Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 10:25 PM EDT

PDB ID	:	6B9P
Title	:	Structure of GH 38 Jack Bean alpha-mannosidase in complex with a 36-valent iminosugar cluster inhibitor
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	:	2.00 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:

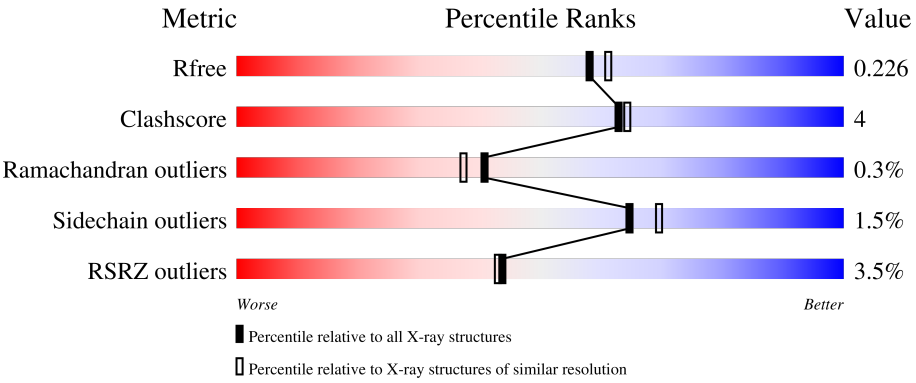
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	3% 86% 9% • 5%
1	B	981	4% 85% 9% • 5%
2	C	12	92% 8%
2	E	12	8% 67% 25%

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Mol	Chain	Length	Quality of chain
3	D	2	50% 50%
3	F	2	50% 50%

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

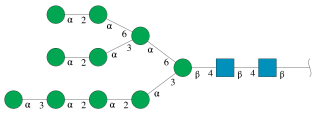
There are 6 unique types of molecules in this entry. The entry contains 16720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	933	Total	C	N	O	S	0	1	0
			7484	4755	1274	1425	30			
1	B	929	Total	C	N	O	S	0	3	0
			7468	4745	1268	1424	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
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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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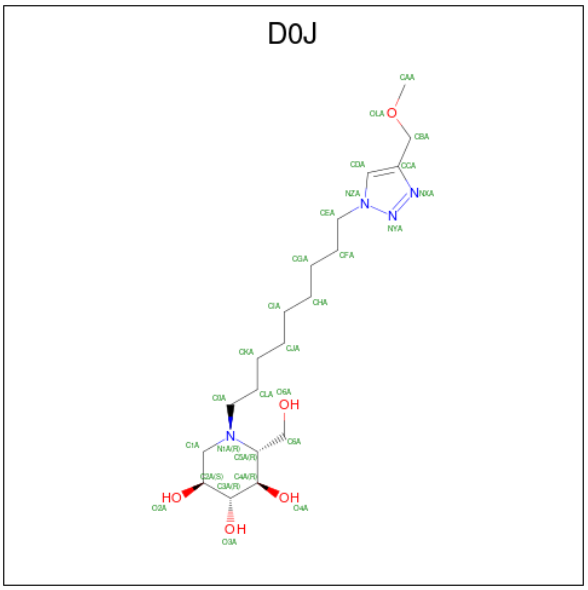
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is (2R,3R,4R,5S)-2-(hydroxymethyl)-1-{9-[4-(methoxymethyl)-1H-1,2,3-triazol-1-yl]nonyl}piperidine-3,4,5-triol (three-letter code: D0J) (formula: $C_{19}H_{36}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 28 19 4 5	0	0
4	B	1	Total C N O 28 19 4 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	694	Total O 694 694	0	0

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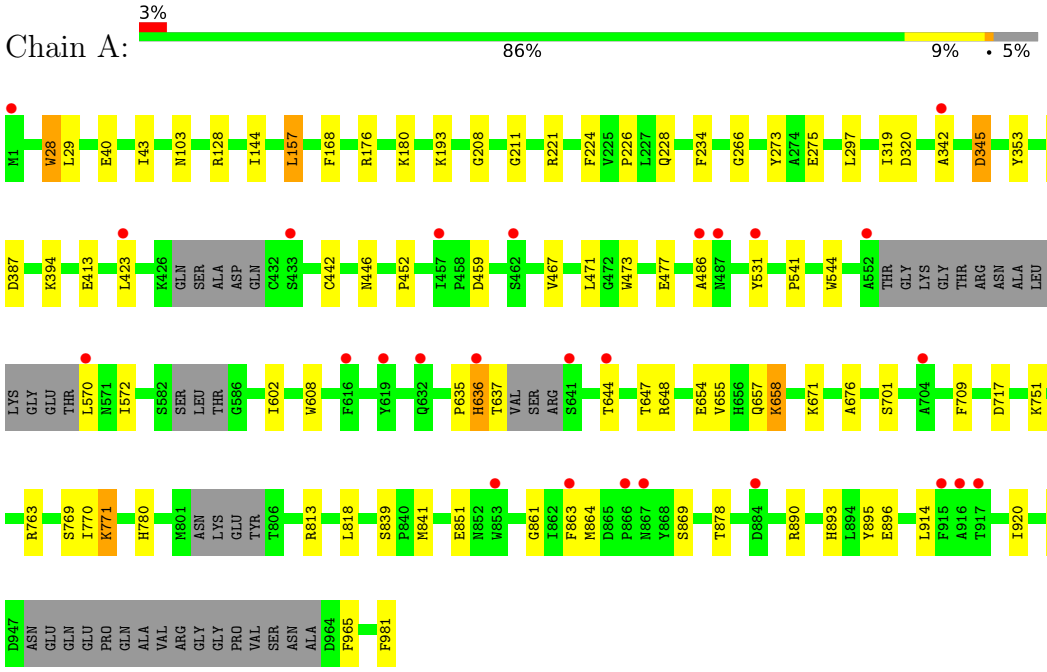
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	673	Total	O	0	0
			673	673		

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.

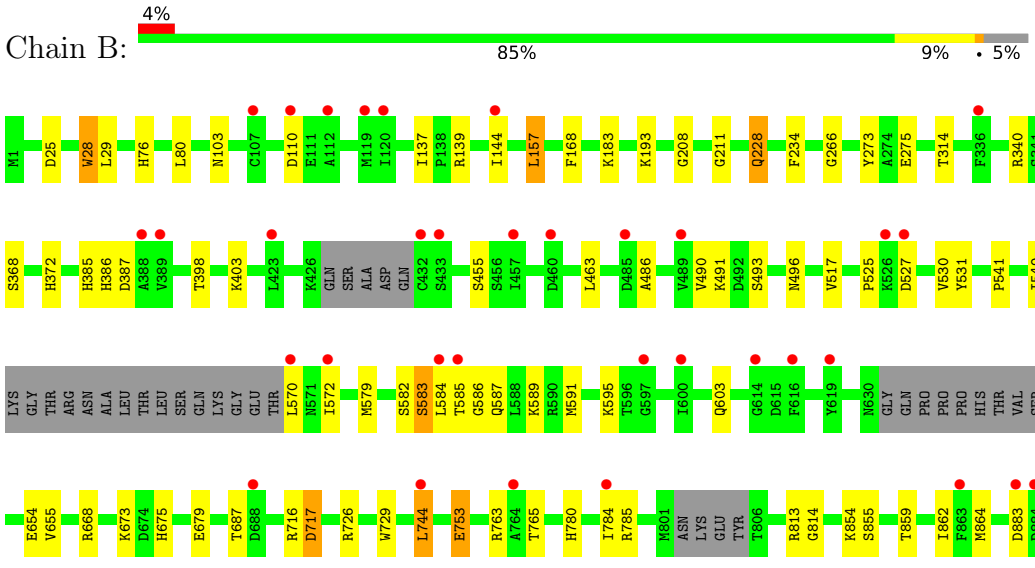
• Molecule 1: Alpha-mannosidase from Canavalia ensiformis (jack bean)

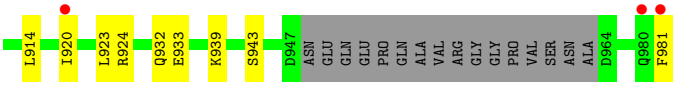
Chain A:



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

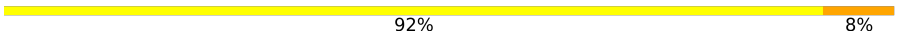
Chain B:





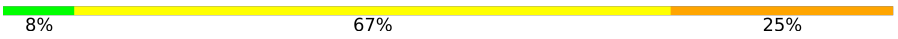
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-be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

Chain C:



• 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:



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

Chain D:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.27Å 119.76Å 277.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.00 48.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.26-2.00) 99.1 (48.26-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.178 , 0.225 0.178 , 0.226	Depositor DCC
R_{free} test set	7562 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16720	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, NAG, BMA, D0J, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.45	0/7676	0.60	1/10406 (0.0%)
1	B	0.43	0/7660	0.59	2/10382 (0.0%)
All	All	0.44	0/15336	0.59	3/20788 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	157	LEU	CA-CB-CG	-8.39	96.00	115.30
1	A	157	LEU	CA-CB-CG	-7.69	97.62	115.30
1	B	744	LEU	CA-CB-CG	5.06	126.94	115.30

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	7484	0	7206	63	0
1	B	7468	0	7199	60	0
2	C	149	0	125	7	0
2	E	138	0	115	8	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	0	0	0
4	B	28	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	694	0	0	8	0
6	B	673	0	0	9	0
All	All	16720	0	14695	129	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 4.

