Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 09:05 AM EDT

PDB ID	:	6VG1
Title	:	xenopus protocadherin 8.1 EC1-6
Authors	:	Harrison, O.J.; Brasch, B.; Shapiro, L.S.
Deposited on	:	2020-01-07
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 (i) 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 (i)) were used in the production of this report:

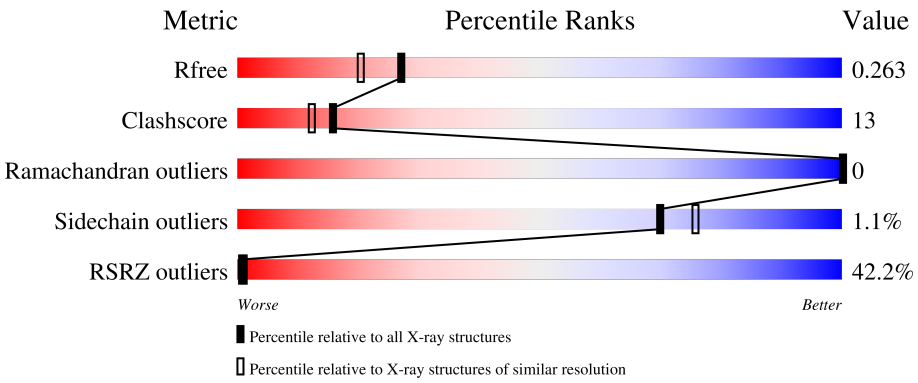
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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	647	34%, 74%, 25%, •
1	B	647	50%, 72%, 27%, •
2	C	4	25%, 25%, 50%
2	D	4	50%, 25%, 25%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19847 atoms, of which 9678 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.

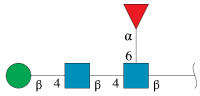
- Molecule 1 is a protein called protocadherin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	642	9697	3078	4771	838	997	13	0	0	0
1	B	641	9691	3075	4770	837	996	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	HIS	-	expression tag	UNP Q6GLU2
A	643	HIS	-	expression tag	UNP Q6GLU2
A	644	HIS	-	expression tag	UNP Q6GLU2
A	645	HIS	-	expression tag	UNP Q6GLU2
A	646	HIS	-	expression tag	UNP Q6GLU2
A	647	HIS	-	expression tag	UNP Q6GLU2
B	642	HIS	-	expression tag	UNP Q6GLU2
B	643	HIS	-	expression tag	UNP Q6GLU2
B	644	HIS	-	expression tag	UNP Q6GLU2
B	645	HIS	-	expression tag	UNP Q6GLU2
B	646	HIS	-	expression tag	UNP Q6GLU2
B	647	HIS	-	expression tag	UNP Q6GLU2

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	4	92	28	43	2	19	0	0	0

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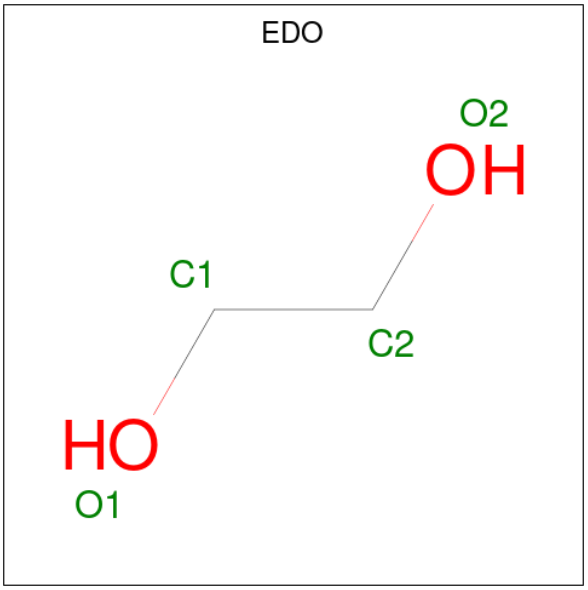
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	D	4	92	28	43	2	19	0	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	10	2	6	2	0	0
3	B	1	10	2	6	2	0	0

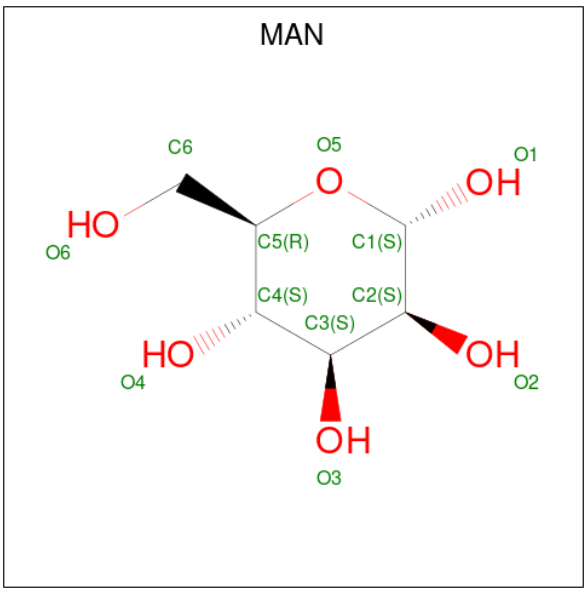
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	15	15	15	0	0
4	B	15	15	15	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	A	1	Total	C	H	O	0	0
			21	6	10	5		
6	B	1	Total	C	H	O	0	0
			20	6	9	5		
6	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	B	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

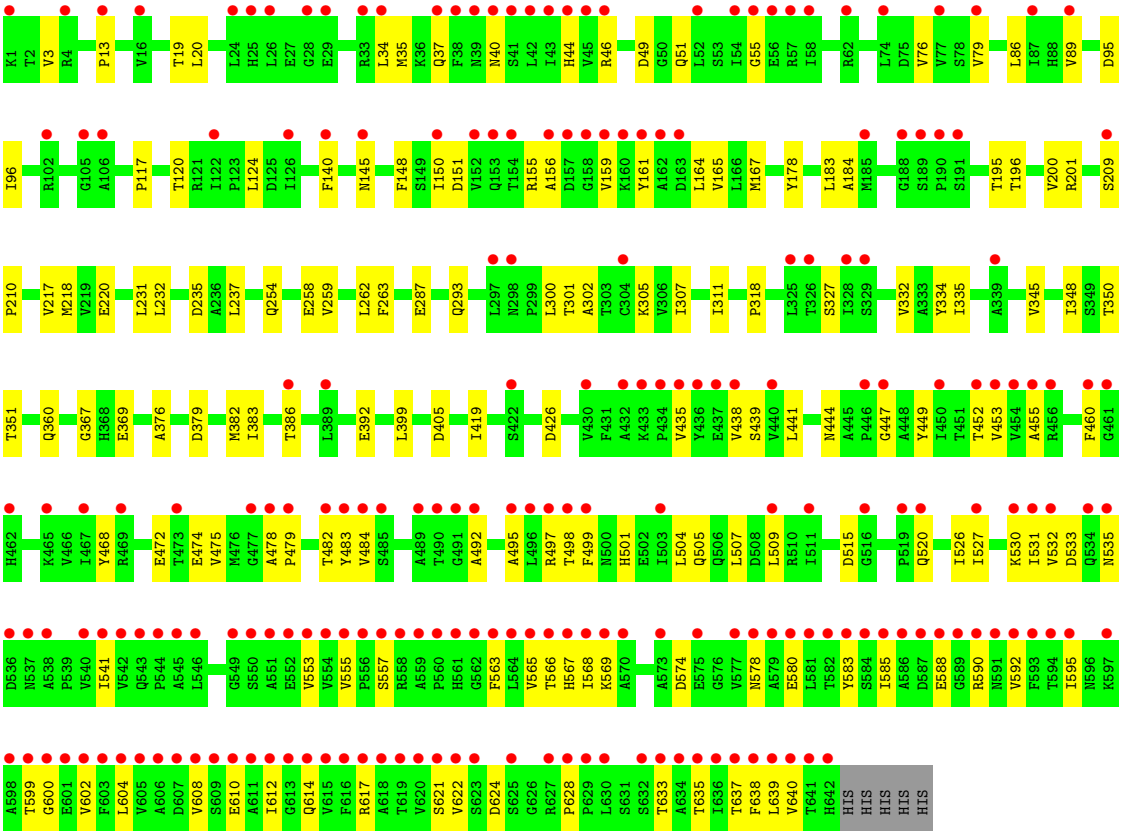
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	81	Total	O	0	0
			81	81		
8	B	57	Total	O	0	0
			57	57		

