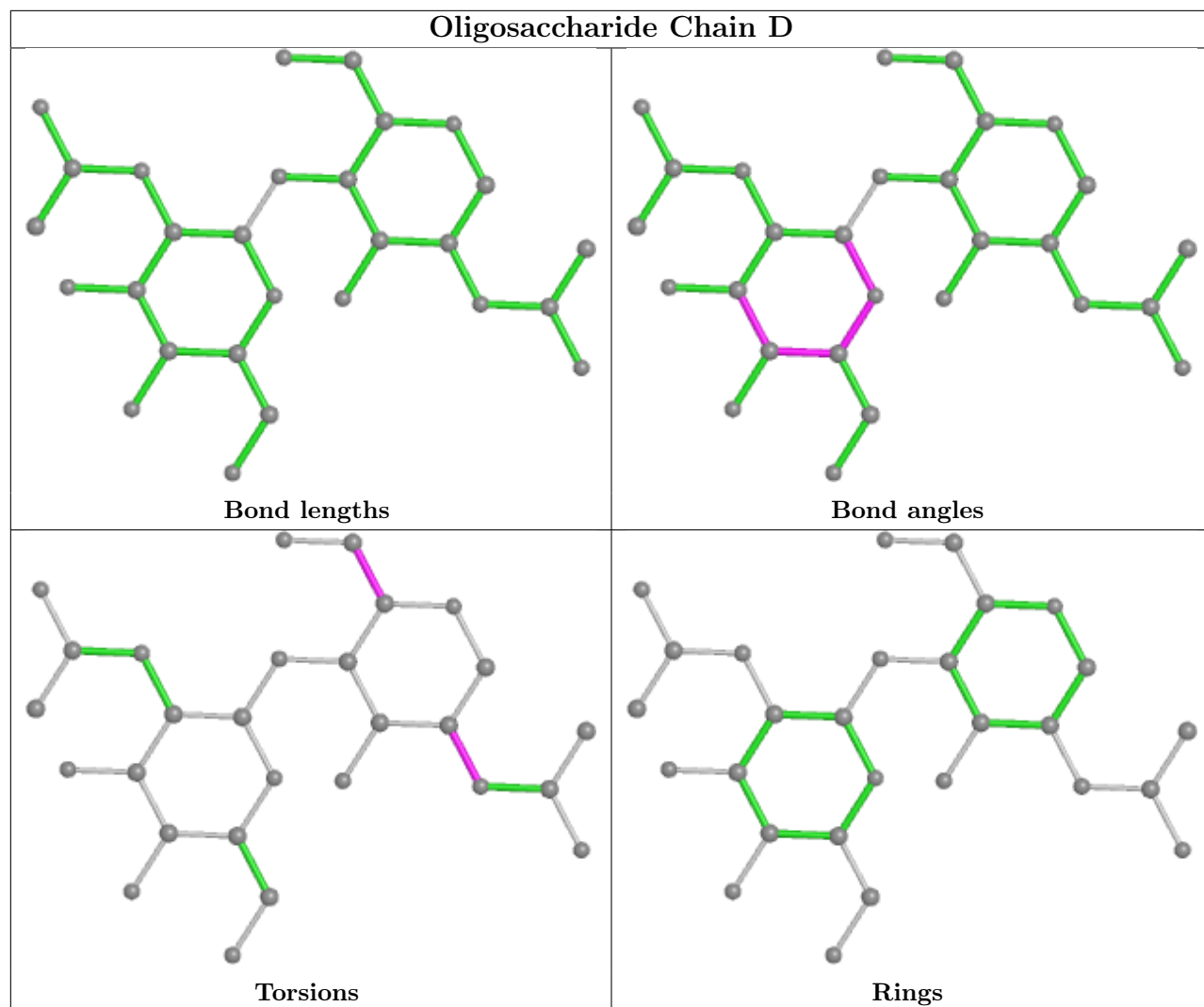
8 monomers are involved in 14 short contacts:

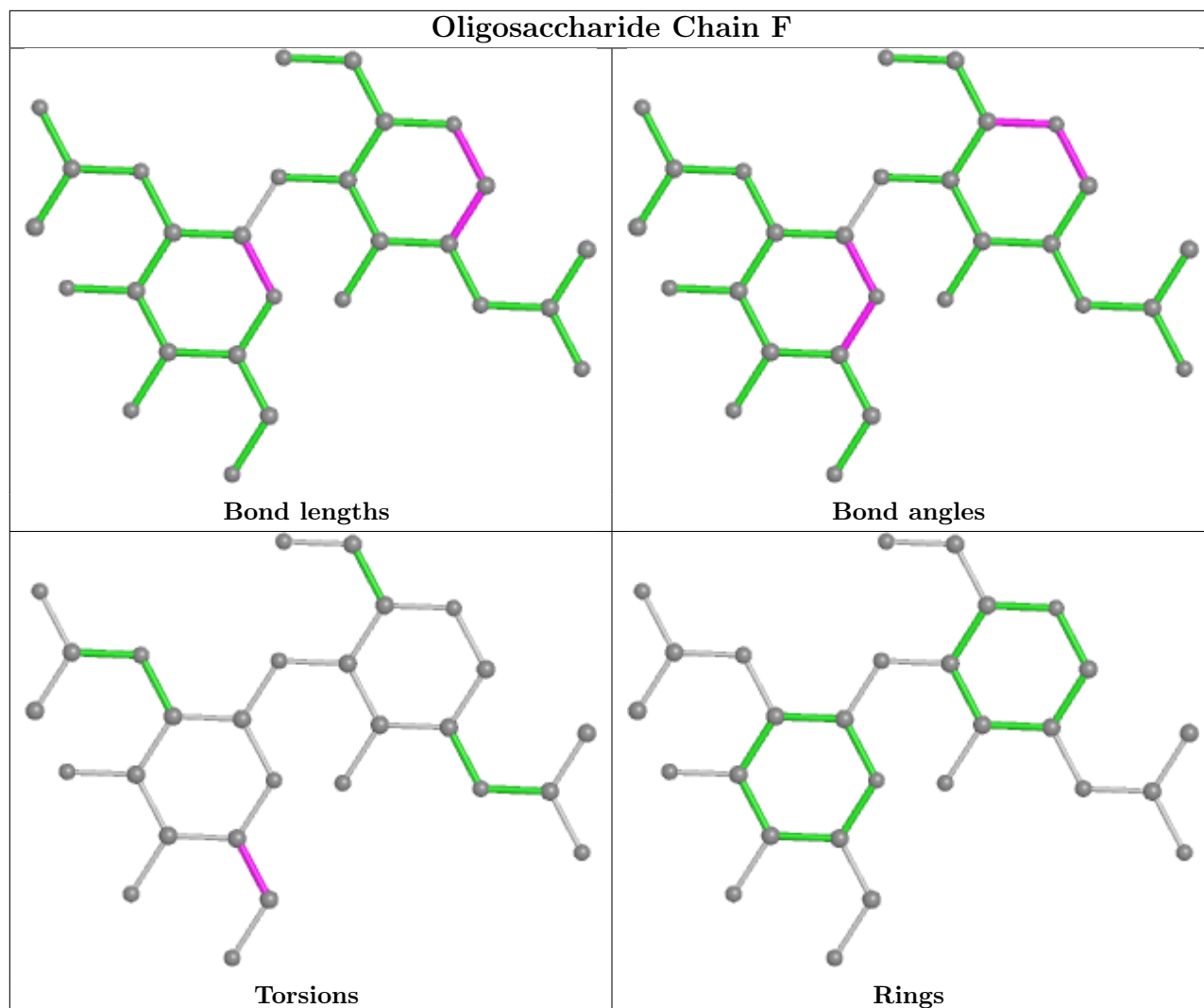
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	MAN	1	0
2	C	2	NAG	3	0
2	C	6[A]	MAN	1	0
2	C	1	NAG	3	0
2	C	6[B]	MAN	1	0
3	F	1	NAG	1	0
2	E	2	NAG	2	0
2	E	1	NAG	3	0

