



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:41 AM UTC

PDB ID : 6DBS / pdb_00006db
Title : Fusion surface structure, function, and dynamics of gamete fusogen HAP2
Authors : Feng, J.; Dong, X.; Springer, T.A.
Deposited on : 2018-05-03
Resolution : 2.60 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

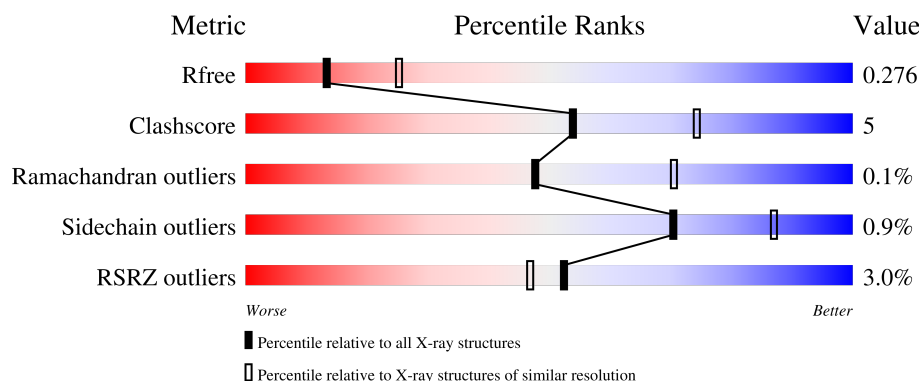
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	565	2% 79% 12% 9%
1	B	565	3% 79% 12% 9%
1	C	565	3% 79% 12% 9%
2	D	3	100%
3	E	4	75% 25%

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Mol	Chain	Length	Quality of chain
3	F	4	 75% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11975 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 Hapless 2.

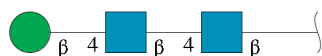
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			3875	2424	664	758	29			
1	C	515	Total	C	N	O	S	0	0	0
			3870	2421	663	757	29			
1	B	515	Total	C	N	O	S	0	0	0
			3870	2421	663	757	29			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP A4GRC6
A	583	HIS	-	expression tag	UNP A4GRC6
A	584	HIS	-	expression tag	UNP A4GRC6
A	585	HIS	-	expression tag	UNP A4GRC6
A	586	HIS	-	expression tag	UNP A4GRC6
A	587	HIS	-	expression tag	UNP A4GRC6
A	588	HIS	-	expression tag	UNP A4GRC6
C	?	-	THR	deletion	UNP A4GRC6
C	583	HIS	-	expression tag	UNP A4GRC6
C	584	HIS	-	expression tag	UNP A4GRC6
C	585	HIS	-	expression tag	UNP A4GRC6
C	586	HIS	-	expression tag	UNP A4GRC6
C	587	HIS	-	expression tag	UNP A4GRC6
C	588	HIS	-	expression tag	UNP A4GRC6
B	?	-	THR	deletion	UNP A4GRC6
B	583	HIS	-	expression tag	UNP A4GRC6
B	584	HIS	-	expression tag	UNP A4GRC6
B	585	HIS	-	expression tag	UNP A4GRC6
B	586	HIS	-	expression tag	UNP A4GRC6
B	587	HIS	-	expression tag	UNP A4GRC6
B	588	HIS	-	expression tag	UNP A4GRC6

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



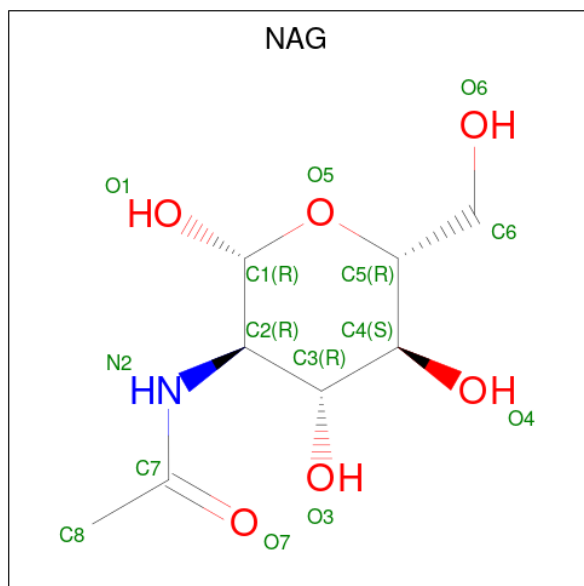
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 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
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

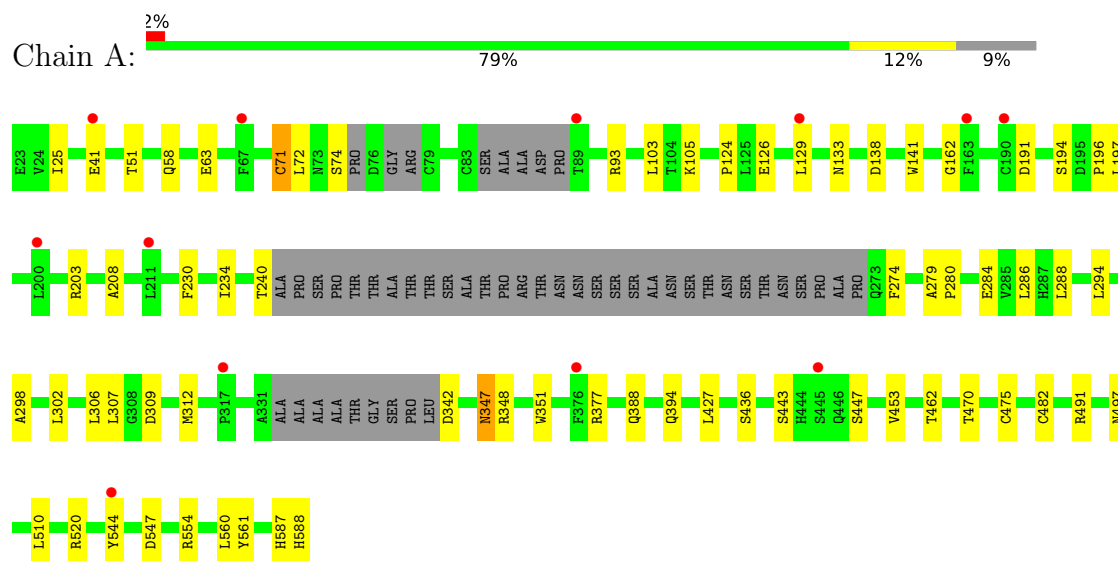
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	C	31	Total O 31 31	0	0
5	B	33	Total O 33 33	0	0