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.

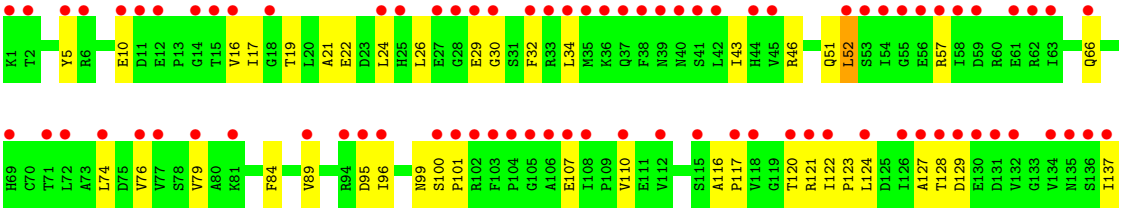
- Molecule 1: protocadherin protein

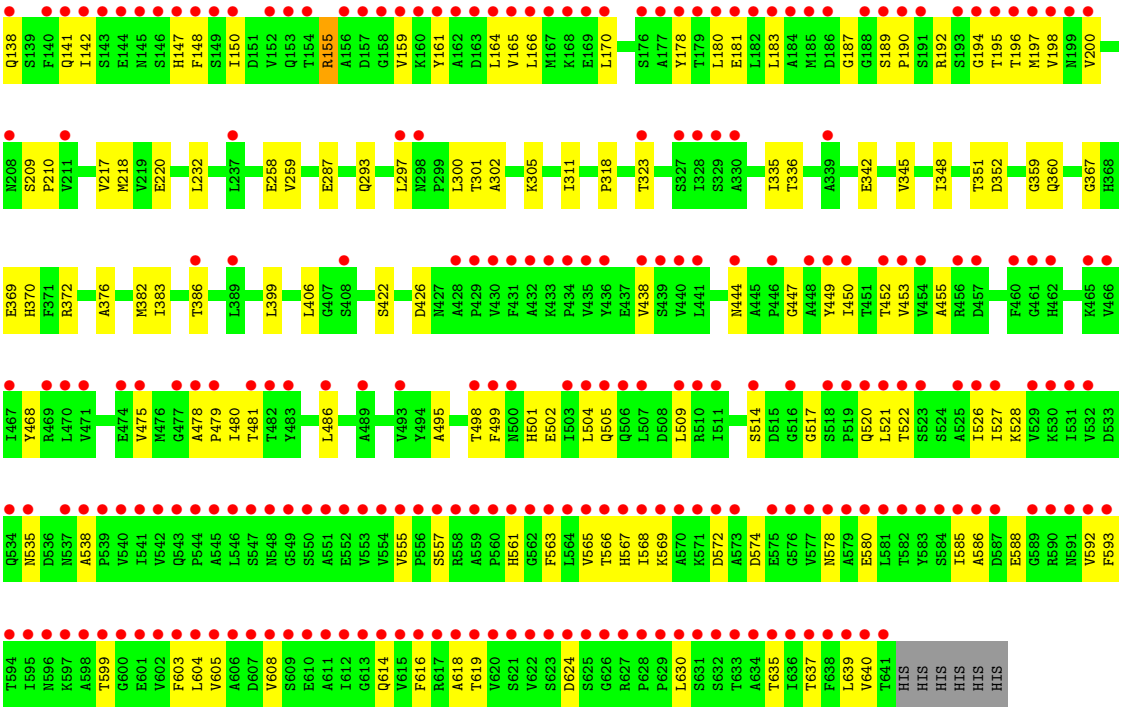
Chain A:



- Molecule 1: protocadherin protein

Chain B:





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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.65Å 42.39Å 167.47Å 90.00° 110.60° 90.00°	Depositor
Resolution (Å)	38.27 – 2.00 38.27 – 2.00	Depositor EDS
% Data completeness (in resolution range)	45.0 (38.27-2.00) 41.9 (38.27-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.253 , 0.297 0.256 , 0.263	Depositor DCC
R_{free} test set	1775 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6680e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.34	0/5010	0.55	0/6823
1	B	0.32	0/5005	0.53	0/6816
All	All	0.33	0/10015	0.54	0/13639

There are no bond length outliers.

There are no bond angle outliers.

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	4926	4771	4831	119	0
1	B	4921	4770	4828	141	0
2	C	49	43	43	1	0
2	D	49	43	43	2	0
3	A	4	6	6	1	0
3	B	4	6	6	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	22	20	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	19	19	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	81	0	0	0	0
8	B	57	0	0	1	0
All	All	10169	9678	9796	260	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 13.