All (129) 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:813:ARG:H	2:E:1:NAG:H81	1.39	0.86
1:B:570:LEU:HG	1:B:583:SER:HB2	1.58	0.85
1:B:862:ILE:HG12	1:B:864:MET:H	1.58	0.69
1:B:579:MET:HG2	1:B:591:MET:HG2	1.74	0.69
1:A:570:LEU:HD21	1:A:648:ARG:NH2	2.11	0.66
1:A:570:LEU:C	1:A:570:LEU:HD13	2.17	0.64
1:A:602:ILE:HD12	1:A:701:SER:HB3	1.81	0.63
1:B:193:LYS:NZ	1:B:896:GLU:OE1	2.32	0.62
1:B:654:GLU:HB3	1:B:668:ARG:HG2	1.81	0.62
1:A:924:ARG:NH1	1:A:933:GLU:OE1	2.33	0.61
1:A:644:THR:HG21	1:A:658:LYS:HD3	1.83	0.60
1:B:490:VAL:HG22	1:B:549:ILE:HG12	1.84	0.59
1:A:541:PRO:HB2	1:A:864:MET:HE1	1.84	0.59
1:B:493:SER:O	1:B:854:LYS:NZ	2.35	0.58
1:B:137:ILE:HD13	1:B:932:GLN:HG2	1.86	0.58
1:B:541:PRO:O	1:B:862:ILE:HG13	2.04	0.58
1:A:221:ARG:HA	6:B:1257:HOH:O	2.05	0.57
1:A:851:GLU:HG2	6:A:1631:HOH:O	2.05	0.57
1:B:862:ILE:HD11	1:B:864:MET:HB2	1.86	0.57
1:A:28:TRP:CE3	1:A:29:LEU:HG	2.40	0.57
1:B:183:LYS:NZ	6:B:1107:HOH:O	2.38	0.56
1:B:753:GLU:H	1:B:753:GLU:CD	2.09	0.56
1:A:813:ARG:HB3	2:C:1:NAG:H81	1.88	0.56
1:B:228:GLN:NE2	1:B:234:PHE:O	2.40	0.55
1:B:668:ARG:NH2	1:B:679:GLU:OE2	2.39	0.55
1:B:28:TRP:CE3	1:B:29:LEU:HG	2.41	0.55
1:B:813:ARG:N	2:E:1:NAG:H81	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ILE:HD13	1:A:655:VAL:HG23	1.90	0.54
1:A:751:LYS:HB3	1:A:756:GLU:HG3	1.88	0.54
1:B:385:HIS:CD2	1:B:387:ASP:H	2.26	0.54
6:B:1197:HOH:O	2:E:1:NAG:H83	2.07	0.54
1:A:128:ARG:NH1	6:A:1111:HOH:O	2.40	0.54
1:A:813:ARG:H	2:C:1:NAG:H81	1.72	0.53
1:A:920:ILE:HD13	1:A:981:PHE:CE1	2.44	0.53
1:B:582:SER:O	1:B:583:SER:HB3	2.07	0.52
1:B:673:LYS:HD2	1:B:675:HIS:CE1	2.44	0.52
1:A:648:ARG:HD3	6:A:1559:HOH:O	2.10	0.52
1:B:647:THR:HB	1:B:654:GLU:HG3	1.92	0.52
1:A:385:HIS:CD2	1:A:387:ASP:H	2.28	0.52
6:A:1710:HOH:O	2:C:2:NAG:H81	2.09	0.52
6:B:1710:HOH:O	2:E:2:NAG:H81	2.09	0.52
1:A:342:ALA:HB1	2:C:2:NAG:H82	1.93	0.51
1:A:544:TRP:CH2	1:A:861:GLY:HA3	2.45	0.50
1:A:657:GLN:C	1:A:658:LYS:HD2	2.32	0.50
1:A:644:THR:CG2	1:A:658:LYS:HD3	2.41	0.50
1:A:608:TRP:O	1:A:635:PRO:HD2	2.12	0.50
3:D:1:NAG:O3	3:D:2:NAG:H61	2.12	0.50
1:B:864:MET:HG2	1:B:914:LEU:HA	1.94	0.49
1:A:636:HIS:ND1	1:A:637:THR:N	2.59	0.49
1:A:893:HIS:HE1	1:A:895:TYR:HB2	1.77	0.49
1:B:144:ILE:HA	1:B:168:PHE:HA	1.94	0.49
1:A:570:LEU:HD21	1:A:648:ARG:HH21	1.77	0.49
1:B:687:THR:OG1	1:B:784:ILE:HD11	2.12	0.49
1:B:193:LYS:HZ2	1:B:717:ASP:HB3	1.78	0.48
1:B:530:VAL:HG23	1:B:531:TYR:CD2	2.47	0.48
1:A:459:ASP:N	6:A:1118:HOH:O	2.44	0.48
1:A:541:PRO:HB2	1:A:864:MET:CE	2.42	0.48
1:B:314:THR:HG22	1:B:943:SER:OG	2.14	0.48
1:A:446:ASN:HD22	2:C:1:NAG:H83	1.78	0.48
1:A:144:ILE:HA	1:A:168:PHE:HA	1.96	0.47
1:B:76:HIS:CE1	1:B:80:LEU:HD11	2.48	0.47
1:B:211:GLY:HA2	1:B:266:GLY:O	2.12	0.47
1:B:343:LEU:HD22	1:B:398:THR:HG23	1.96	0.47
1:B:342:ALA:HB1	2:E:2:NAG:H82	1.95	0.47
1:A:486:ALA:HB2	1:A:531:TYR:CE2	2.49	0.47
1:A:193:LYS:HE2	1:A:896:GLU:OE1	2.15	0.47
1:A:754:LYS:HG2	1:A:755:SER:OG	2.15	0.46
1:A:878:THR:HB	1:A:890:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ILE:O	1:A:771:LYS:HD2	2.16	0.46
1:A:676:ALA:HB3	1:A:818:LEU:CD1	2.45	0.46
1:A:467:VAL:O	1:A:544:TRP:HA	2.15	0.46
1:A:818:LEU:O	1:A:818:LEU:HD12	2.15	0.46
1:B:589:LYS:NZ	1:B:603:GLN:HG2	2.31	0.46
1:A:920:ILE:HB	1:A:965:PHE:CE2	2.51	0.45
6:A:1577:HOH:O	2:C:2:NAG:H83	2.16	0.45
1:B:273:TYR:CZ	1:B:275:GLU:HB3	2.51	0.45
1:B:572:ILE:HD13	1:B:655:VAL:HG23	1.97	0.45
1:B:110:ASP:HB2	1:B:386:HIS:HA	1.99	0.45
1:A:771:LYS:HD3	6:A:1521:HOH:O	2.17	0.44
1:A:471:LEU:HD21	1:A:839:SER:HB2	1.99	0.44
1:A:570:LEU:HD13	1:A:570:LEU:O	2.17	0.44
1:A:709:PHE:CD1	1:A:769:SER:HB3	2.53	0.44
1:B:486:ALA:HB2	1:B:531:TYR:CE2	2.52	0.44
1:B:744:LEU:HB2	1:B:765:THR:O	2.16	0.44
1:A:345:ASP:HB2	1:A:763:ARG:CZ	2.47	0.44
1:A:671:LYS:NZ	6:A:1129:HOH:O	2.47	0.44
1:B:493:SER:HB2	1:B:859:THR:HG21	2.00	0.44
1:B:586:GLY:O	1:B:587:GLN:HB3	2.17	0.44
1:A:211:GLY:HA2	1:A:266:GLY:O	2.19	0.43
1:B:862:ILE:HG12	1:B:864:MET:N	2.28	0.43
1:B:668:ARG:NE	6:B:1121:HOH:O	2.46	0.43
6:B:1595:HOH:O	2:E:2:NAG:H83	2.18	0.43
1:A:477:GLU:HB3	1:A:841:MET:SD	2.59	0.43
1:B:367:LYS:NZ	1:B:883:ASP:HA	2.33	0.43
1:A:176:ARG:HG2	1:A:180:LYS:HD2	2.00	0.43
1:A:864:MET:HG2	1:A:914:LEU:HA	2.00	0.43
1:A:224:PHE:O	1:A:226:PRO:HD3	2.19	0.43
1:A:570:LEU:C	1:A:570:LEU:CD1	2.86	0.43
1:B:589:LYS:HA	1:B:589:LYS:HD3	1.86	0.43
1:A:29:LEU:HD22	1:A:394:LYS:HE2	2.00	0.42
1:A:273:TYR:CZ	1:A:275:GLU:HB3	2.54	0.42
1:A:658:LYS:HD2	1:A:658:LYS:N	2.34	0.42
1:A:676:ALA:HB3	1:A:818:LEU:HD11	2.00	0.42
1:B:491:LYS:HA	1:B:496:ASN:O	2.20	0.42
1:B:920:ILE:HD13	1:B:981:PHE:CE1	2.54	0.42
1:B:340:ARG:HD3	1:B:398:THR:HG21	2.01	0.42
1:B:726:ARG:HG3	1:B:729:TRP:CZ2	2.55	0.42
1:A:473:TRP:C	1:A:541:PRO:HB3	2.40	0.42
1:B:139:ARG:NE	6:B:1125:HOH:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:ARG:HD2	1:B:933:GLU:OE2	2.20	0.41
1:B:585:THR:O	1:B:585:THR:OG1	2.36	0.41
1:A:234:PHE:CD1	2:E:7:MAN:H4	2.55	0.41
1:B:673:LYS:HA	1:B:673:LYS:HD3	1.85	0.41
1:B:939:LYS:HD3	6:B:1199:HOH:O	2.20	0.41
1:B:584:LEU:HA	1:B:584:LEU:HD12	1.84	0.41
1:B:517:VAL:HG11	1:B:525:PRO:HB3	2.02	0.41
1:B:763:ARG:NH2	1:B:814:GLY:HA3	2.35	0.41
1:A:423:LEU:HD13	1:A:863:PHE:CZ	2.56	0.41
1:A:647:THR:HB	1:A:654:GLU:HB2	2.03	0.41
1:B:25:ASP:OD2	4:B:1001:D0J:O2A	2.38	0.41
1:A:442:CYS:SG	1:A:452:PRO:HD2	2.61	0.41
1:A:813:ARG:N	2:C:1:NAG:H81	2.36	0.41
1:A:319:ILE:HG22	1:A:320:ASP:N	2.36	0.41
1:A:353:TYR:OH	1:A:413:GLU:HA	2.21	0.41
1:B:403:LYS:NZ	2:E:7:MAN:O2	2.39	0.40
1:B:463:LEU:HB3	1:B:549:ILE:HB	2.02	0.40
1:B:367:LYS:HD2	1:B:368:SER:H	1.86	0.40
1:B:595:LYS:NZ	6:B:1155:HOH:O	2.54	0.40
1:A:40:GLU:HB3	1:A:43:ILE:HD12	2.04	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	920/981 (94%)	879 (96%)	38 (4%)	3 (0%)	41	37
1	B	920/981 (94%)	882 (96%)	35 (4%)	3 (0%)	41	37
All	All	1840/1962 (94%)	1761 (96%)	73 (4%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