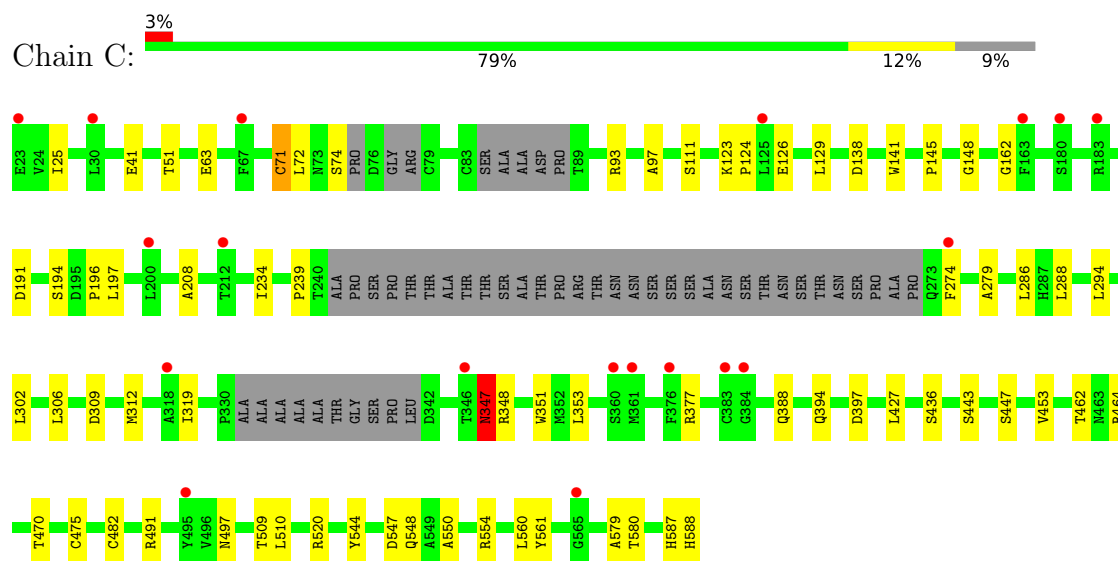
3 Residue-property plots [i](#)

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.

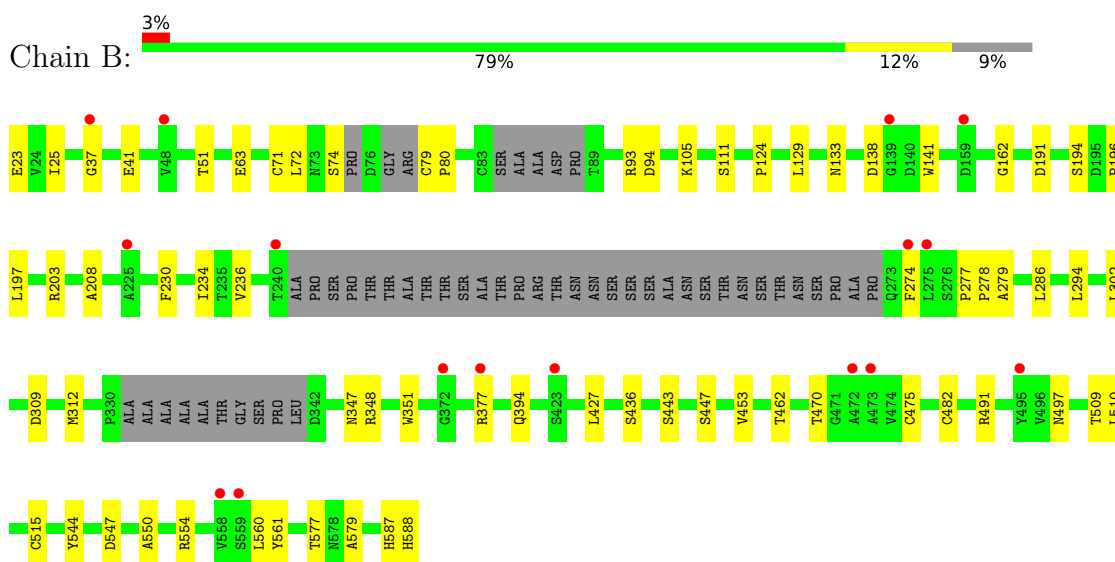
• Molecule 1: Hapless 2



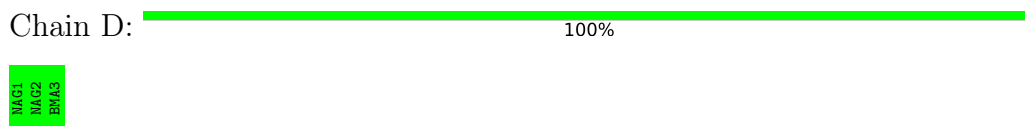
• Molecule 1: Hapless 2



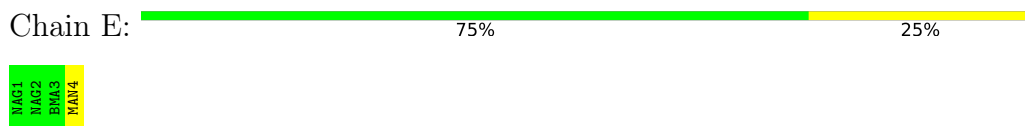
• Molecule 1: Hapless 2



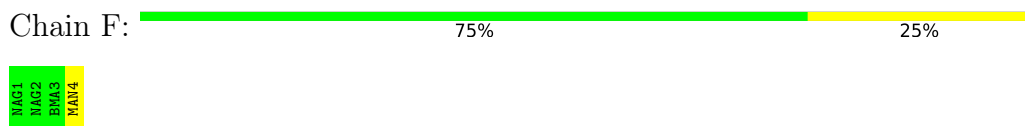
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 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