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









5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	935/981 (95%)	-0.23	24 (2%) 56 53	12, 24, 48, 79	0
1	B	937/981 (95%)	0.00	35 (3%) 41 38	13, 26, 51, 103	0
All	All	1872/1962 (95%)	-0.11	59 (3%) 47 44	12, 25, 50, 103	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	PHE	7.4
1	B	432	CYS	6.9
1	B	804	GLU	6.1
1	B	433	SER	6.0
1	B	633	PRO	5.6
1	A	917	THR	5.4
1	A	636	HIS	5.3
1	B	805	TYR	5.0
1	B	636	HIS	4.7
1	B	632	GLN	4.6
1	B	635	PRO	4.4
1	B	884	ASP	4.3
1	A	619	TYR	4.2
1	A	428	SER	4.0
1	B	917	THR	3.8
1	B	631	GLY	3.7
1	A	427	GLN	3.6
1	B	619	TYR	3.5
1	B	459	ASP	3.3
1	B	594	SER	3.2
1	A	853	TRP	3.2
1	B	688	ASP	3.2
1	B	630	ASN	3.2
1	B	585	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	632	GLN	3.1
1	B	964	ASP	2.8
1	A	570	LEU	2.8
1	A	433	SER	2.8
1	B	617	SER	2.8
1	A	635	PRO	2.7
1	A	583	SER	2.7
1	A	460	ASP	2.7
1	B	886	LEU	2.6
1	B	852	ASN	2.6
1	B	640	ARG	2.6
1	B	530	VAL	2.6
1	B	920	ILE	2.6
1	B	1	MET	2.5
1	A	494	SER	2.5
1	B	485	ASP	2.5
1	B	980	GLN	2.5
1	A	867	ASN	2.4
1	B	551	GLU	2.3
1	A	432	CYS	2.3
1	A	631	GLY	2.3
1	A	637	THR	2.3
1	A	633	PRO	2.3
1	A	550	SER	2.3
1	A	981	PHE	2.2
1	A	531	TYR	2.2
1	B	981	PHE	2.2
1	A	644	THR	2.2
1	A	915	PHE	2.2
1	B	853	TRP	2.1
1	B	863	TYR	2.1
1	B	883	ASP	2.1
1	B	460	ASP	2.1
1	A	851	GLU	2.0
1	B	753	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 i