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

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	810/849 (95%)	798 (98%)	12 (2%)	65	69
1	B	809/849 (95%)	796 (98%)	13 (2%)	62	67
All	All	1619/1698 (95%)	1594 (98%)	25 (2%)	65	69

All (25) 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	345	ASP
1	A	367	LYS
1	A	636	HIS
1	A	658	LYS
1	A	717	ASP
1	A	754	LYS
1	A	771	LYS
1	A	780	HIS
1	A	869	SER
1	B	157	LEU
1	B	228	GLN
1	B	372	HIS
1	B	455	SER
1	B	527	ASP
1	B	583	SER

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Mol	Chain	Res	Type
1	B	716	ARG
1	B	717	ASP
1	B	753	GLU
1	B	780	HIS
1	B	785	ARG
1	B	855	SER
1	B	923	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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	0.56	0	17,19,21	0.72	0
2	MAN	C	10	2	11,11,12	1.04	0	15,15,17	1.16	1 (6%)
2	MAN	C	11	2	11,11,12	0.94	1 (9%)	15,15,17	1.25	1 (6%)
2	MAN	C	12	2	11,11,12	0.51	0	15,15,17	1.32	1 (6%)
2	NAG	C	2	2	14,14,15	0.65	0	17,19,21	0.96	1 (5%)
2	BMA	C	3	2	11,11,12	1.00	1 (9%)	15,15,17	1.28	1 (6%)
2	MAN	C	4	2	11,11,12	0.85	0	15,15,17	1.38	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	C	5	2	11,11,12	1.20	1 (9%)	15,15,17	1.17	1 (6%)
2	MAN	C	6[A]	2	11,11,12	1.71	2 (18%)	15,15,17	1.22	1 (6%)
2	MAN	C	6[B]	2	11,11,12	1.19	2 (18%)	15,15,17	1.55	4 (26%)
2	MAN	C	7	2	11,11,12	2.32	4 (36%)	15,15,17	1.70	2 (13%)
2	MAN	C	8	2	11,11,12	0.61	0	15,15,17	1.31	2 (13%)
2	MAN	C	9	2	11,11,12	0.60	0	15,15,17	1.23	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.61	0	17,19,21	0.65	0
3	NAG	D	2	3	14,14,15	1.27	1 (7%)	17,19,21	1.22	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	0.87	1 (5%)
2	MAN	E	10	2	11,11,12	0.77	0	15,15,17	1.26	2 (13%)
2	MAN	E	11	2	11,11,12	0.78	0	15,15,17	1.05	1 (6%)
2	MAN	E	12	2	11,11,12	1.10	1 (9%)	15,15,17	1.14	3 (20%)
2	NAG	E	2	2	14,14,15	0.95	1 (7%)	17,19,21	0.65	0
2	BMA	E	3	2	11,11,12	0.76	0	15,15,17	0.85	0
2	MAN	E	4	2	11,11,12	0.62	0	15,15,17	1.16	1 (6%)
2	MAN	E	5	2	11,11,12	1.12	1 (9%)	15,15,17	1.32	2 (13%)
2	MAN	E	6	2	11,11,12	1.23	0	15,15,17	1.56	2 (13%)
2	MAN	E	7	2	11,11,12	2.53	6 (54%)	15,15,17	1.81	4 (26%)
2	MAN	E	8	2	11,11,12	0.94	0	15,15,17	1.17	1 (6%)
2	MAN	E	9	2	11,11,12	0.71	0	15,15,17	1.47	2 (13%)
3	NAG	F	1	3	14,14,15	0.41	0	17,19,21	0.59	0
3	NAG	F	2	3	14,14,15	1.38	2 (14%)	17,19,21	0.95	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	-	2/6/23/26	0/1/1/1
2	MAN	C	10	2	-	1/2/19/22	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	-	2/2/19/22	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

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	MAN	C2-C3	4.85	1.59	1.52
3	D	2	NAG	O5-C1	4.31	1.50	1.43
3	F	2	NAG	O5-C1	4.21	1.50	1.43
2	C	7	MAN	C2-C3	3.88	1.58	1.52
2	E	7	MAN	O3-C3	3.86	1.52	1.43
2	E	7	MAN	C1-C2	3.80	1.60	1.52
2	C	7	MAN	O5-C1	-3.79	1.37	1.43
2	C	7	MAN	O3-C3	3.35	1.50	1.43
2	C	6[A]	MAN	C2-C3	3.26	1.57	1.52
2	C	7	MAN	C4-C3	3.19	1.60	1.52
2	C	6[A]	MAN	O5-C1	-3.17	1.38	1.43
2	E	5	MAN	O5-C5	3.06	1.49	1.43
2	E	2	NAG	O5-C1	-3.05	1.38	1.43
2	C	5	MAN	C2-C3	3.00	1.56	1.52
2	C	6[B]	MAN	C1-C2	2.90	1.58	1.52
3	F	2	NAG	C1-C2	2.70	1.56	1.52
2	E	7	MAN	O2-C2	-2.36	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	MAN	O5-C5	2.32	1.48	1.43
2	E	12	MAN	O5-C1	-2.20	1.40	1.43
2	E	1	NAG	C1-C2	2.14	1.55	1.52
2	E	7	MAN	C4-C5	2.10	1.57	1.53
2	C	3	BMA	C4-C5	2.04	1.57	1.53
2	C	6[B]	MAN	O5-C5	2.02	1.47	1.43
2	E	7	MAN	O5-C5	2.02	1.47	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	7	MAN	C1-C2-C3	5.01	115.82	109.67
2	E	6	MAN	C1-O5-C5	4.82	118.72	112.19
3	D	2	NAG	C1-O5-C5	4.80	118.69	112.19
2	E	9	MAN	C1-O5-C5	4.27	117.98	112.19
2	C	7	MAN	C1-C2-C3	4.11	114.72	109.67
2	C	6[B]	MAN	C1-O5-C5	3.97	117.57	112.19
2	E	4	MAN	O2-C2-C3	-3.88	102.36	110.14
2	C	12	MAN	C1-O5-C5	3.79	117.32	112.19
2	C	11	MAN	O2-C2-C3	-3.77	102.58	110.14
2	C	8	MAN	C1-O5-C5	3.58	117.04	112.19
3	F	2	NAG	C1-O5-C5	3.52	116.97	112.19
2	C	3	BMA	C1-O5-C5	3.40	116.80	112.19
2	C	9	MAN	C1-O5-C5	3.35	116.74	112.19
2	C	4	MAN	O2-C2-C3	-3.33	103.46	110.14
2	C	2	NAG	C1-O5-C5	3.23	116.57	112.19
2	E	8	MAN	C1-O5-C5	3.14	116.44	112.19
2	C	5	MAN	C1-O5-C5	3.13	116.43	112.19
2	E	11	MAN	O2-C2-C3	-3.05	104.03	110.14
2	E	9	MAN	O2-C2-C3	-2.88	104.36	110.14
2	C	4	MAN	C1-O5-C5	2.88	116.09	112.19
2	E	10	MAN	O2-C2-C3	-2.86	104.42	110.14
2	C	6[B]	MAN	C1-C2-C3	2.77	113.07	109.67
2	E	5	MAN	C1-O5-C5	2.72	115.88	112.19
2	E	5	MAN	O2-C2-C3	-2.71	104.71	110.14
2	E	12	MAN	C1-O5-C5	2.68	115.82	112.19
2	E	1	NAG	C1-O5-C5	2.57	115.67	112.19
2	C	10	MAN	C1-O5-C5	2.56	115.67	112.19
2	E	7	MAN	O2-C2-C3	-2.47	105.19	110.14
2	C	9	MAN	O2-C2-C3	-2.45	105.23	110.14
2	E	10	MAN	C1-O5-C5	2.41	115.46	112.19
2	E	6	MAN	O5-C1-C2	2.38	114.44	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	7	MAN	O2-C2-C3	-2.38	105.38	110.14
2	E	7	MAN	O5-C1-C2	2.35	114.40	110.77
2	C	6[B]	MAN	O2-C2-C3	-2.25	105.64	110.14
2	E	7	MAN	O3-C3-C2	2.23	114.26	109.99
2	E	12	MAN	O2-C2-C1	2.17	113.59	109.15
2	C	8	MAN	O2-C2-C3	-2.10	105.93	110.14
2	E	12	MAN	O2-C2-C3	-2.10	105.94	110.14
2	C	6[A]	MAN	C2-C3-C4	2.06	114.45	110.89
2	C	6[B]	MAN	O2-C2-C1	2.03	113.30	109.15