- Molecule 3: 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.22Å 117.60Å 115.21Å 90.00° 123.79° 90.00°	Depositor
Resolution (Å)	48.99 – 2.60 48.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.99-2.60) 97.1 (48.99-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX V1.0	Depositor
R, R_{free}	0.237 , 0.276 0.239 , 0.276	Depositor DCC
R_{free} test set	1840 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+3/2*k-l,1/2*h+1/2*k+1,1/2*h-1/2*k 0.000 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.000 for -h-k-l,l,k 0.000 for -h+k-l,-l,-k 0.000 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.000 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.460 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.468 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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	0.10	0/3955	0.30	0/5387
1	B	0.10	0/3950	0.30	0/5380
1	C	0.11	0/3950	0.31	1/5380 (0.0%)
All	All	0.10	0/11855	0.30	1/16147 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	ASN	CB-CA-C	-6.33	109.29	116.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ALA	Peptide
1	B	279	ALA	Peptide
1	C	279	ALA	Peptide

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	3875	0	3757	44	0
1	B	3870	0	3752	43	0
1	C	3870	0	3752	44	0
2	D	39	0	34	0	0
3	E	50	0	43	0	0
3	F	50	0	43	0	0
4	A	42	0	39	0	0
4	B	42	0	39	0	0
4	C	42	0	39	0	0
5	A	31	0	0	3	0
5	B	33	0	0	1	0
5	C	31	0	0	2	0
All	All	11975	0	11498	115	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 5.