All (260) 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:572:ASP:OD2	1:B:578:ASN:O	1.73	1.06
1:B:574:ASP:OD2	1:B:578:ASN:OD1	1.84	0.94
1:A:567:HIS:HE1	1:A:599:THR:HG22	1.32	0.92
1:B:220:GLU:HB3	1:B:311:ILE:HD11	1.56	0.86
1:B:557:SER:O	1:B:608:VAL:HG21	1.76	0.84
1:B:618:ALA:O	1:B:635:THR:OG1	1.94	0.83
1:A:567:HIS:CE1	1:A:599:THR:HG22	2.19	0.77
1:B:614:GLN:O	1:B:639:LEU:HD13	1.85	0.76
1:B:557:SER:HB2	1:B:608:VAL:HG11	1.68	0.75
1:A:565:VAL:CG2	1:A:602:VAL:HG13	2.16	0.75
1:B:10:GLU:OE1	1:B:57:ARG:NH2	2.20	0.74
1:A:155:ARG:HB2	1:A:159:VAL:HG22	1.69	0.73
1:A:392:GLU:OE2	1:A:426:ASP:OD1	2.06	0.73
1:A:156:ALA:N	1:B:287:GLU:OE1	2.15	0.73
1:A:612:ILE:HA	1:A:640:VAL:HG23	1.69	0.73
1:A:37:GLN:HE21	1:A:40:ASN:HA	1.54	0.72
1:B:293:GLN:HG3	1:B:301:THR:HG22	1.69	0.72
1:A:515:ASP:O	1:A:520:GLN:NE2	2.22	0.71
1:A:327:SER:HB2	1:A:332:VAL:O	1.91	0.70
2:C:1:NAG:H62	2:C:4:FUC:O2	1.91	0.70
1:B:592:VAL:O	1:B:604:LEU:HD12	1.92	0.70
1:B:369:GLU:O	1:B:386:THR:HG21	1.92	0.69
1:A:220:GLU:HB3	1:A:311:ILE:HD11	1.76	0.67
1:A:617:ARG:HG2	1:A:637:THR:HG22	1.76	0.67
1:A:583:TYR:HD1	1:A:622:VAL:HG12	1.59	0.67
1:B:538:ALA:HB2	1:B:630:LEU:HD23	1.77	0.66
1:A:592:VAL:O	1:A:604:LEU:HD12	1.96	0.66
1:B:148:PHE:CE2	1:B:200:VAL:HG11	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:PHE:O	1:B:637:THR:HG22	1.96	0.65
1:A:19:THR:HG22	1:A:51:GLN:HG3	1.77	0.65
1:A:117:PRO:O	1:A:120:THR:HG23	1.99	0.63
1:A:565:VAL:HG23	1:A:602:VAL:HG13	1.80	0.63
1:B:574:ASP:CG	1:B:578:ASN:OD1	2.37	0.63
1:A:441:LEU:HD23	1:A:532:VAL:CG2	2.29	0.63
1:A:583:TYR:CD1	1:A:622:VAL:HG12	2.34	0.63
1:B:74:LEU:O	1:B:89:VAL:HG12	1.98	0.63
1:B:455:ALA:N	1:B:468:TYR:OH	2.31	0.63
1:B:585:ILE:HD11	1:B:593:PHE:HB2	1.81	0.62
1:A:555:VAL:N	1:A:639:LEU:O	2.33	0.61
1:B:110:VAL:HG11	1:B:122:ILE:HG21	1.82	0.61
1:B:100:SER:HB3	1:B:192:ARG:HB3	1.83	0.60
1:A:563:PHE:HD2	1:A:565:VAL:HG13	1.67	0.60
1:B:148:PHE:HE2	1:B:200:VAL:HG11	1.66	0.60
1:B:287:GLU:OE2	1:B:305:LYS:HE3	2.02	0.60
1:B:639:LEU:HD12	1:B:640:VAL:H	1.66	0.60
1:B:121:ARG:HG2	1:B:165:VAL:HG22	1.85	0.59
1:A:555:VAL:O	1:A:640:VAL:HA	2.03	0.59
1:B:21:ALA:HA	1:B:26:LEU:HD12	1.85	0.58
1:A:499:PHE:HB3	1:A:531:ILE:HD13	1.85	0.58
1:B:565:VAL:HG23	1:B:566:THR:H	1.68	0.58
1:B:567:HIS:CD2	1:B:569:LYS:HG3	2.39	0.58
1:A:574:ASP:CG	1:A:578:ASN:OD1	2.40	0.58
1:A:293:GLN:HG3	1:A:301:THR:HG22	1.85	0.57
1:A:621:SER:OG	1:A:633:THR:HG22	2.04	0.57
1:A:482:THR:HG21	1:A:497:ARG:HH21	1.70	0.56
1:A:217:VAL:HG11	1:A:232:LEU:CD2	2.35	0.56
1:A:305:LYS:HE2	1:A:307:ILE:HD11	1.87	0.56
1:A:148:PHE:HB3	1:A:164:LEU:HD11	1.87	0.56
1:A:452:THR:HG22	1:A:492:ALA:HA	1.87	0.56
1:B:585:ILE:HG23	1:B:585:ILE:O	2.05	0.56
1:B:586:ALA:HB3	1:B:619:THR:OG1	2.06	0.56
1:B:444:ASN:O	1:B:498:THR:HG22	2.06	0.56
1:A:455:ALA:N	1:A:468:TYR:OH	2.35	0.55
1:B:360:GLN:O	1:B:406:LEU:HD23	2.06	0.55
1:A:217:VAL:HG11	1:A:232:LEU:HD21	1.88	0.55
1:B:447:GLY:N	1:B:495:ALA:O	2.39	0.55
1:B:599:THR:HG22	1:B:599:THR:O	2.07	0.55
1:A:46:ARG:HD2	1:A:49:ASP:OD2	2.06	0.55
1:A:585:ILE:O	1:A:585:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:PRO:HD2	1:B:192:ARG:O	2.08	0.54
1:A:567:HIS:HD2	1:A:569:LYS:HE2	1.72	0.54
1:B:593:PHE:CE1	1:B:604:LEU:HD13	2.42	0.54
1:A:369:GLU:O	1:A:386:THR:HG21	2.08	0.54
1:A:568:ILE:HG22	1:A:600:GLY:O	2.08	0.54
1:B:189:SER:HB2	1:B:190:PRO:HD3	1.90	0.53
1:B:376:ALA:HB2	1:B:382:MET:HG3	1.89	0.53
1:A:444:ASN:O	1:A:498:THR:HG22	2.08	0.53
1:A:155:ARG:HG3	1:A:159:VAL:CG2	2.38	0.53
1:B:34:LEU:HD23	1:B:76:VAL:HG12	1.90	0.53
1:A:155:ARG:HD3	1:B:287:GLU:OE2	2.08	0.53
1:B:258:GLU:HG3	1:B:259:VAL:N	2.24	0.53
1:A:535:ASN:ND2	1:A:628:PRO:O	2.33	0.53
1:A:583:TYR:HB3	1:A:595:ILE:HD11	1.91	0.53
1:A:484:VAL:HG21	1:A:509:LEU:CD2	2.39	0.53
1:B:195:THR:HG22	1:B:196:THR:N	2.23	0.52
1:B:19:THR:OG1	1:B:22:GLU:HB2	2.10	0.52
2:D:4:FUC:H63	2:D:4:FUC:H2	1.91	0.52
1:B:148:PHE:CE1	1:B:166:LEU:HD13	2.44	0.52