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6[B]	MAN	C4-C5-C6-O6
2	E	6	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	6[B]	MAN	O5-C5-C6-O6
2	C	6[A]	MAN	C4-C5-C6-O6
2	E	6	MAN	C4-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	D	2	NAG	O5-C5-C6-O6
2	C	6[A]	MAN	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	E	10	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
2	E	10	MAN	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7
2	C	10	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

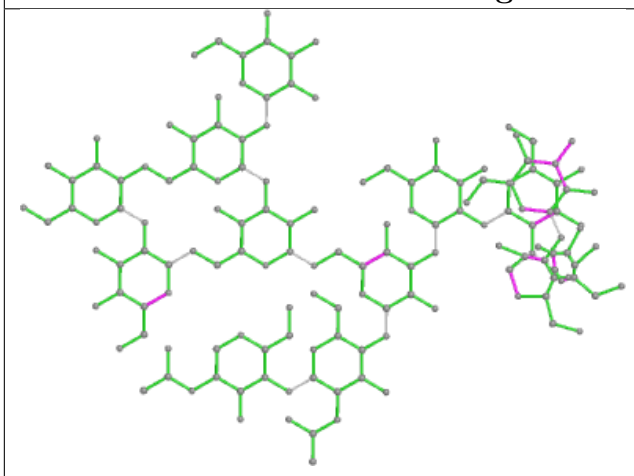
Mol	Chain	Res	Type	Atoms
2	C	6[B]	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 16 short contacts:

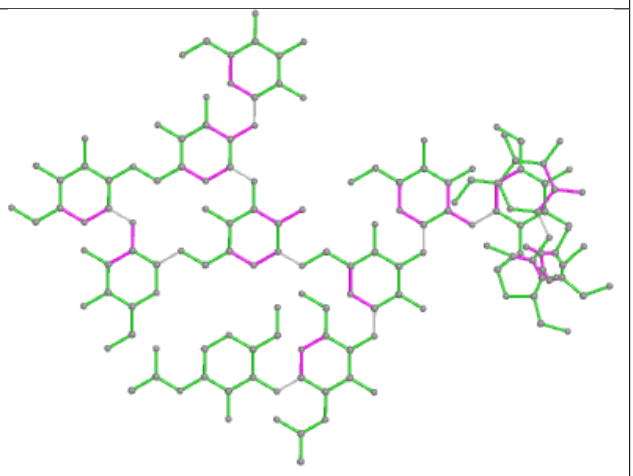
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	MAN	2	0
2	E	2	NAG	3	0
2	C	1	NAG	4	0
2	C	2	NAG	3	0
3	D	2	NAG	1	0
3	D	1	NAG	1	0
2	E	1	NAG	3	0