All (115) 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:C:348:ARG:NH1	1:C:436:SER:O	2.14	0.79
1:A:348:ARG:NH1	1:A:436:SER:O	2.17	0.76
1:B:348:ARG:NH1	1:B:436:SER:O	2.18	0.75
1:B:129:LEU:HB2	1:B:208:ALA:HB3	1.68	0.74
1:B:515:CYS:SG	5:B:701:HOH:O	2.48	0.72
1:A:129:LEU:HB2	1:A:208:ALA:HB3	1.72	0.71
1:B:162:GLY:O	1:B:377:ARG:NH1	2.26	0.69
1:C:129:LEU:HB2	1:C:208:ALA:HB3	1.75	0.68
1:A:162:GLY:O	1:A:377:ARG:NH1	2.28	0.67
1:A:280:PRO:O	5:A:701:HOH:O	2.13	0.66
1:C:162:GLY:O	1:C:377:ARG:NH1	2.30	0.64
1:B:138:ASP:HB2	1:B:377:ARG:HH12	1.61	0.64
1:B:302:LEU:HD13	1:B:453:VAL:HG22	1.82	0.62
1:A:138:ASP:HB2	1:A:377:ARG:HH12	1.63	0.61
1:C:138:ASP:HB2	1:C:377:ARG:HH12	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD13	1:C:453:VAL:HG22	1.84	0.58
1:A:274:PHE:HB3	1:C:41:GLU:HG3	1.84	0.58
1:A:133:ASN:O	1:A:203:ARG:NH2	2.31	0.58
1:B:312:MET:HE3	1:B:443:SER:HB3	1.86	0.56
1:C:312:MET:HE3	1:C:443:SER:HB3	1.88	0.56
1:B:234:ILE:HB	1:B:286:LEU:HB2	1.88	0.55
1:A:312:MET:HE3	1:A:443:SER:HB3	1.89	0.55
1:B:196:PRO:HG2	1:B:197:LEU:HD12	1.88	0.55
1:A:510:LEU:HD13	1:A:560:LEU:HD13	1.88	0.55
1:A:63:GLU:HG2	1:A:462:THR:HG23	1.89	0.54
1:C:274:PHE:HB3	1:B:41:GLU:HG3	1.88	0.54
1:A:196:PRO:HG2	1:A:197:LEU:HD12	1.89	0.54
1:C:234:ILE:HB	1:C:286:LEU:HB2	1.89	0.53
1:A:342:ASP:N	5:A:704:HOH:O	2.41	0.53
1:A:41:GLU:HG3	1:B:274:PHE:HB3	1.90	0.53
1:C:510:LEU:HD13	1:C:560:LEU:HD13	1.91	0.53
1:C:196:PRO:HG2	1:C:197:LEU:HD12	1.90	0.52
1:A:191:ASP:O	1:A:194:SER:OG	2.25	0.51
1:B:63:GLU:HG2	1:B:462:THR:HG23	1.92	0.51
1:C:63:GLU:HG2	1:C:462:THR:HG23	1.92	0.51
1:B:510:LEU:HD13	1:B:560:LEU:HD13	1.92	0.51
1:B:547:ASP:OD2	1:B:554:ARG:NH2	2.43	0.51
1:A:74:SER:HB2	1:A:93:ARG:HE	1.76	0.51
1:C:74:SER:HB2	1:C:93:ARG:HE	1.77	0.50
1:C:124:PRO:HD2	1:C:394:GLN:HG3	1.94	0.50
1:A:274:PHE:HB2	1:C:41:GLU:HA	1.94	0.50
1:C:123:LYS:NZ	1:C:397:ASP:OD2	2.44	0.50
1:A:25:ILE:HG23	1:C:51:THR:HG21	1.94	0.49
1:A:309:ASP:HA	1:A:447:SER:HA	1.95	0.49
1:C:274:PHE:HB2	1:B:41:GLU:HA	1.94	0.49
1:A:41:GLU:HA	1:B:274:PHE:HB2	1.95	0.48
1:A:51:THR:HG21	1:B:25:ILE:HG23	1.95	0.48
1:A:284:GLU:OE2	1:A:298:ALA:N	2.47	0.48
1:C:191:ASP:O	1:C:194:SER:OG	2.27	0.48
1:A:302:LEU:HD13	1:A:453:VAL:HG22	1.96	0.48
1:A:547:ASP:OD2	1:A:554:ARG:NH2	2.47	0.48
1:C:72:LEU:O	1:C:93:ARG:HB3	2.14	0.48
1:A:348:ARG:HA	1:A:351:TRP:CD1	2.50	0.47
1:C:580:THR:N	5:C:701:HOH:O	2.31	0.47
1:A:240:THR:HG22	5:A:701:HOH:O	2.15	0.47
1:C:547:ASP:OD2	1:C:554:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PRO:HD2	1:B:394:GLN:HG3	1.96	0.47
1:A:124:PRO:HD2	1:A:394:GLN:HG3	1.95	0.47
1:C:548:GLN:O	5:C:701:HOH:O	2.20	0.46
1:B:309:ASP:HA	1:B:447:SER:HA	1.98	0.46
1:A:491:ARG:HD3	1:A:544:TYR:CE2	2.51	0.46
1:B:133:ASN:O	1:B:203:ARG:NH2	2.37	0.46
1:B:191:ASP:O	1:B:194:SER:OG	2.27	0.46
1:C:288:LEU:HD23	1:C:306:LEU:HB2	1.97	0.46
1:A:520:ARG:NH2	1:C:111:SER:O	2.49	0.46
1:B:470:THR:N	1:B:497:ASN:O	2.47	0.46
1:B:72:LEU:O	1:B:93:ARG:HB3	2.17	0.45
1:A:561:TYR:CD2	1:C:294:LEU:HD11	2.51	0.45
1:C:97:ALA:HB1	1:C:239:PRO:HG2	1.98	0.45
1:A:470:THR:N	1:A:497:ASN:O	2.50	0.44
1:C:587:HIS:O	1:C:588:HIS:ND1	2.51	0.44
1:C:348:ARG:HA	1:C:351:TRP:CD1	2.52	0.44
1:B:79:CYS:HB3	1:B:80:PRO:HD3	1.99	0.44
1:A:105:LYS:HE3	1:A:230:PHE:CD2	2.53	0.44
1:A:491:ARG:HD3	1:A:544:TYR:CZ	2.52	0.44
1:A:475:CYS:HA	1:A:482:CYS:HA	2.00	0.44
1:C:309:ASP:HA	1:C:447:SER:HA	2.00	0.44
1:C:470:THR:N	1:C:497:ASN:O	2.48	0.44
1:B:509:THR:HB	1:B:561:TYR:HB2	1.99	0.44
1:A:72:LEU:O	1:A:93:ARG:HB3	2.17	0.44
1:A:234:ILE:HB	1:A:286:LEU:HB2	1.99	0.43
1:C:491:ARG:HD3	1:C:544:TYR:CE2	2.53	0.43
1:B:72:LEU:HB2	1:B:94:ASP:HB2	2.01	0.43
1:C:561:TYR:CD2	1:B:294:LEU:HD11	2.53	0.43
1:A:288:LEU:HD23	1:A:306:LEU:HB2	2.00	0.43
1:C:520:ARG:NH2	1:B:111:SER:O	2.52	0.43
1:A:284:GLU:CD	1:A:298:ALA:H	2.26	0.43
1:A:587:HIS:O	1:A:588:HIS:ND1	2.52	0.43
1:B:475:CYS:HA	1:B:482:CYS:HA	2.00	0.43
1:B:587:HIS:O	1:B:588:HIS:ND1	2.52	0.42
1:A:294:LEU:HD11	1:B:561:TYR:CD2	2.54	0.42
1:C:319:ILE:HB	1:C:353:LEU:HD21	2.02	0.42
1:B:348:ARG:HA	1:B:351:TRP:CD1	2.54	0.42
1:C:126:GLU:HB3	1:C:388:GLN:OE1	2.20	0.42
1:C:475:CYS:HA	1:C:482:CYS:HA	2.00	0.42
1:B:491:ARG:HD3	1:B:544:TYR:CZ	2.54	0.42
1:B:550:ALA:HB2	1:B:579:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ARG:HH11	1:B:577:THR:HG21	1.85	0.42
1:A:347:ASN:HB3	1:A:348:ARG:H	1.77	0.41
1:C:550:ALA:HB2	1:C:579:ALA:HB2	2.02	0.41
1:C:464:ARG:O	1:B:37:GLY:N	2.43	0.41
1:B:236:VAL:HG21	1:B:302:LEU:HD23	2.02	0.41
1:C:491:ARG:HD3	1:C:544:TYR:CZ	2.56	0.41
1:B:491:ARG:HD3	1:B:544:TYR:CE2	2.55	0.41
1:C:509:THR:HB	1:C:561:TYR:HB2	2.02	0.41
1:C:25:ILE:HG23	1:B:51:THR:HG21	2.02	0.41
1:C:145:PRO:HG2	1:C:148:GLY:H	1.86	0.41
1:C:347:ASN:HB3	1:C:348:ARG:H	1.45	0.41
1:B:74:SER:HB2	1:B:93:ARG:HE	1.85	0.41
1:A:58:GLN:NE2	1:A:103:LEU:O	2.54	0.40
1:A:126:GLU:HB3	1:A:388:GLN:OE1	2.21	0.40
1:A:307:LEU:HD21	1:B:23:GLU:HG2	2.03	0.40
1:A:309:ASP:OD1	1:A:447:SER:HB3	2.21	0.40
1:B:277:PRO:HA	1:B:278:PRO:HD3	1.97	0.40
1:B:105:LYS:HE3	1:B:230:PHE:CD2	2.56	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	505/565 (89%)	477 (94%)	27 (5%)	1 (0%)	43	66
1	B	504/565 (89%)	476 (94%)	28 (6%)	0	100	100
1	C	504/565 (89%)	476 (94%)	27 (5%)	1 (0%)	43	66
All	All	1513/1695 (89%)	1429 (94%)	82 (5%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	CYS
1	C	71	CYS

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	430/466 (92%)	426 (99%)	4 (1%)	70	87
1	B	430/466 (92%)	426 (99%)	4 (1%)	70	87
1	C	430/466 (92%)	426 (99%)	4 (1%)	70	87
All	All	1290/1398 (92%)	1278 (99%)	12 (1%)	70	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	CYS
1	A	141	TRP
1	A	347	ASN
1	A	427	LEU
1	C	71	CYS
1	C	141	TRP
1	C	347	ASN
1	C	427	LEU
1	B	71	CYS
1	B	141	TRP
1	B	347	ASN
1	B	427	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	C	287	HIS
1	C	444	HIS
1	C	584	HIS

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Mol	Chain	Res	Type
1	B	287	HIS
1	B	584	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.46	0
2	BMA	D	3	2	11,11,12	0.55	0	15,15,17	0.68	0
3	NAG	E	1	3,1	14,14,15	0.31	0	17,19,21	0.43	0
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.48	0
3	BMA	E	3	3	11,11,12	0.56	0	15,15,17	0.81	0
3	MAN	E	4	3	11,11,12	0.74	0	15,15,17	1.16	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	BMA	F	3	3	11,11,12	0.56	0	15,15,17	0.82	0
3	MAN	F	4	3	11,11,12	0.75	0	15,15,17	1.17	2 (13%)