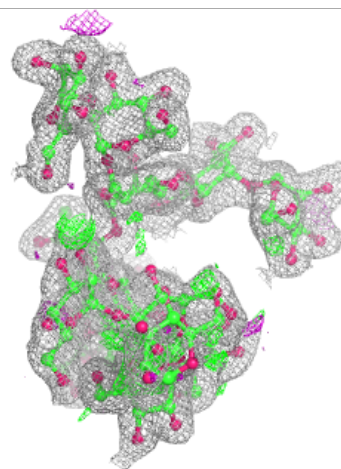
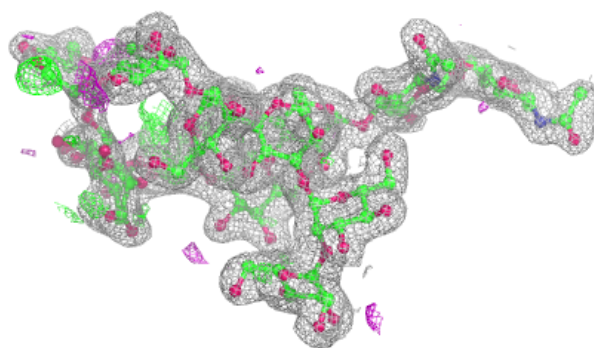
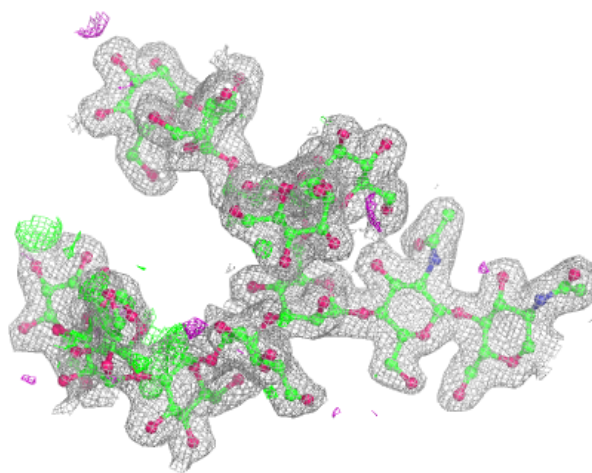
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.01	1.18	100,133,145,147	0
3	NAG	D	2	14/15	0.41	0.42	76,87,94,95	0
3	NAG	F	1	14/15	0.57	0.47	88,106,117,130	0
2	MAN	C	6[A]	11/12	0.75	0.24	43,46,48,49	11
2	MAN	C	6[B]	11/12	0.75	0.24	45,47,50,50	11
3	NAG	D	1	14/15	0.75	0.17	56,64,74,79	0
2	MAN	C	7	11/12	0.79	0.14	31,43,48,52	0
2	MAN	E	6	11/12	0.79	0.30	49,53,58,61	0
2	MAN	E	7	11/12	0.83	0.18	29,46,52,61	0
2	MAN	C	5	11/12	0.84	0.11	27,38,43,44	0
2	MAN	E	5	11/12	0.89	0.11	24,39,46,47	0
2	MAN	E	10	11/12	0.89	0.13	34,39,43,45	0
2	MAN	E	9	11/12	0.94	0.09	28,32,36,37	0
2	NAG	E	2	14/15	0.95	0.11	15,22,31,38	0
2	NAG	E	1	14/15	0.95	0.12	21,24,28,39	0
2	NAG	C	2	14/15	0.96	0.11	21,24,33,38	0
2	MAN	C	4	11/12	0.96	0.07	26,31,40,42	0
2	MAN	E	4	11/12	0.96	0.09	24,30,37,41	0
2	MAN	C	9	11/12	0.96	0.07	25,25,30,30	0
2	MAN	C	8	11/12	0.97	0.07	17,19,22,25	0
2	BMA	E	3	11/12	0.97	0.07	18,22,27,29	0
2	BMA	C	3	11/12	0.97	0.07	18,18,23,24	0
2	MAN	C	10	11/12	0.97	0.07	28,31,38,44	0
2	MAN	C	12	11/12	0.97	0.06	17,18,20,21	0
2	NAG	C	1	14/15	0.97	0.10	21,24,28,34	0
2	MAN	C	11	11/12	0.98	0.06	17,20,24,25	0
2	MAN	E	8	11/12	0.98	0.07	17,20,24,24	0
2	MAN	E	11	11/12	0.98	0.05	18,21,24,26	0
2	MAN	E	12	11/12	0.98	0.07	15,17,20,22	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.

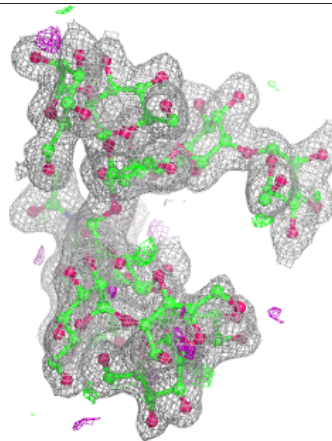
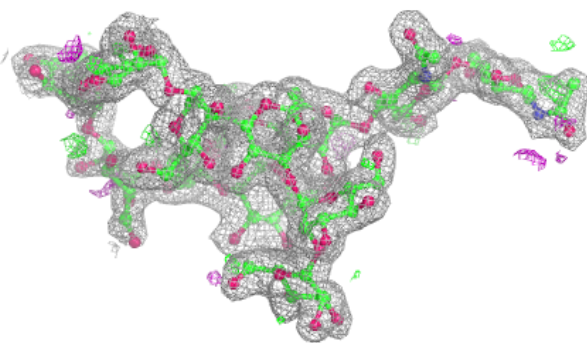
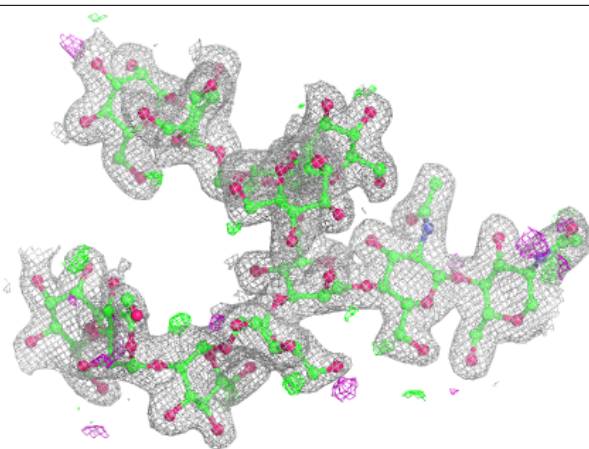
Electron density around Chain C:

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



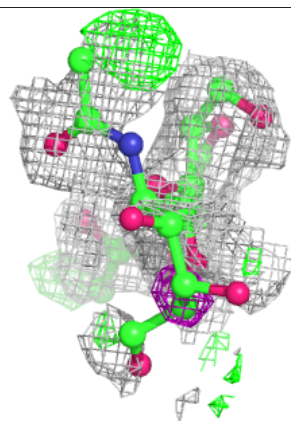
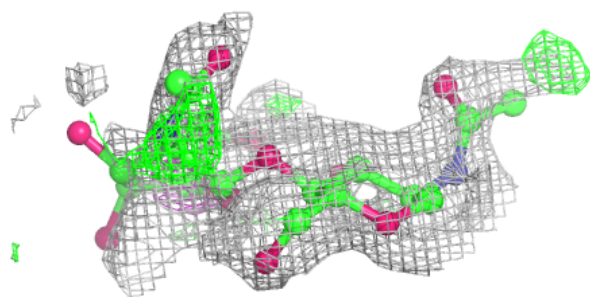
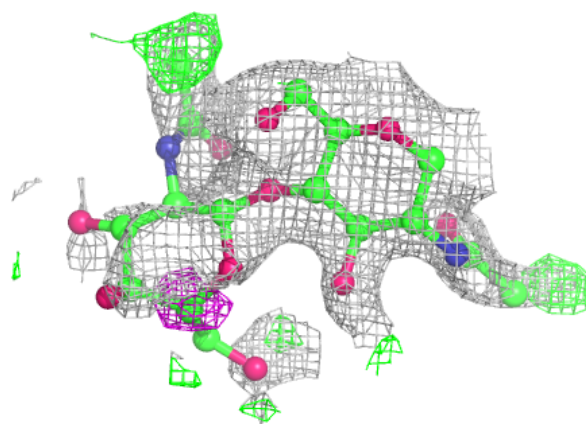
Electron density around Chain E:

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

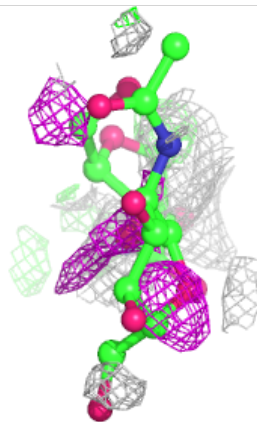
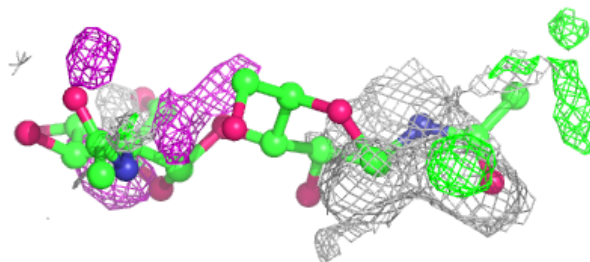
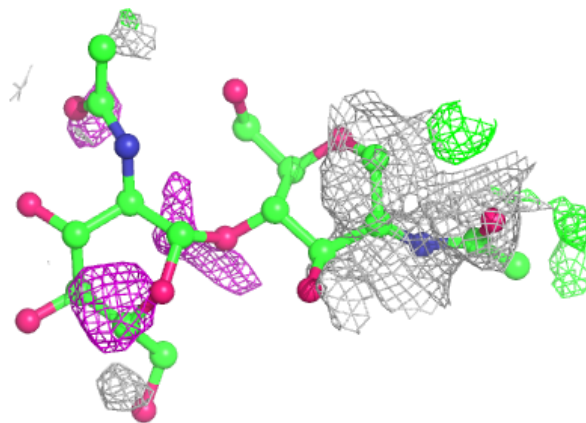


Electron density around Chain D:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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	ZN	A	1001	1/1	1.00	0.09	16,16,16,16	0
4	ZN	B	1001	1/1	1.00	0.08	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.