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

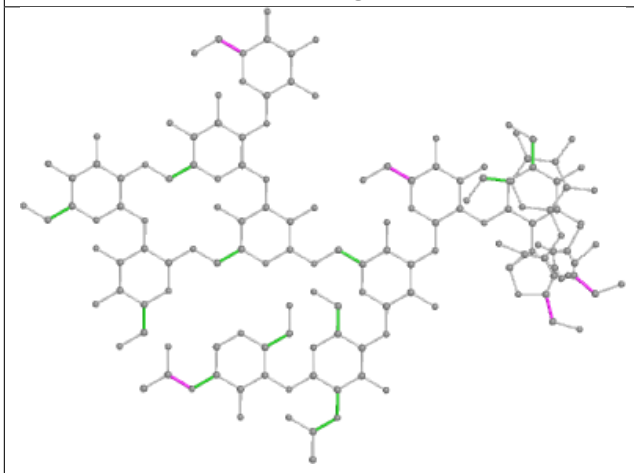
Oligosaccharide Chain C



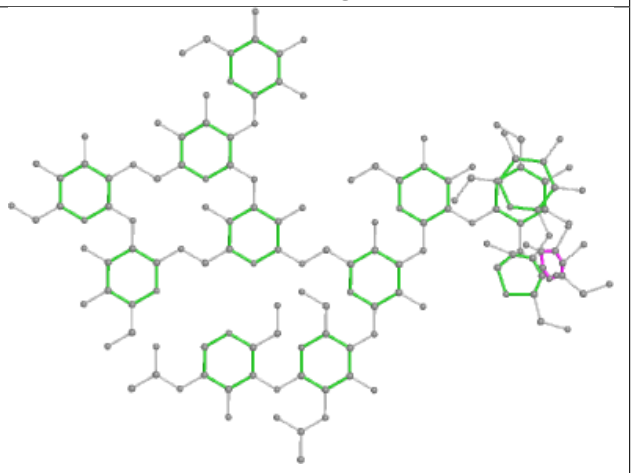
Bond lengths



Bond angles

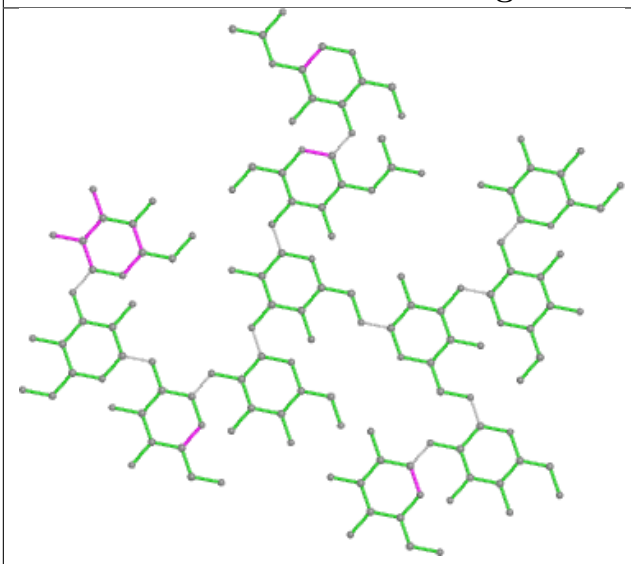


Torsions

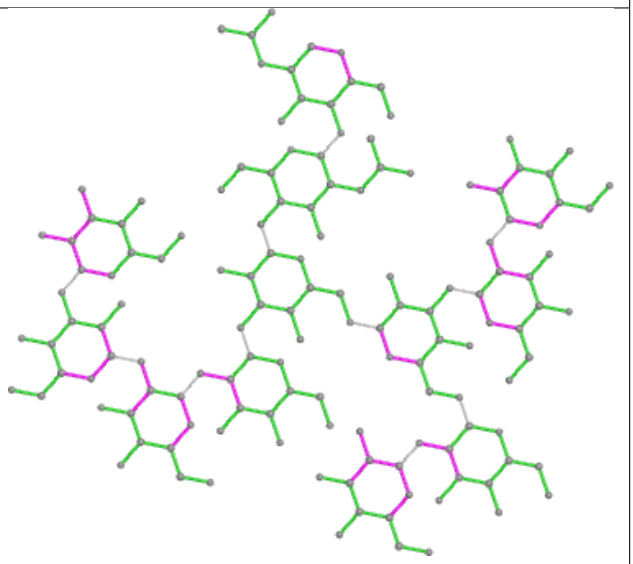


Rings

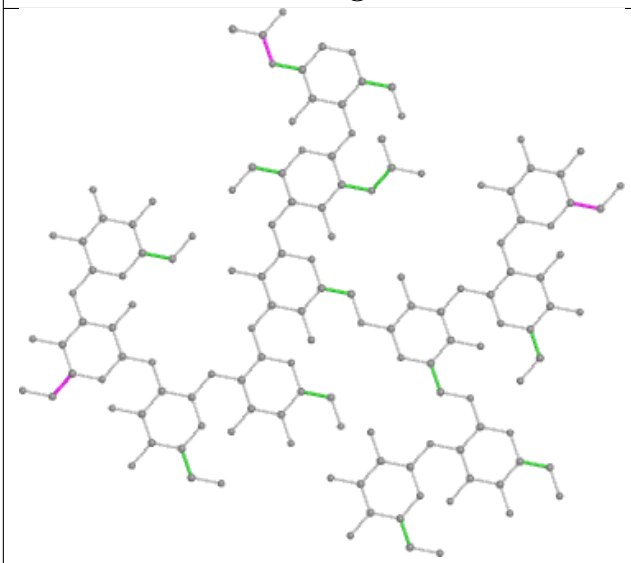
Oligosaccharide Chain E



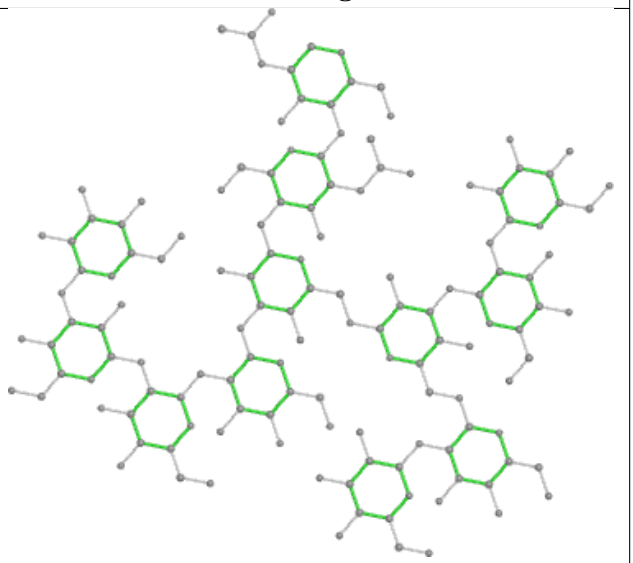
Bond lengths



Bond angles

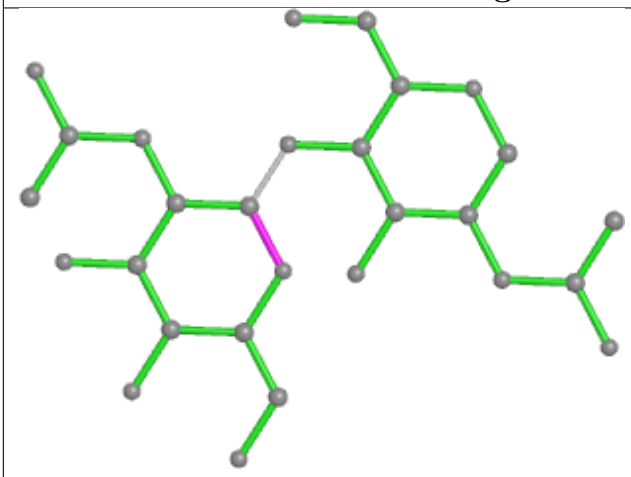


Torsions

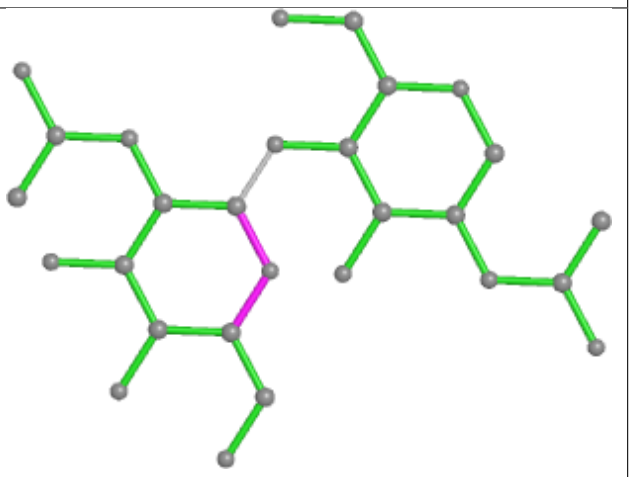


Rings

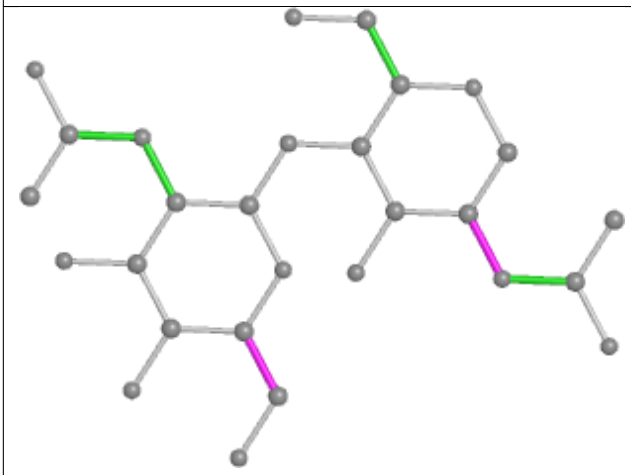
Oligosaccharide Chain D



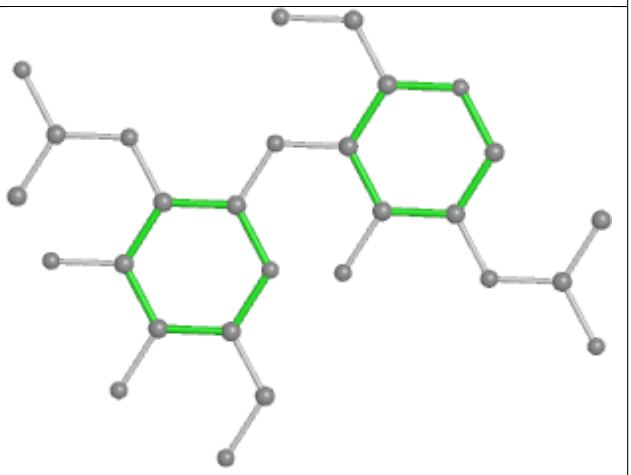
Bond lengths



Bond angles

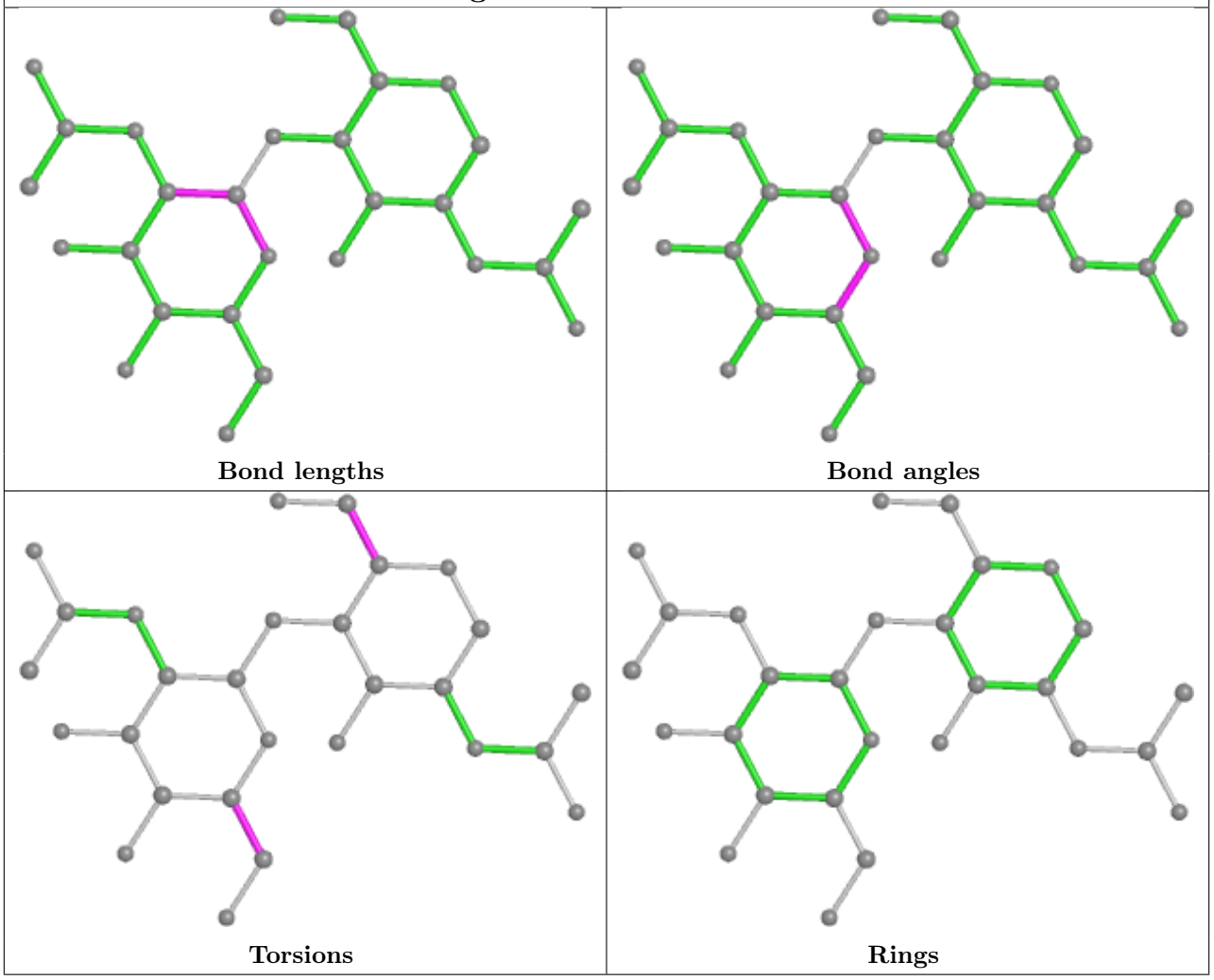


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	D0J	B	1001	5	29,29,29	1.63	3 (10%)	30,37,37	1.97	8 (26%)
4	D0J	A	1001	5	29,29,29	1.14	2 (6%)	30,37,37	1.64	5 (16%)