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	D	1	2,1	-	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	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	1/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	3.54	116.93	112.19
3	E	4	MAN	C1-O5-C5	3.49	116.87	112.19
3	E	4	MAN	O2-C2-C3	-2.14	105.72	110.15
3	F	4	MAN	O2-C2-C3	-2.12	105.77	110.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

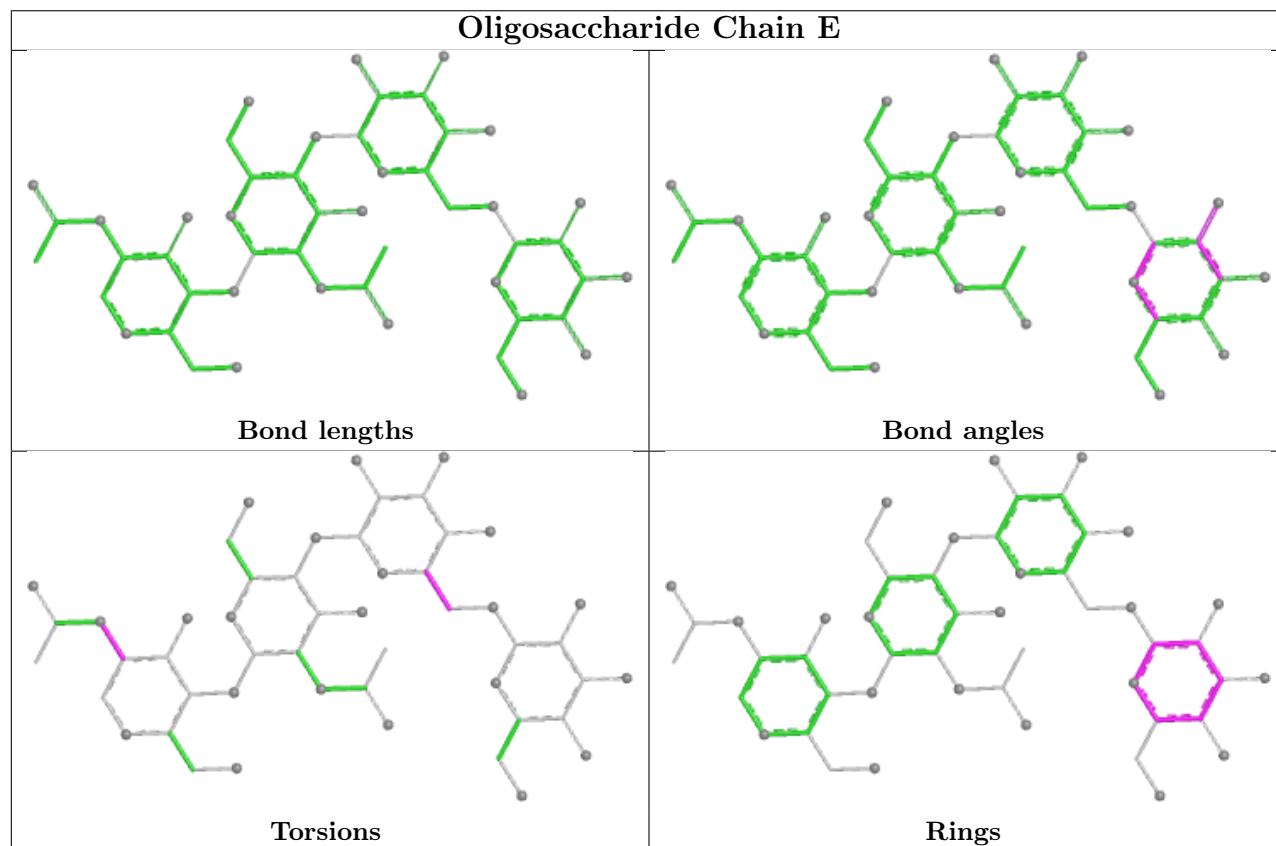
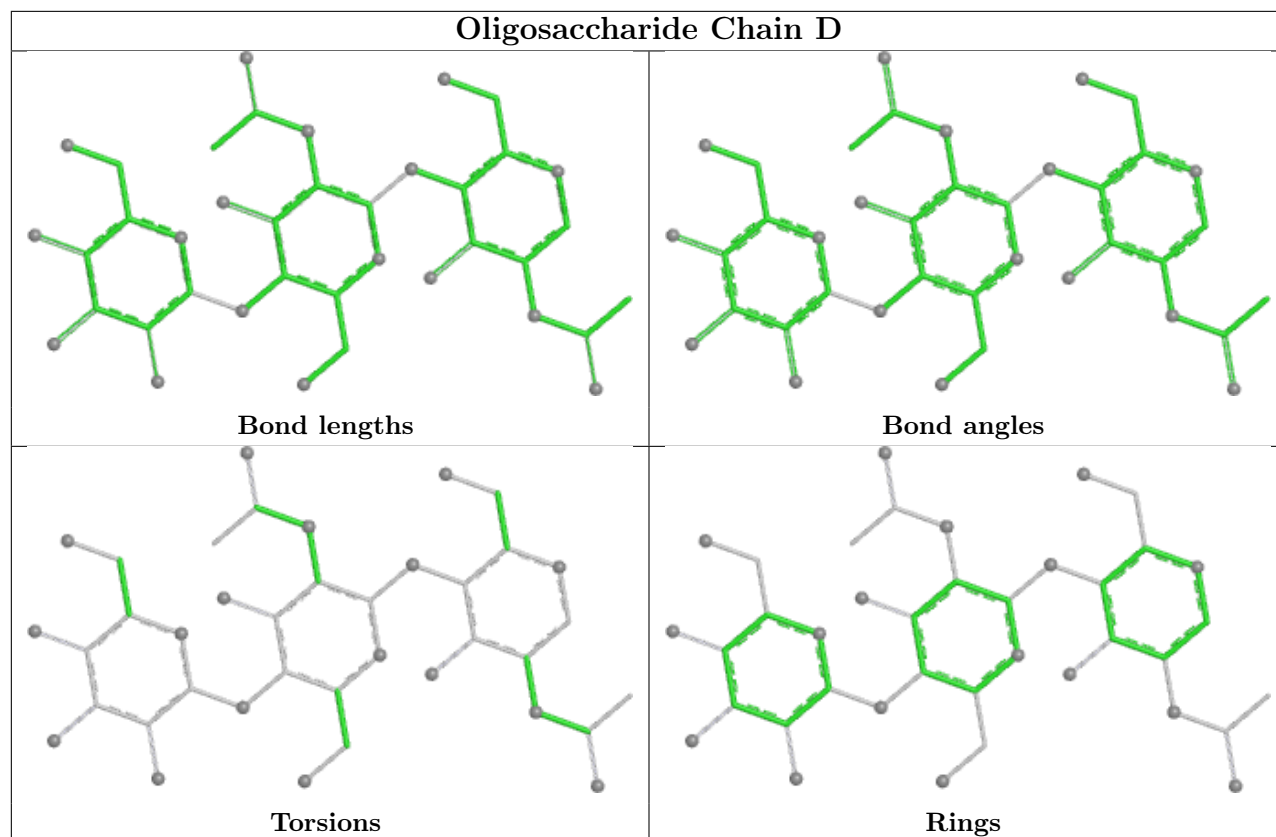
Mol	Chain	Res	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	E	3	BMA	C4-C5-C6-O6