1:A:565:VAL:HG23	1:A:566:THR:N	2.25	0.52
1:A:565:VAL:HG23	1:A:566:THR:H	1.74	0.52
1:B:46:ARG:NH2	1:B:51:GLN:OE1	2.43	0.52
1:A:478:ALA:HB1	1:A:479:PRO:HD2	1.92	0.52
1:A:287:GLU:HG3	1:A:307:ILE:CD1	2.40	0.52
1:B:555:VAL:HG21	1:B:565:VAL:HG12	1.91	0.52
1:B:117:PRO:O	1:B:120:THR:HG23	2.10	0.51
1:A:124:LEU:HD11	1:A:164:LEU:HB2	1.93	0.51
1:B:100:SER:HB3	1:B:192:ARG:HE	1.74	0.51
1:B:535:ASN:OD1	1:B:578:ASN:ND2	2.43	0.51
1:B:449:TYR:CE1	1:B:452:THR:HG23	2.46	0.51
1:A:444:ASN:HD21	1:A:499:PHE:HD2	1.58	0.51
1:B:210:PRO:O	1:B:302:ALA:HB2	2.10	0.51
1:A:449:TYR:CE1	1:A:452:THR:HG23	2.46	0.51
1:B:287:GLU:OE2	1:B:305:LYS:CE	2.59	0.51
1:B:499:PHE:HD1	1:B:504:LEU:HD23	1.76	0.51
1:B:370:HIS:C	1:B:386:THR:HG22	2.31	0.50
1:A:449:TYR:HE1	1:A:452:THR:HG23	1.75	0.50
1:A:588:GLU:HG3	1:A:590:ARG:O	2.11	0.50
1:B:557:SER:HB2	1:B:608:VAL:CG1	2.39	0.50
1:B:129:ASP:HB2	1:B:137:ILE:HG13	1.92	0.50
1:A:155:ARG:HG2	1:A:161:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:ILE:HG23	1:B:568:ILE:O	2.12	0.50
1:B:128:THR:N	1:B:137:ILE:HD11	2.27	0.49
1:B:178:TYR:HB2	1:B:200:VAL:HB	1.93	0.49
1:B:449:TYR:OH	1:B:452:THR:HG23	2.13	0.49
1:A:557:SER:O	1:A:608:VAL:HG11	2.12	0.49
1:B:342:GLU:HG2	1:B:372:ARG:HH12	1.77	0.49
1:B:567:HIS:CD2	1:B:569:LYS:HE2	2.48	0.49
1:A:447:GLY:N	1:A:495:ALA:O	2.45	0.49
1:B:499:PHE:CD1	1:B:504:LEU:HD23	2.48	0.49
1:B:565:VAL:HG23	1:B:566:THR:N	2.27	0.49
1:A:210:PRO:O	1:A:302:ALA:HB2	2.12	0.49
1:A:612:ILE:CA	1:A:640:VAL:HG23	2.39	0.49
1:B:517:GLY:O	1:B:520:GLN:HG2	2.13	0.49
1:A:145:ASN:HD21	1:A:148:PHE:HB2	1.78	0.48
1:A:530:LYS:HE2	1:A:532:VAL:HG12	1.95	0.48
1:A:568:ILE:HG23	1:A:568:ILE:O	2.13	0.48
1:A:567:HIS:CE1	1:A:599:THR:O	2.66	0.48
1:A:635:THR:O	1:A:635:THR:HG23	2.12	0.48
1:B:79:VAL:HG23	1:B:79:VAL:O	2.13	0.48
1:B:129:ASP:CB	1:B:137:ILE:HG13	2.42	0.48
1:B:370:HIS:HA	1:B:386:THR:HG22	1.95	0.48
1:B:635:THR:HG23	1:B:635:THR:O	2.13	0.48
1:B:166:LEU:HD21	1:B:170:LEU:HG	1.96	0.48
1:B:367:GLY:HA3	1:B:399:LEU:HD23	1.94	0.48
1:A:580:GLU:O	1:A:624:ASP:HA	2.14	0.48
1:B:585:ILE:HD11	1:B:593:PHE:CB	2.44	0.48
1:B:195:THR:HG21	6:B:722:MAN:H5	1.95	0.48
1:A:610:GLU:HG3	1:A:614:GLN:HG3	1.96	0.48
1:B:370:HIS:O	1:B:386:THR:HG22	2.13	0.48
1:A:399:LEU:HD11	1:A:419:ILE:HD12	1.95	0.47
1:A:585:ILE:O	1:A:585:ILE:CG2	2.62	0.47
1:B:217:VAL:HG11	1:B:232:LEU:HD21	1.96	0.47
1:A:585:ILE:H	1:A:595:ILE:HG21	1.79	0.47
1:B:444:ASN:HD21	1:B:499:PHE:HD2	1.62	0.47
1:A:617:ARG:HG2	1:A:637:THR:CG2	2.45	0.47
1:A:95:ASP:OD1	1:A:96:ILE:N	2.48	0.47
1:A:376:ALA:HB2	1:A:382:MET:HG3	1.97	0.47
1:A:475:VAL:O	1:A:475:VAL:HG13	2.14	0.47
1:A:557:SER:O	1:A:608:VAL:HG21	2.15	0.47
1:A:501:HIS:CD2	1:A:505:GLN:HG3	2.50	0.47
1:B:323:THR:HG23	1:B:323:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:SER:CB	1:A:332:VAL:O	2.63	0.47
1:B:127:ALA:CB	1:B:137:ILE:HD13	2.45	0.47
1:B:335:ILE:HD12	1:B:345:VAL:HG22	1.96	0.47
1:B:95:ASP:OD1	1:B:96:ILE:N	2.48	0.46
1:B:127:ALA:HB3	1:B:137:ILE:HD13	1.97	0.46
1:B:181:GLU:OE2	6:B:722:MAN:H5	2.15	0.46
1:B:110:VAL:CG1	1:B:122:ILE:HG21	2.46	0.46
1:A:335:ILE:HD12	1:A:345:VAL:HG22	1.96	0.46
1:B:217:VAL:HG11	1:B:232:LEU:CD2	2.45	0.46
1:B:438:VAL:HG11	1:B:450:ILE:CG2	2.46	0.46
1:A:483:TYR:CZ	1:A:497:ARG:NH1	2.83	0.46
1:B:181:GLU:HG2	1:B:195:THR:CG2	2.46	0.46
1:A:258:GLU:HG3	1:A:259:VAL:N	2.31	0.46
1:A:140:PHE:HB3	1:A:150:ILE:CD1	2.46	0.46
1:B:220:GLU:CB	1:B:311:ILE:HD11	2.38	0.46
1:A:165:VAL:HG12	1:A:167:MET:HE2	1.98	0.45
1:A:34:LEU:HD23	1:A:76:VAL:HG12	1.97	0.45
1:A:585:ILE:CG2	1:A:595:ILE:HB	2.46	0.45
1:A:254:GLN:HG2	1:B:123:PRO:CB	2.46	0.45
1:B:348:ILE:HD11	1:B:383:ILE:HD11	1.98	0.45
1:A:140:PHE:CE1	1:A:184:ALA:HB2	2.51	0.45
1:B:124:LEU:HD11	1:B:164:LEU:HB2	1.99	0.45
1:B:588:GLU:HB3	1:B:618:ALA:HB2	1.98	0.45
1:B:183:LEU:HD12	1:B:183:LEU:O	2.17	0.45
1:A:3:VAL:HG13	1:A:89:VAL:HG23	1.99	0.45
1:A:318:PRO:HA	1:A:351:THR:O	2.17	0.45
1:A:327:SER:HA	1:A:334:TYR:HD2	1.81	0.45