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	D0J	B	1001	5	-	1/15/37/37	0/2/2/2
4	D0J	A	1001	5	-	2/15/37/37	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	D0J	NXA-NYA	-6.81	1.22	1.34
4	A	1001	D0J	NXA-NYA	-3.06	1.28	1.34
4	A	1001	D0J	CEA-NZA	2.60	1.52	1.47
4	B	1001	D0J	NYA-NZA	-2.57	1.29	1.34
4	B	1001	D0J	C4A-C5A	-2.30	1.48	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	D0J	NXA-NYA-NZA	5.78	111.67	107.31
4	B	1001	D0J	O2A-C2A-C1A	3.88	117.09	109.62
4	A	1001	D0J	NXA-NYA-NZA	3.55	109.99	107.31
4	A	1001	D0J	O2A-C2A-C1A	3.29	115.96	109.62
4	B	1001	D0J	C1A-C2A-C3A	-3.25	106.53	110.24
4	B	1001	D0J	CLA-C0A-N1A	-3.18	105.19	113.88
4	A	1001	D0J	C6A-C5A-N1A	-3.14	105.84	112.55
4	A	1001	D0J	CEA-NZA-CDA	-3.06	122.63	129.82
4	B	1001	D0J	O4A-C4A-C5A	-2.80	104.78	109.77
4	A	1001	D0J	O4A-C4A-C5A	-2.64	105.06	109.77
4	B	1001	D0J	C6A-C5A-N1A	-2.13	108.00	112.55
4	B	1001	D0J	CGA-CFA-CEA	-2.12	104.27	112.32
4	B	1001	D0J	O2A-C2A-C3A	2.00	114.15	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	D0J	CFA-CEA-NZA-CDA
4	A	1001	D0J	CFA-CEA-NZA-NYA
4	B	1001	D0J	CFA-CEA-NZA-NYA

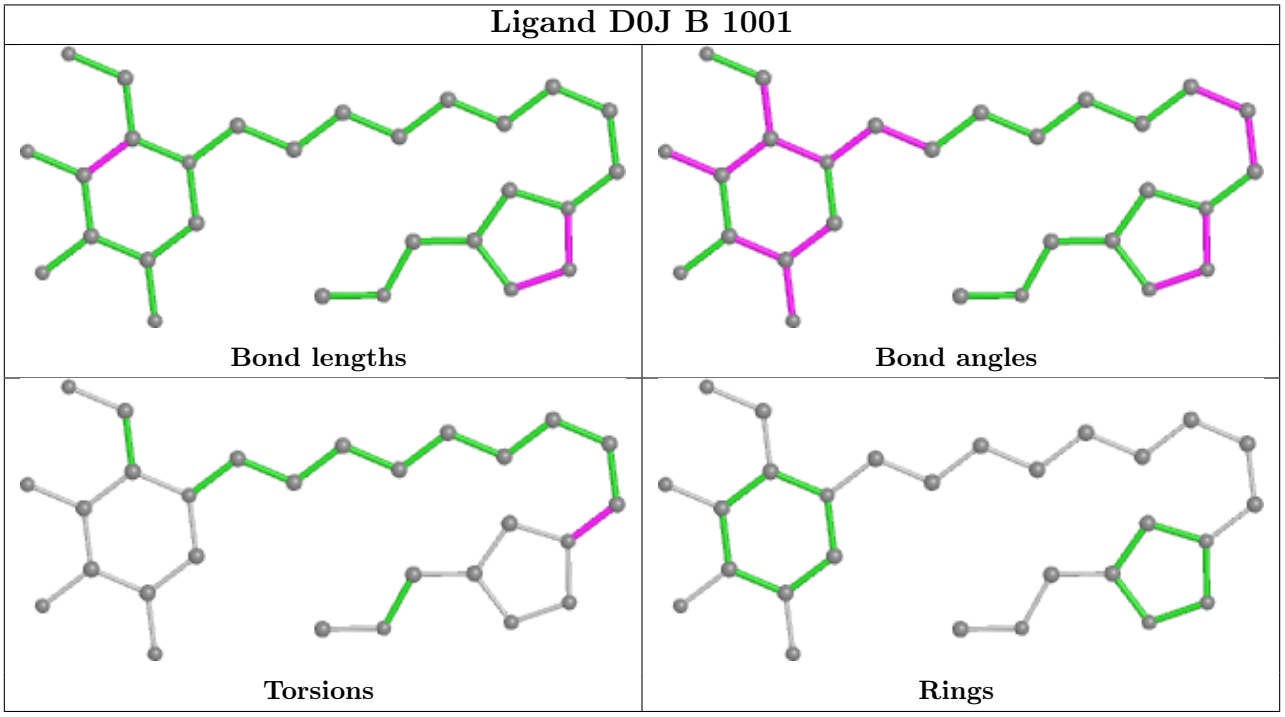
There are no ring outliers.

1 monomer is involved in 1 short contact:

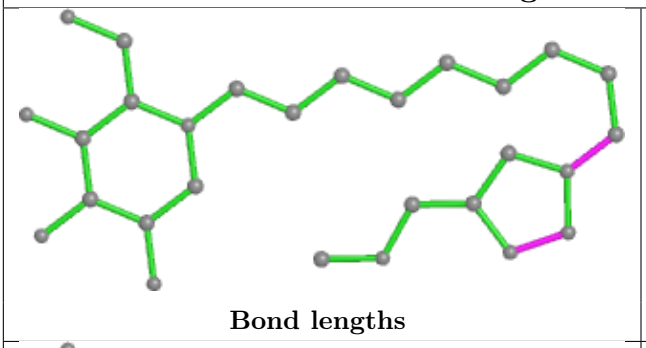
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	D0J	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

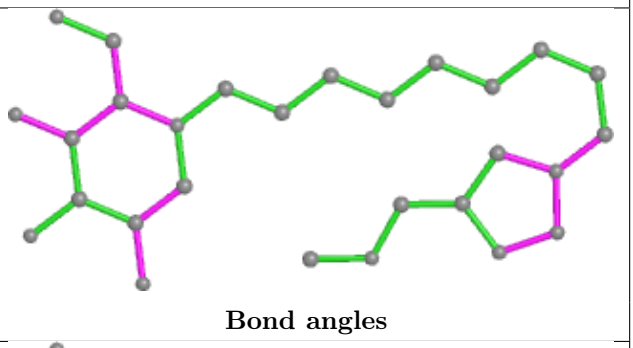
Ligand D0J B 1001



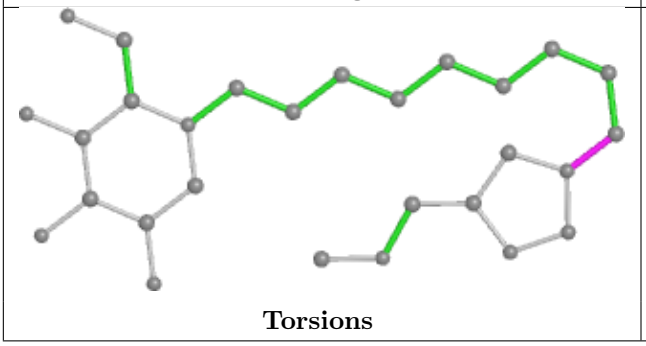
Ligand D0J A 1001



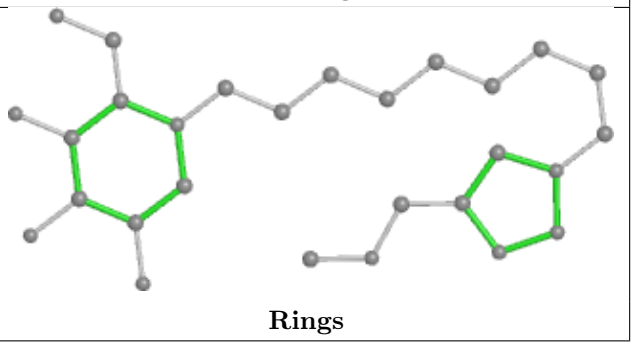
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	933/981 (95%)	0.08	26 (2%)	53	51	16, 28, 51, 74	0
1	B	929/981 (94%)	0.26	39 (4%)	36	35	16, 30, 51, 77	0
All	All	1862/1962 (94%)	0.17	65 (3%)	44	43	16, 29, 51, 77	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	PHE	5.9
1	A	636	HIS	5.8
1	B	432	CYS	4.7
1	A	853	TRP	4.6
1	A	644	THR	4.3
1	B	619	TYR	4.1
1	B	570	LEU	4.0
1	A	619	TYR	3.9
1	B	433	SER	3.9
1	B	884	ASP	3.7
1	B	688	ASP	3.5
1	A	632	GLN	3.2
1	B	600	ILE	3.2
1	B	107	CYS	3.1
1	A	867	ASN	3.0
1	A	866	PRO	3.0
1	A	486	ALA	2.9
1	A	863	PHE	2.9
1	B	552	ALA	2.9
1	A	487	ASN	2.8
1	B	527	ASP	2.8
1	B	457	ILE	2.7
1	B	389	VAL	2.7
1	A	570	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	531	TYR	2.7
1	B	980	GLN	2.7
1	B	764	ALA	2.6
1	B	784	ILE	2.6
1	B	597	GLY	2.6
1	B	886	LEU	2.6
1	B	920	ILE	2.6
1	B	981	PHE	2.5
1	A	552	ALA	2.5
1	B	744	LEU	2.5
1	B	584	LEU	2.5
1	B	585	THR	2.5
1	B	119	MET	2.4
1	A	916	ALA	2.4
1	A	433	SER	2.4
1	B	336	PHE	2.4
1	B	489	VAL	2.4
1	A	1	MET	2.3
1	B	460	ASP	2.3
1	A	616	PHE	2.3
1	A	915	PHE	2.3
1	A	423	LEU	2.3
1	B	423	LEU	2.2
1	B	112	ALA	2.2
1	B	110	ASP	2.2
1	A	342	ALA	2.2
1	B	883	ASP	2.2
1	A	917	THR	2.2
1	A	457	ILE	2.1
1	B	388	ALA	2.1
1	A	641	SER	2.1
1	A	884	ASP	2.1
1	B	863	PHE	2.1
1	A	462	SER	2.1
1	B	614	GLY	2.1
1	B	120	ILE	2.1
1	B	144	ILE	2.1
1	B	485	ASP	2.0
1	A	704	ALA	2.0
1	B	572	ILE	2.0
1	B	526	LYS	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)