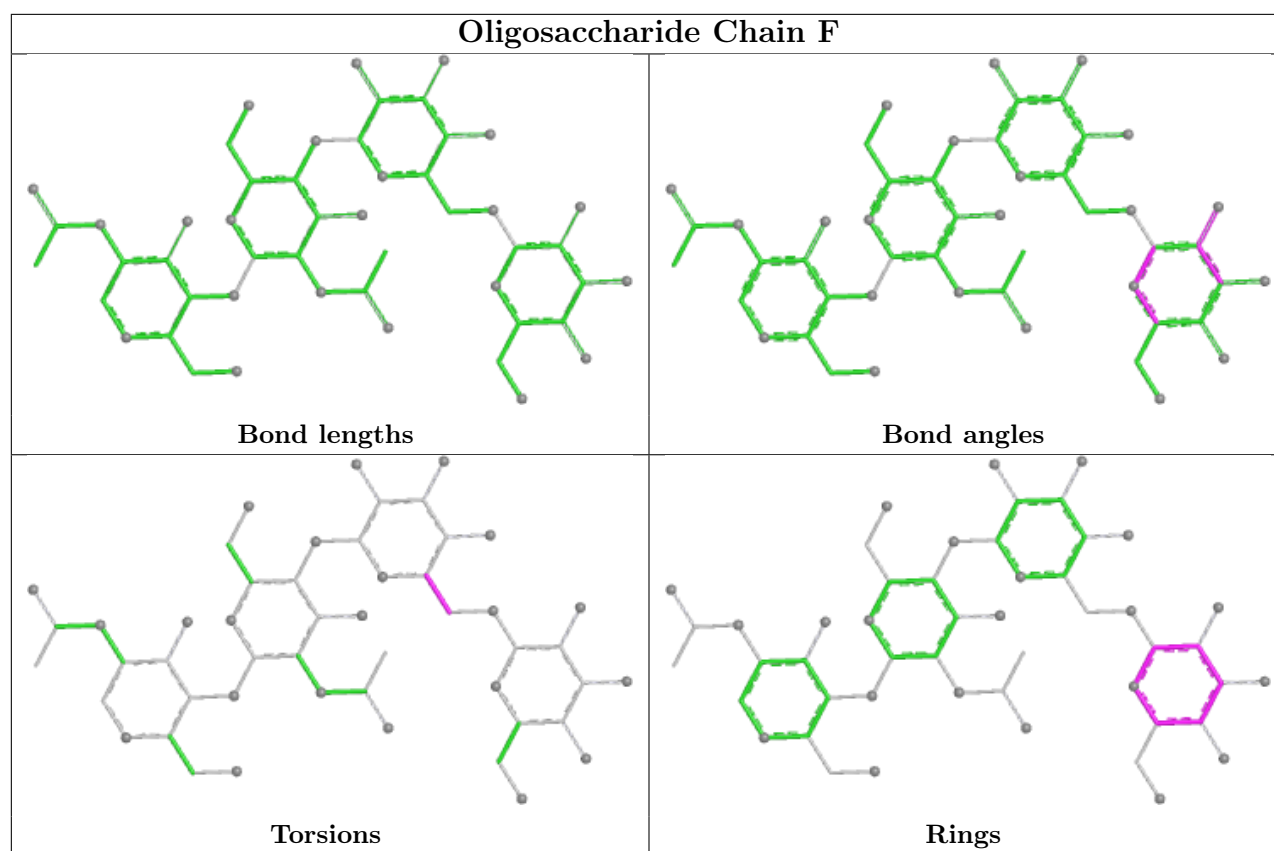
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	MAN	C1-C2-C3-C4-C5-O5
3	E	4	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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](#)

9 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	C	606	1	14,14,15	0.35	0	17,19,21	0.47	0
4	NAG	B	601	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	A	604	1	14,14,15	0.27	0	17,19,21	0.35	0
4	NAG	A	605	1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	B	606	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	A	606	1	14,14,15	0.49	0	17,19,21	0.52	0
4	NAG	C	605	1	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	C	607	1	14,14,15	0.46	0	17,19,21	0.54	0
4	NAG	B	607	1	14,14,15	0.42	0	17,19,21	0.51	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	C	606	1	-	1/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
4	NAG	A	605	1	-	2/6/23/26	0/1/1/1
4	NAG	B	606	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	1/6/23/26	0/1/1/1
4	NAG	C	605	1	-	2/6/23/26	0/1/1/1
4	NAG	C	607	1	-	2/6/23/26	0/1/1/1
4	NAG	B	607	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	C	605	NAG	C4-C5-C6-O6
4	A	605	NAG	O5-C5-C6-O6
4	C	605	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
4	C	606	NAG	O5-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	A	605	NAG	C4-C5-C6-O6
4	A	604	NAG	O5-C5-C6-O6
4	C	607	NAG	O5-C5-C6-O6
4	C	607	NAG	C3-C2-N2-C7
4	B	607	NAG	C3-C2-N2-C7
4	A	606	NAG	C3-C2-N2-C7

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 [i](#)