1:B:514:SER:HB3	1:B:522:THR:HG22	1.99	0.45
1:B:453:VAL:HG11	1:B:527:ILE:HD11	2.00	0.44
1:B:501:HIS:CD2	1:B:505:GLN:HG3	2.51	0.44
1:B:578:ASN:O	1:B:578:ASN:ND2	2.50	0.44
1:A:350:THR:O	1:A:379:ASP:HB3	2.17	0.44
1:A:209:SER:HB3	1:A:300:LEU:HB3	1.99	0.44
1:B:107:GLU:HG2	1:B:197:MET:HB2	1.99	0.44
1:B:180:LEU:O	1:B:198:VAL:HB	2.17	0.44
1:B:526:ILE:HD12	1:B:528:LYS:HE3	2.00	0.44
1:A:35:MET:HE1	1:A:86:LEU:HD11	1.98	0.44
1:B:481:THR:HG22	1:B:481:THR:O	2.17	0.44
1:B:79:VAL:HG12	1:B:84:PHE:CD1	2.53	0.44
1:A:44:HIS:CD2	1:A:55:GLY:HA2	2.53	0.44
1:A:79:VAL:HG23	1:A:79:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:C	1:A:183:LEU:HD12	2.38	0.44
1:B:99:ASN:ND2	8:B:807:HOH:O	2.50	0.44
1:A:195:THR:HG22	1:A:196:THR:N	2.33	0.43
1:B:30:GLY:HA3	1:B:32:PHE:CE2	2.53	0.43
1:A:178:TYR:HB2	1:A:200:VAL:HB	2.00	0.43
1:B:142:ILE:HD13	1:B:150:ILE:CG2	2.48	0.43
1:B:155:ARG:HD3	1:B:159:VAL:HG23	2.00	0.43
1:B:555:VAL:O	1:B:640:VAL:HA	2.18	0.43
1:B:116:ALA:HB1	1:B:120:THR:HG21	1.99	0.43
2:D:4:FUC:H63	2:D:4:FUC:C2	2.47	0.43
1:B:580:GLU:O	1:B:624:ASP:HA	2.19	0.43
1:B:614:GLN:HB3	1:B:616:PHE:CE2	2.53	0.43
1:A:20:LEU:CD1	1:A:76:VAL:HG21	2.48	0.43
1:A:472:GLU:OE2	1:A:479:PRO:CB	2.66	0.43
1:B:24:LEU:HB2	1:B:26:LEU:HG	2.01	0.43
1:A:360:GLN:O	1:A:405:ASP:HA	2.18	0.43
1:A:585:ILE:HG22	1:A:595:ILE:HB	2.01	0.43
1:A:639:LEU:HD23	1:A:640:VAL:N	2.33	0.43
1:B:475:VAL:O	1:B:475:VAL:HG13	2.19	0.43
1:B:155:ARG:HD3	1:B:159:VAL:CG2	2.48	0.43
1:B:449:TYR:HE1	1:B:452:THR:HG23	1.84	0.42
1:B:468:TYR:HB3	1:B:486:LEU:HD21	2.01	0.42
1:B:563:PHE:O	1:B:603:PHE:CD1	2.72	0.42
1:A:348:ILE:HD11	1:A:383:ILE:HD11	2.02	0.42
1:B:101:PRO:O	1:B:194:GLY:HA3	2.20	0.42
1:A:533:ASP:OD2	1:A:574:ASP:HB3	2.20	0.42
1:B:155:ARG:HG2	1:B:161:TYR:CE2	2.54	0.42
1:B:209:SER:HB3	1:B:300:LEU:HB3	2.01	0.42
1:A:254:GLN:OE1	1:A:254:GLN:N	2.51	0.42
1:B:141:GLN:OE1	1:B:183:LEU:HD11	2.19	0.42
1:B:142:ILE:HD13	1:B:150:ILE:HG23	2.01	0.42
1:A:13:PRO:HB3	1:A:55:GLY:O	2.20	0.42
1:A:453:VAL:CG1	1:A:527:ILE:HD11	2.50	0.42
1:A:140:PHE:HB3	1:A:150:ILE:HD12	2.02	0.42
1:A:504:LEU:HD21	1:A:507:LEU:HD13	2.02	0.42
1:B:183:LEU:HB3	1:B:195:THR:HG23	2.01	0.42
1:B:502:GLU:H	1:B:502:GLU:CD	2.23	0.42
1:B:5:TYR:HB3	1:B:17:ILE:CG2	2.50	0.42
1:B:29:GLU:HG2	1:B:30:GLY:N	2.35	0.42
1:A:195:THR:HB	6:A:723:MAN:C5	2.50	0.41
1:B:66:GLN:HG3	1:B:66:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:HA	1:B:351:THR:O	2.21	0.41
1:A:235:ASP:H	3:A:705:EDO:H11	1.86	0.41
1:B:480:ILE:HD11	1:B:509:LEU:CD2	2.51	0.41
1:A:553:VAL:O	1:A:638:PHE:HA	2.20	0.41
1:B:561:HIS:CD2	1:B:605:VAL:HA	2.54	0.41
1:A:155:ARG:HG2	1:A:161:TYR:HE2	1.83	0.41
1:A:217:VAL:HG11	1:A:232:LEU:HD22	2.03	0.41
1:B:138:GLN:HG3	1:B:187:GLY:HA3	2.02	0.41
1:B:147:HIS:HB3	1:B:166:LEU:CD1	2.50	0.41
1:A:438:VAL:HG22	1:A:439:SER:N	2.36	0.41
1:B:148:PHE:CZ	1:B:200:VAL:HG11	2.56	0.41
1:B:258:GLU:HG3	1:B:259:VAL:HG23	2.03	0.41
1:A:541:ILE:HD13	1:A:568:ILE:HD11	2.03	0.41
1:B:16:VAL:HG13	1:B:51:GLN:HE21	1.86	0.41
1:B:336:THR:HA	1:B:422:SER:HB3	2.02	0.41
1:B:478:ALA:HB1	1:B:479:PRO:HD2	2.03	0.41
1:A:367:GLY:HA3	1:A:399:LEU:HD23	2.02	0.41
1:B:367:GLY:HA3	1:B:399:LEU:CD2	2.51	0.41
1:B:148:PHE:HE2	1:B:200:VAL:HG21	1.86	0.40
1:A:183:LEU:HD12	1:A:183:LEU:O	2.21	0.40
1:A:474:GLU:N	1:A:474:GLU:OE1	2.54	0.40
1:B:370:HIS:CA	1:B:386:THR:HG22	2.51	0.40
1:A:435:VAL:HG22	1:A:526:ILE:HD11	2.04	0.40
1:B:352:ASP:HB3	1:B:359:GLY:HA2	2.02	0.40
1:B:150:ILE:HG22	1:B:164:LEU:HD12	2.02	0.40
1:A:231:LEU:HD21	1:A:263:PHE:HE1	1.87	0.40
1:B:43:ILE:HG21	1:B:52:LEU:CD1	2.52	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	640/647 (99%)	612 (96%)	28 (4%)	0	100	100
1	B	639/647 (99%)	615 (96%)	24 (4%)	0	100	100
All	All	1279/1294 (99%)	1227 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	549/555 (99%)	543 (99%)	6 (1%)	70	76
1	B	549/555 (99%)	543 (99%)	6 (1%)	70	76
All	All	1098/1110 (99%)	1086 (99%)	12 (1%)	70	76