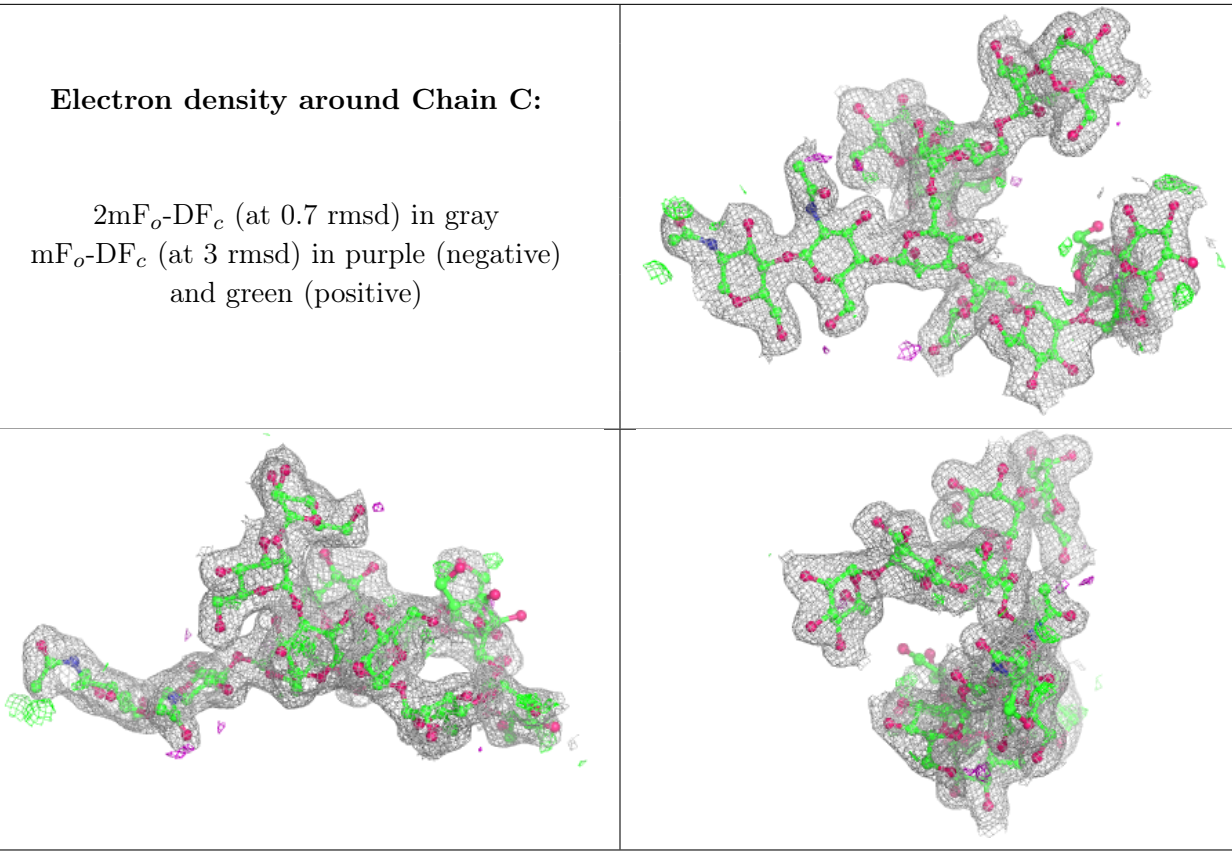
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.24	0.69	60,92,99,100	0
3	NAG	D	2	14/15	0.33	0.44	92,105,113,114	0
3	NAG	F	1	14/15	0.38	0.60	85,98,102,103	0
2	MAN	C	6[B]	11/12	0.73	0.31	52,54,56,57	11
2	MAN	C	6[A]	11/12	0.73	0.31	50,54,56,56	11
2	MAN	E	6	11/12	0.74	0.20	52,57,61,64	0
2	MAN	E	7	11/12	0.77	0.24	31,49,54,54	0
2	MAN	C	7	11/12	0.79	0.16	37,48,54,55	0
3	NAG	D	1	14/15	0.80	0.20	70,83,89,95	0
2	MAN	E	5	11/12	0.91	0.10	29,42,48,53	0
2	MAN	C	5	11/12	0.92	0.09	29,41,45,50	0
2	MAN	E	9	11/12	0.93	0.10	29,31,36,37	0
2	MAN	E	10	11/12	0.93	0.12	34,37,44,44	0
2	MAN	C	4	11/12	0.93	0.11	29,35,43,44	0
2	MAN	C	9	11/12	0.94	0.10	28,31,35,36	0
2	NAG	C	2	14/15	0.94	0.12	23,27,34,38	0
2	MAN	C	10	11/12	0.95	0.08	28,33,37,46	0
2	MAN	E	11	11/12	0.95	0.09	21,23,25,27	0
2	NAG	E	1	14/15	0.95	0.12	24,27,30,36	0
2	NAG	E	2	14/15	0.95	0.12	21,26,32,36	0
2	MAN	E	8	11/12	0.95	0.10	20,24,27,27	0
2	MAN	E	4	11/12	0.95	0.08	28,34,40,43	0
2	MAN	E	12	11/12	0.96	0.11	17,20,23,24	0
2	MAN	C	11	11/12	0.96	0.08	22,24,26,32	0
2	MAN	C	12	11/12	0.96	0.07	18,20,23,23	0
2	BMA	C	3	11/12	0.96	0.10	20,24,25,26	0
2	MAN	C	8	11/12	0.96	0.11	22,24,27,30	0
2	BMA	E	3	11/12	0.97	0.08	23,25,28,28	0
2	NAG	C	1	14/15	0.97	0.15	22,25,30,35	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.

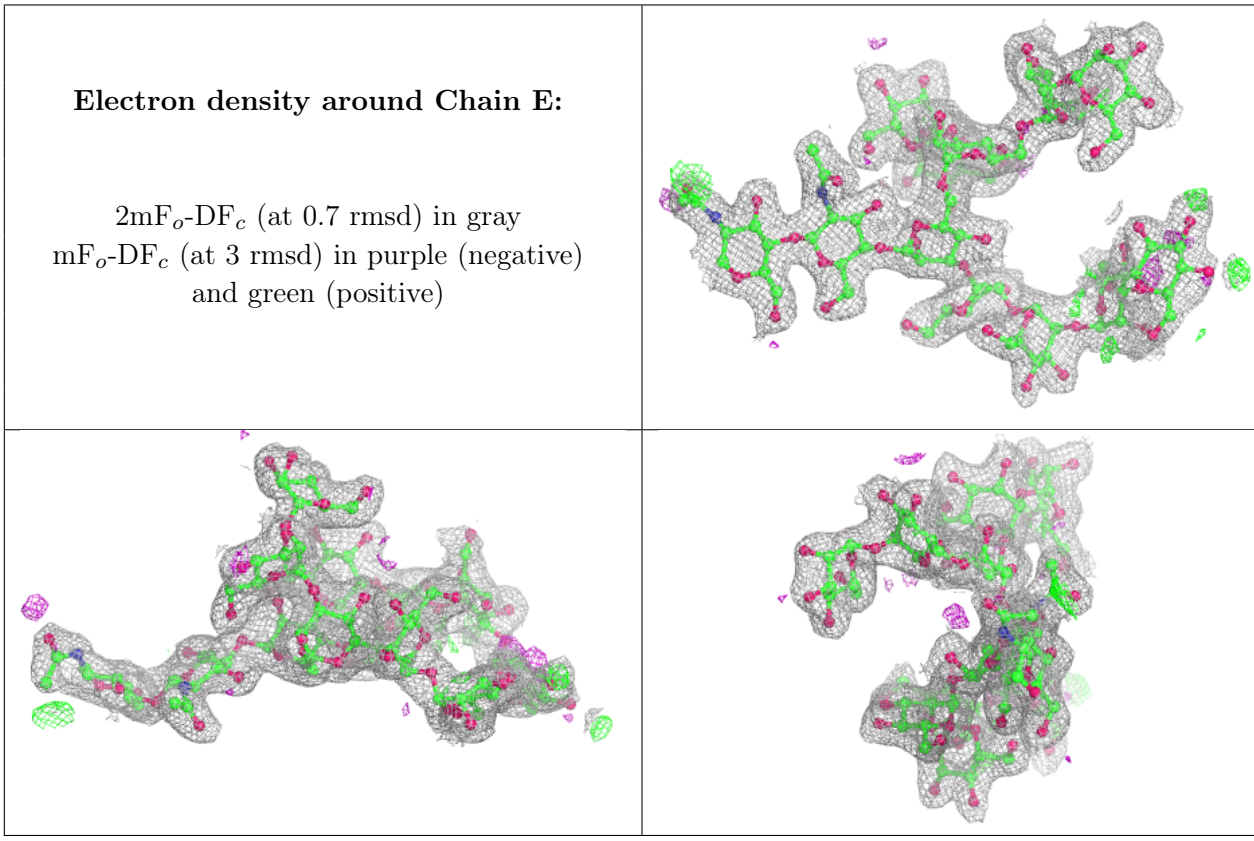
Electron density around Chain C:

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



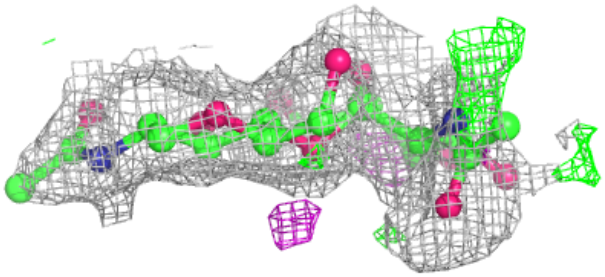
Electron density around Chain E:

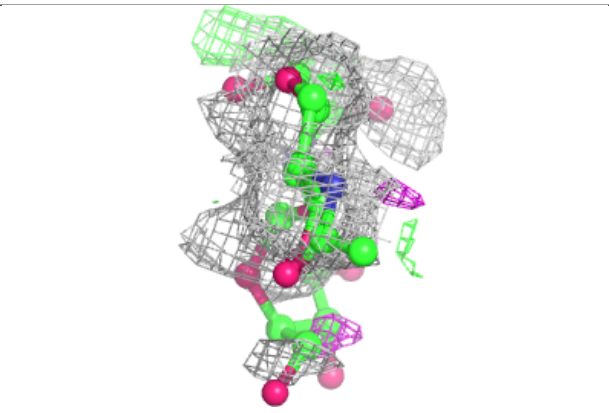
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain D:

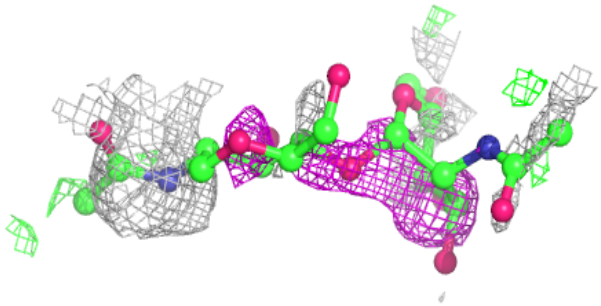
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

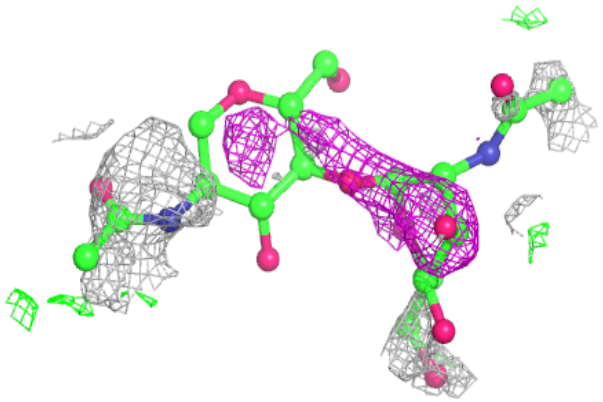




Electron density around Chain F:

$2mF_o$-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)

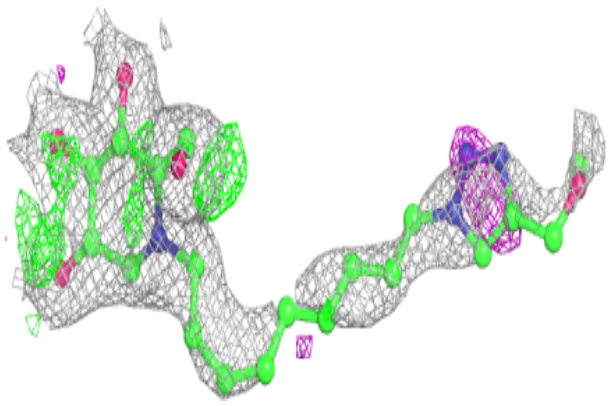
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

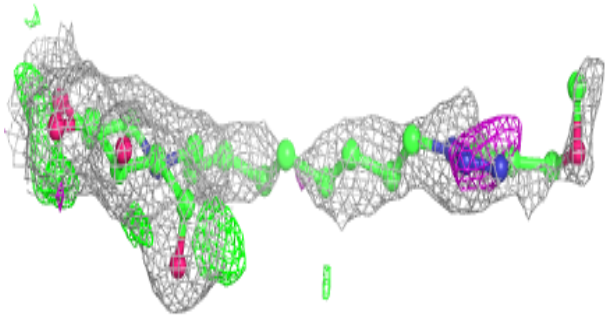
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	D0J	B	1001	28/28	0.73	0.30	19,36,74,78	0
4	D0J	A	1001	28/28	0.83	0.24	17,32,76,82	0
5	ZN	B	1002	1/1	0.99	0.11	20,20,20,20	0
5	ZN	A	1002	1/1	1.00	0.10	18,18,18,18	0

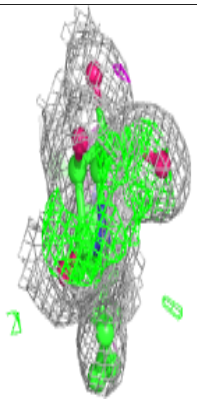
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around D0J B 1001:

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

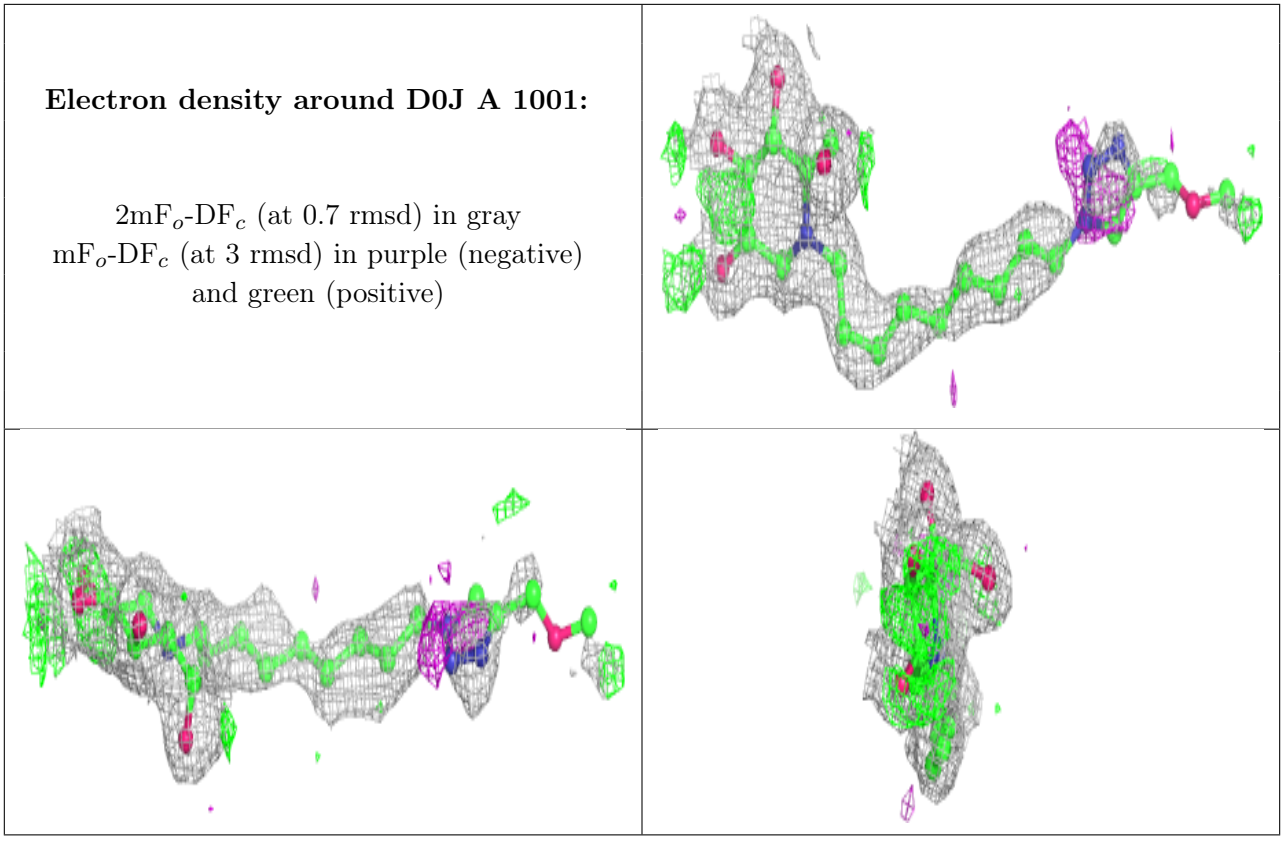






Electron density around D0J A 1001:

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



6.5 Other polymers (i)

There are no such residues in this entry.