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	516/565 (91%)	0.36	12 (2%) 61 55	77, 110, 189, 270	0
1	B	515/565 (91%)	0.37	16 (3%) 51 45	78, 110, 189, 291	0
1	C	515/565 (91%)	0.38	19 (3%) 45 39	80, 110, 186, 277	0
All	All	1546/1695 (91%)	0.37	47 (3%) 52 47	77, 110, 189, 291	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	384	GLY	5.9
1	B	274	PHE	3.7
1	A	200	LEU	3.2
1	C	274	PHE	3.1
1	C	200	LEU	3.1
1	A	190	CYS	3.0
1	C	360	SER	2.9
1	A	129	LEU	2.8
1	B	473	ALA	2.8
1	C	346	THR	2.8
1	B	139	GLY	2.7
1	A	67	PHE	2.7
1	B	48	VAL	2.7
1	C	180	SER	2.6
1	C	383	CYS	2.5
1	A	211	LEU	2.5
1	B	275	LEU	2.5
1	C	376	PHE	2.5
1	C	125	LEU	2.4
1	C	361	MET	2.4
1	C	318	ALA	2.4
1	C	163	PHE	2.4
1	C	495	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	317	PRO	2.4
1	A	163	PHE	2.4
1	B	472	ALA	2.3
1	C	565	GLY	2.3
1	B	37	GLY	2.3
1	B	372	GLY	2.3
1	B	225	ALA	2.2
1	A	376	PHE	2.2
1	A	445	SER	2.2
1	B	423	SER	2.2
1	C	23	GLU	2.2
1	A	41	GLU	2.1
1	B	240	THR	2.1
1	B	495	TYR	2.1
1	C	183	ARG	2.1
1	A	89	THR	2.1
1	A	544	TYR	2.1
1	B	377	ARG	2.1
1	B	159	ASP	2.0
1	C	212	THR	2.0
1	C	30	LEU	2.0
1	C	67	PHE	2.0
1	B	559	SER	2.0
1	B	558	VAL	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.

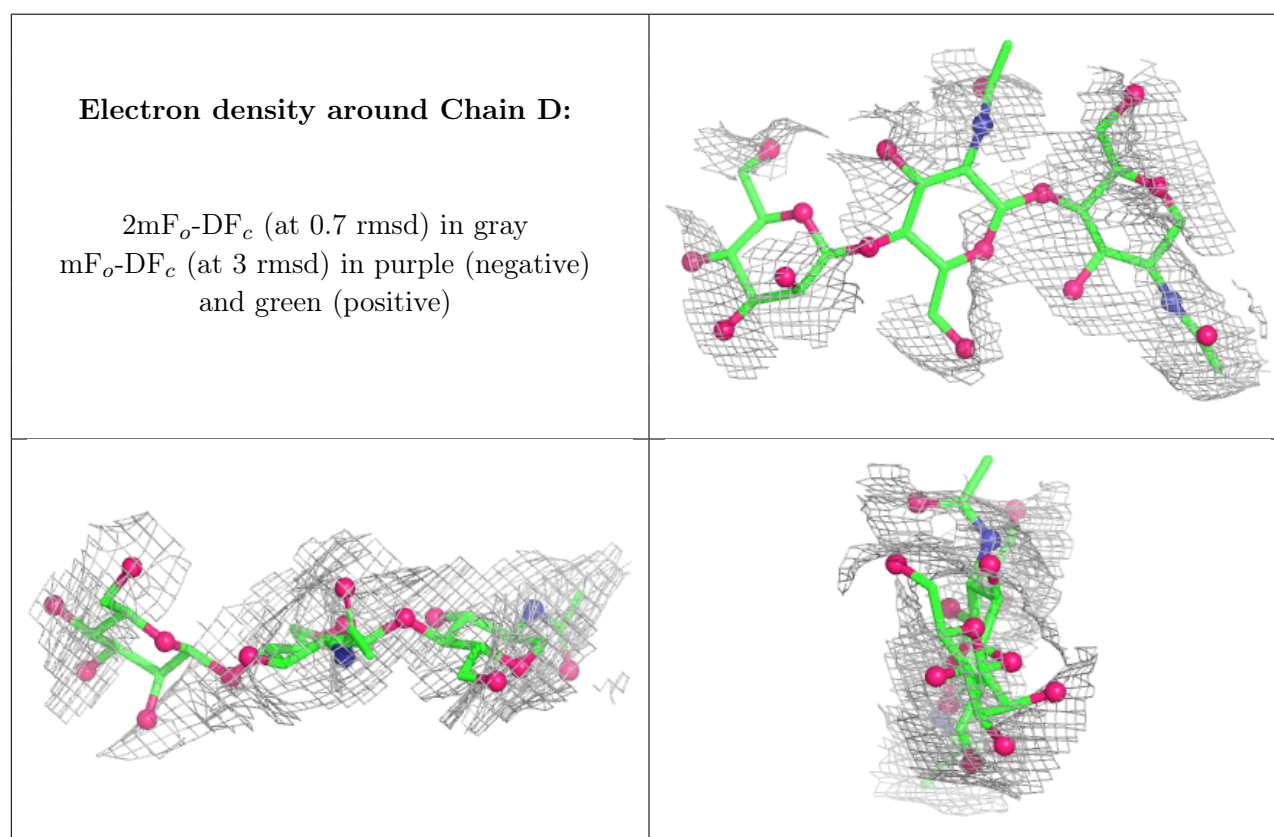
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	D	3	11/12	0.89	0.10	175,186,198,199	0
3	NAG	F	1	14/15	0.92	0.13	84,117,150,151	0
3	MAN	E	4	11/12	0.93	0.11	237,243,246,246	0
3	BMA	E	3	11/12	0.93	0.08	204,213,222,230	0