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

Mol	Chain	Res	Type
1	A	151	ASP
1	A	201	ARG
1	A	218	MET
1	A	237	LEU
1	A	262	LEU
1	A	460	PHE
1	B	52	LEU
1	B	155	ARG
1	B	218	MET
1	B	297	LEU
1	B	426	ASP
1	B	521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	44	HIS
1	A	83	GLN
1	A	147	HIS
1	A	277	GLN
1	B	229	HIS
1	B	277	GLN
1	B	368	HIS
1	B	444	ASN
1	B	506	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)

8 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	0.63	0	17,19,21	0.91	1 (5%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	0.52	0
2	BMA	C	3	2	11,11,12	0.98	0	15,15,17	0.78	1 (6%)
2	FUC	C	4	2	10,10,11	2.25	2 (20%)	14,14,16	1.89	2 (14%)
2	NAG	D	1	2,1	14,14,15	0.38	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	0.52	0
2	BMA	D	3	2	11,11,12	0.86	1 (9%)	15,15,17	0.97	0
2	FUC	D	4	2	10,10,11	1.33	2 (20%)	14,14,16	2.01	2 (14%)

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	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUC	D	4	2	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	FUC	C2-C3	5.01	1.60	1.52
2	C	4	FUC	C1-C2	3.91	1.61	1.52
2	D	4	FUC	O3-C3	2.65	1.49	1.43
2	D	4	FUC	O2-C2	2.34	1.48	1.43
2	D	3	BMA	C1-C2	2.05	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	FUC	O2-C2-C1	5.76	122.41	109.22
2	D	4	FUC	C1-C2-C3	5.73	117.98	109.64
2	D	4	FUC	C2-C3-C4	3.44	116.91	110.86
2	C	4	FUC	O2-C2-C3	-2.69	104.58	110.15
2	C	1	NAG	C4-C3-C2	2.14	114.15	111.02
2	C	3	BMA	O2-C2-C3	-2.08	105.84	110.15

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

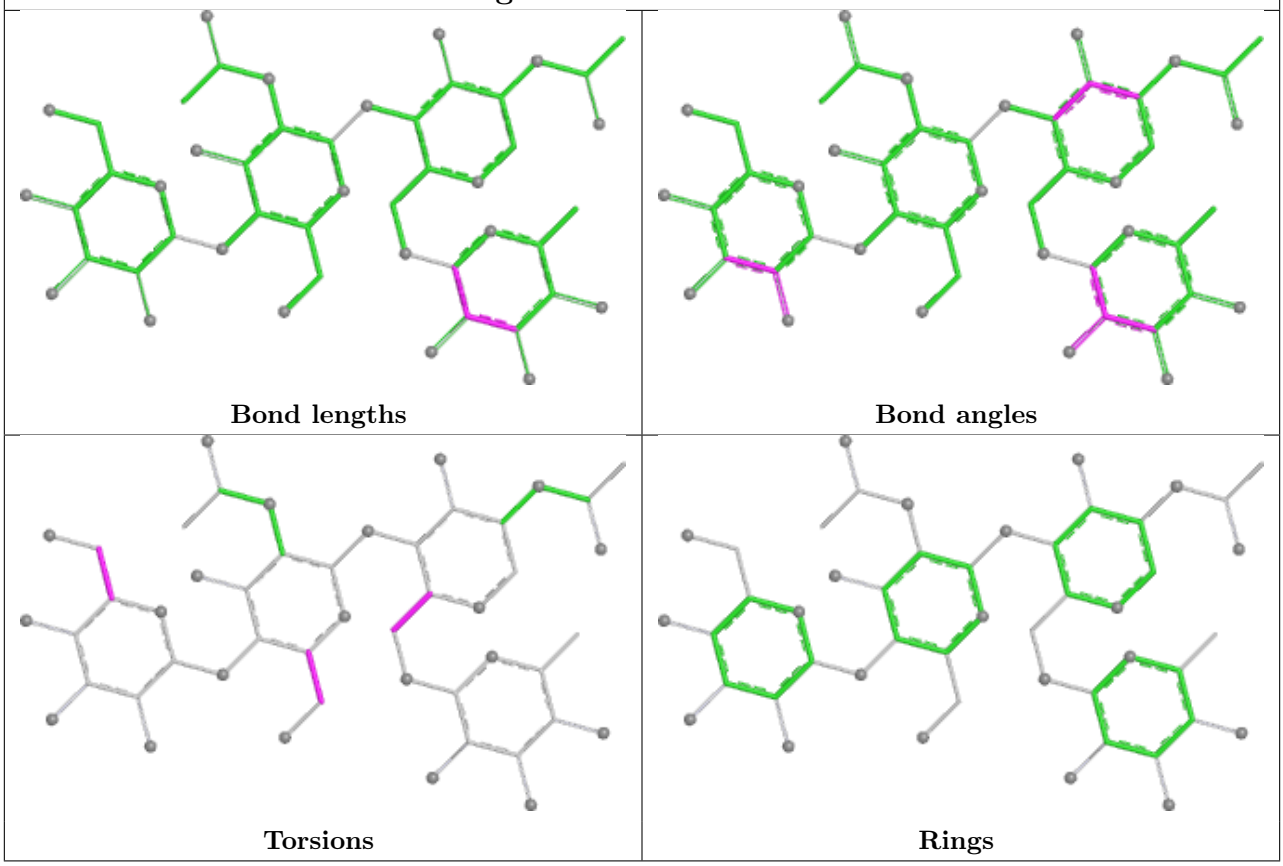
There are no ring outliers.

3 monomers are involved in 3 short contacts:

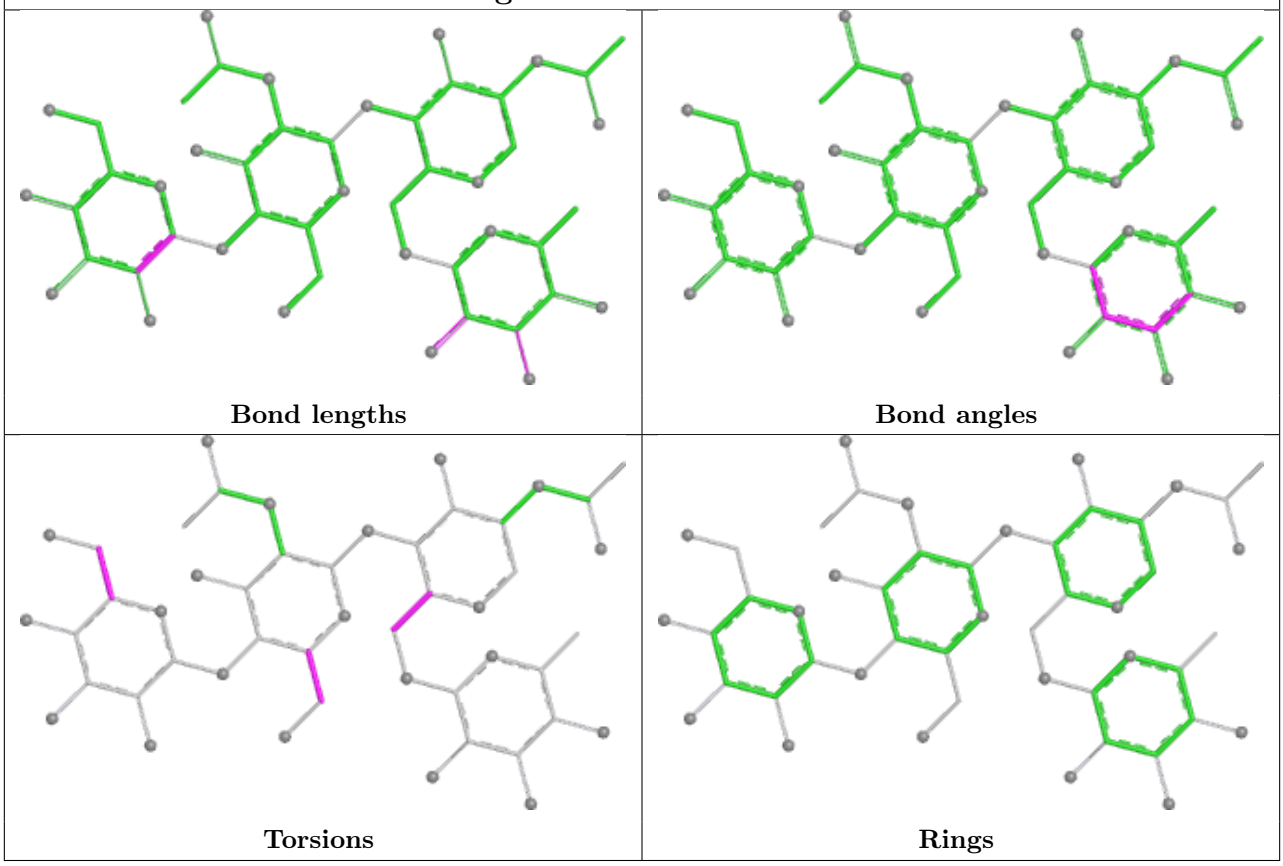
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	4	FUC	2	0
2	C	4	FUC	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 34 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	EDO	A	705	-	3,3,3	0.46	0	2,2,2	0.60	0
6	MAN	A	722	1	11,11,12	0.90	0	15,15,17	1.11	1 (6%)
3	EDO	B	724	-	3,3,3	0.46	0	2,2,2	0.49	0
6	MAN	B	722	1	11,11,12	1.27	1 (9%)	15,15,17	1.10	1 (6%)
6	MAN	A	723	1	11,11,12	1.01	0	15,15,17	1.35	3 (20%)
6	MAN	B	721	1	11,11,12	1.60	2 (18%)	15,15,17	1.32	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	705	-	-	0/1/1/1	-
6	MAN	A	722	1	-	0/2/19/22	0/1/1/1
3	EDO	B	724	-	-	1/1/1/1	-
6	MAN	B	722	1	-	0/2/19/22	0/1/1/1
6	MAN	A	723	1	-	2/2/19/22	0/1/1/1
6	MAN	B	721	1	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	721	MAN	O4-C4	3.13	1.50	1.43
6	B	721	MAN	O5-C1	-2.96	1.38	1.43
6	B	722	MAN	C2-C3	2.18	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	723	MAN	C1-O5-C5	3.48	116.85	112.19
6	A	722	MAN	C1-O5-C5	2.51	115.55	112.19
6	B	721	MAN	O2-C2-C3	-2.19	105.62	110.15
6	A	723	MAN	C2-C3-C4	2.19	114.71	110.86
6	A	723	MAN	O5-C5-C4	-2.14	105.63	110.83
6	B	721	MAN	C1-O5-C5	2.13	115.04	112.19
6	B	722	MAN	C1-O5-C5	2.09	114.99	112.19
6	B	721	MAN	O4-C4-C3	-2.06	105.51	110.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	723	MAN	O5-C5-C6-O6
6	A	723	MAN	C4-C5-C6-O6
6	B	721	MAN	O5-C5-C6-O6
3	B	724	EDO	O1-C1-C2-O2
6	B	721	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	EDO	1	0
6	B	722	MAN	2	0
6	A	723	MAN	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	642/647 (99%)	1.65	217 (33%)	1	1	12, 65, 130, 196	0
1	B	641/647 (99%)	2.32	324 (50%)	0	1	21, 81, 156, 231	0
All	All	1283/1294 (99%)	1.99	541 (42%)	1	1	12, 72, 145, 231	0