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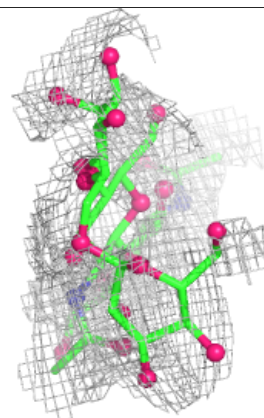
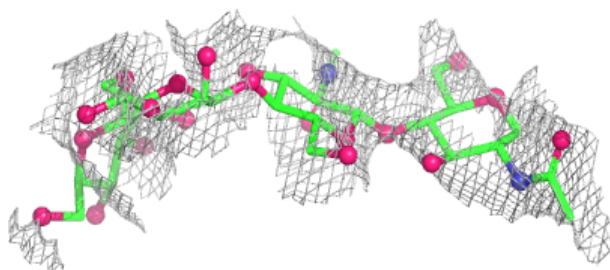
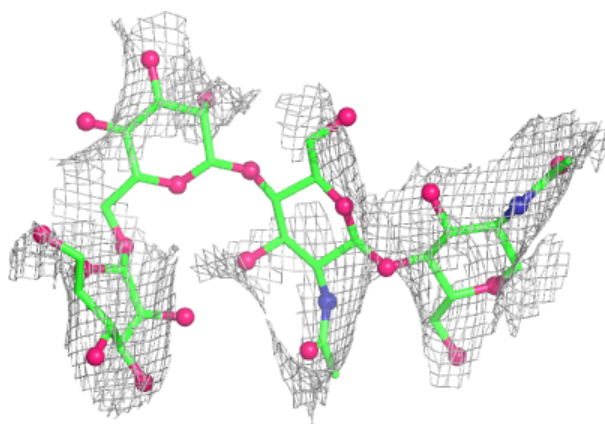
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.95	0.07	132,160,165,173	0
3	BMA	F	3	11/12	0.95	0.08	199,206,216,219	0
3	MAN	F	4	11/12	0.95	0.08	221,227,230,232	0
3	NAG	E	1	14/15	0.96	0.09	79,113,154,158	0
3	NAG	F	2	14/15	0.96	0.07	132,161,171,186	0
2	NAG	D	1	14/15	0.97	0.08	90,122,150,152	0
3	NAG	E	2	14/15	0.97	0.08	136,164,174,189	0

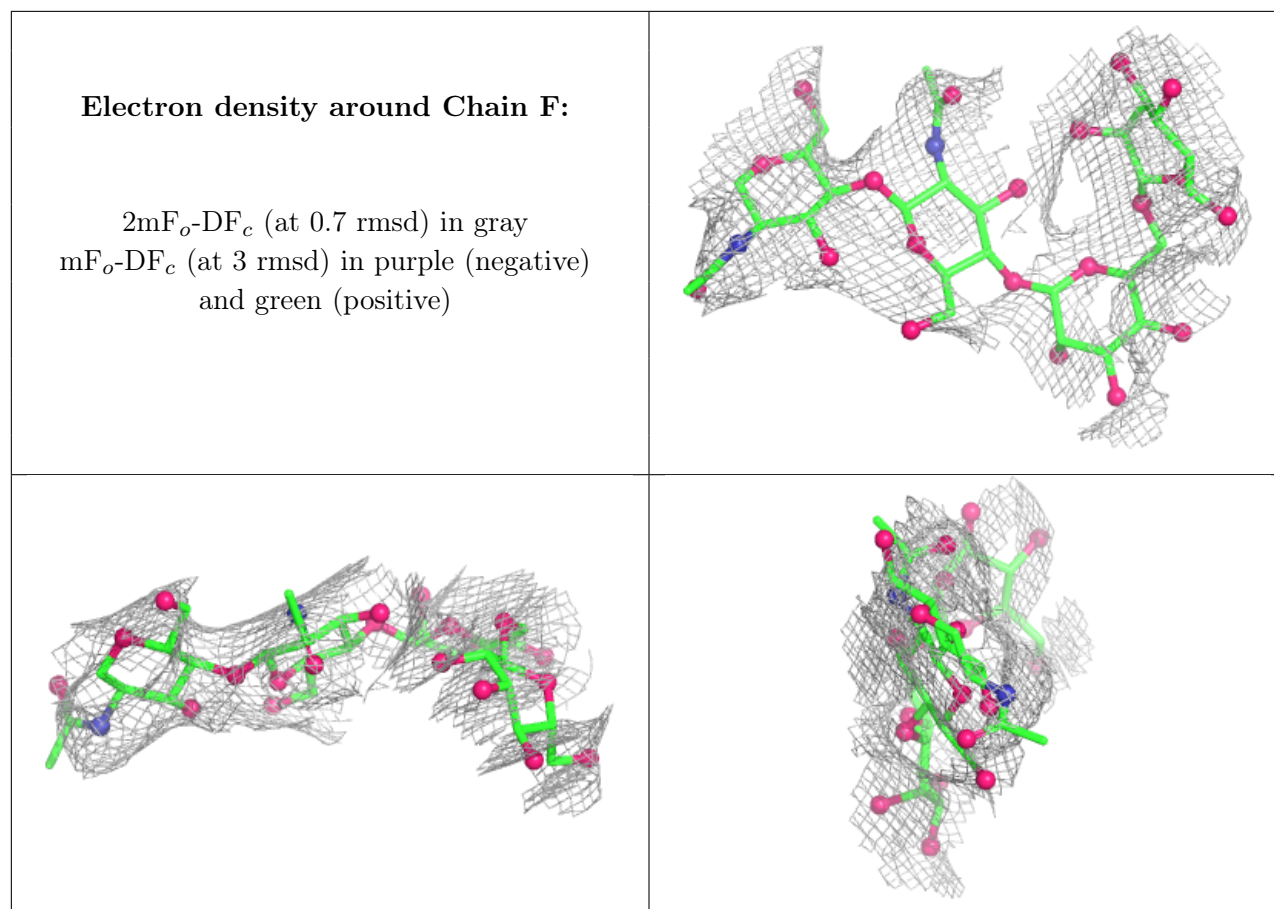
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	605	14/15	0.88	0.11	127,151,162,164	0
4	NAG	A	604	14/15	0.91	0.12	129,157,178,181	0
4	NAG	B	606	14/15	0.91	0.12	142,160,172,174	0
4	NAG	B	607	14/15	0.93	0.07	109,126,140,141	0
4	NAG	C	607	14/15	0.94	0.09	113,131,150,153	0
4	NAG	B	601	14/15	0.94	0.14	136,164,190,193	0
4	NAG	C	606	14/15	0.95	0.12	139,181,195,195	0
4	NAG	A	605	14/15	0.96	0.10	150,177,207,208	0
4	NAG	A	606	14/15	0.96	0.07	106,128,147,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.