All (541) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	PHE	10.1
1	B	556	PRO	8.6
1	A	616	PHE	8.5
1	B	555	VAL	8.4
1	B	568	ILE	8.1
1	B	605	VAL	8.0
1	A	38	PHE	8.0
1	A	642	HIS	7.8
1	B	598	ALA	7.7
1	A	618	ALA	7.6
1	B	622	VAL	7.6
1	B	595	ILE	7.6
1	B	554	VAL	7.6
1	A	546	LEU	7.4
1	A	563	PHE	7.3
1	B	560	PRO	7.3
1	B	581	LEU	7.3
1	B	545	ALA	7.2
1	B	563	PHE	7.2
1	A	582	THR	7.2
1	B	621	SER	7.2
1	A	586	ALA	7.2
1	B	564	LEU	7.0
1	B	641	THR	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	540	VAL	6.8
1	B	577	VAL	6.8
1	B	612	ILE	6.8
1	B	592	VAL	6.6
1	A	159	VAL	6.5
1	B	615	VAL	6.4
1	A	602	VAL	6.4
1	B	602	VAL	6.4
1	B	38	PHE	6.3
1	A	636	ILE	6.3
1	B	618	ALA	6.2
1	B	559	ALA	6.2
1	A	615	VAL	6.2
1	B	583	TYR	6.1
1	B	142	ILE	6.1
1	A	554	VAL	6.0
1	B	638	PHE	6.0
1	B	118	VAL	5.9
1	B	440	VAL	5.9
1	B	566	THR	5.9
1	A	162	ALA	5.9
1	B	611	ALA	5.8
1	B	127	ALA	5.8
1	B	608	VAL	5.8
1	B	96	ILE	5.8
1	B	585	ILE	5.8
1	B	185	MET	5.8
1	B	147	HIS	5.8
1	B	607	ASP	5.8
1	B	603	PHE	5.7
1	B	606	ALA	5.7
1	B	546	LEU	5.7
1	B	150	ILE	5.7
1	B	193	SER	5.7
1	B	436	TYR	5.7
1	A	603	PHE	5.7
1	B	541	ILE	5.7
1	B	553	VAL	5.6
1	B	146	SER	5.6
1	B	625	SER	5.6
1	A	585	ILE	5.6
1	B	636	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	5.5
1	B	632	SER	5.5
1	B	557	SER	5.4
1	B	168	LYS	5.4
1	B	594	THR	5.4
1	B	177	ALA	5.3
1	B	580	GLU	5.3
1	B	558	ARG	5.3
1	A	555	VAL	5.1
1	B	619	THR	5.1
1	B	593	PHE	5.1
1	A	564	LEU	5.1
1	B	184	ALA	5.1
1	A	640	VAL	5.1
1	B	565	VAL	5.1
1	A	126	ILE	5.1
1	B	532	VAL	5.1
1	B	620	VAL	5.0
1	A	606	ALA	5.0
1	A	535	ASN	5.0
1	B	183	LEU	4.9
1	B	478	ALA	4.9
1	B	519	PRO	4.9
1	A	587	ASP	4.9
1	B	582	THR	4.9
1	B	126	ILE	4.8
1	B	52	LEU	4.8
1	B	570	ALA	4.8
1	A	608	VAL	4.8
1	B	33	ARG	4.8
1	B	630	LEU	4.8
1	B	639	LEU	4.8
1	B	148	PHE	4.8
1	B	1	LYS	4.8
1	B	597	LYS	4.8
1	A	604	LEU	4.7
1	A	630	LEU	4.7
1	B	586	ALA	4.7
1	A	632	SER	4.7
1	B	44	HIS	4.7
1	A	578	ASN	4.7
1	B	34	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	456	ARG	4.7
1	B	330	ALA	4.7
1	B	634	ALA	4.7
1	B	561	HIS	4.7
1	B	591	ASN	4.7
1	B	599	THR	4.7
1	B	190	PRO	4.6
1	B	149	SER	4.6
1	B	567	HIS	4.6
1	B	600	GLY	4.6
1	B	58	ILE	4.6
1	A	591	ASN	4.6
1	A	553	VAL	4.6
1	A	589	GLY	4.6
1	A	599	THR	4.6
1	A	559	ALA	4.6
1	B	499	PHE	4.5
1	B	198	VAL	4.5
1	B	441	LEU	4.5
1	A	605	VAL	4.5
1	B	237	LEU	4.4
1	B	134	VAL	4.4
1	B	575	GLU	4.4
1	B	587	ASP	4.4
1	A	160	LYS	4.4
1	B	166	LEU	4.4
1	B	180	LEU	4.4
1	A	612	ILE	4.4
1	A	37	GLN	4.4
1	A	1	LYS	4.4
1	B	16	VAL	4.3
1	B	143	SER	4.3
1	A	597	LYS	4.3
1	A	452	THR	4.3
1	A	595	ILE	4.3
1	B	40	ASN	4.3
1	A	189	SER	4.3
1	A	556	PRO	4.3
1	B	529	VAL	4.3
1	A	558	ARG	4.3
1	B	596	ASN	4.3
1	A	566	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	100	SER	4.2
1	B	604	LEU	4.2
1	B	37	GLN	4.2
1	B	520	GLN	4.2
1	B	140	PHE	4.2
1	A	456	ARG	4.2
1	B	162	ALA	4.2
1	B	633	THR	4.2
1	A	625	SER	4.2
1	A	560	PRO	4.2
1	B	181	GLU	4.2
1	B	156	ALA	4.2
1	B	578	ASN	4.2
1	A	641	THR	4.1
1	B	576	GLY	4.1
1	B	613	GLY	4.1
1	A	467	ILE	4.1
1	A	519	PRO	4.1
1	B	55	GLY	4.1
1	B	165	VAL	4.1
1	A	611	ALA	4.1
1	B	182	LEU	4.1
1	A	152	VAL	4.1
1	B	628	PRO	4.0
1	A	638	PHE	4.0
1	A	634	ALA	4.0
1	B	329	SER	4.0
1	B	467	ILE	4.0
1	B	477	GLY	4.0
1	A	577	VAL	4.0
1	B	579	ALA	4.0
1	B	160	LYS	4.0
1	A	24	LEU	4.0
1	A	609	SER	3.9
1	B	551	ALA	3.9
1	B	503	ILE	3.9
1	B	562	GLY	3.9
1	B	129	ASP	3.9
1	A	622	VAL	3.9
1	B	635	THR	3.9
1	A	25	HIS	3.9
1	B	539	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	573	ALA	3.9
1	B	154	THR	3.9
1	B	102	ARG	3.9
1	A	460	PHE	3.9
1	B	45	VAL	3.8
1	A	469	ARG	3.8
1	B	590	ARG	3.8
1	A	157	ASP	3.8
1	B	518	SER	3.8
1	B	609	SER	3.8
1	A	593	PHE	3.8
1	B	197	MET	3.8
1	A	562	GLY	3.8
1	B	194	GLY	3.8
1	B	623	SER	3.8
1	A	544	PRO	3.7
1	B	144	GLU	3.7
1	B	69	HIS	3.7
1	B	526	ILE	3.7
1	B	141	GLN	3.7
1	B	164	LEU	3.7
1	A	598	ALA	3.7
1	B	30	GLY	3.7
1	B	104	PRO	3.7
1	B	601	GLU	3.7
1	B	610	GLU	3.7
1	A	635	THR	3.7
1	A	52	LEU	3.7
1	B	179	THR	3.7
1	A	567	HIS	3.6
1	B	614	GLN	3.6
1	B	41	SER	3.6
1	B	108	ILE	3.6
1	B	170	LEU	3.6
1	B	589	GLY	3.6
1	A	607	ASP	3.6
1	B	629	PRO	3.6
1	A	57	ARG	3.6
1	B	297	LEU	3.6
1	B	448	ALA	3.6
1	B	117	PRO	3.6
1	B	453	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	511	ILE	3.5
1	A	614	GLN	3.5
1	B	42	LEU	3.5
1	B	535	ASN	3.5
1	B	531	ILE	3.5
1	B	167	MET	3.5
1	A	489	ALA	3.5
1	A	610	GLU	3.5
1	A	532	VAL	3.5
1	A	540	VAL	3.5
1	B	542	VAL	3.5
1	B	640	VAL	3.5
1	B	462	HIS	3.5
1	B	56	GLU	3.5
1	B	449	TYR	3.5
1	A	190	PRO	3.4
1	A	628	PRO	3.4
1	A	328	ILE	3.4
1	A	581	LEU	3.4
1	A	579	ALA	3.4
1	B	538	ALA	3.4
1	B	544	PRO	3.4
1	A	161	TYR	3.4
1	A	33	ARG	3.4
1	A	590	ARG	3.4
1	B	543	GLN	3.3
1	A	44	HIS	3.3
1	A	433	LYS	3.3
1	B	627	ARG	3.3
1	A	600	GLY	3.3
1	B	461	GLY	3.3
1	A	542	VAL	3.3
1	A	565	VAL	3.3
1	A	39	ASN	3.3
1	B	145	ASN	3.3
1	A	479	PRO	3.3
1	B	327	SER	3.3
1	A	56	GLU	3.3
1	B	11	ASP	3.3
1	A	613	GLY	3.3
1	A	483	TYR	3.3
1	B	530	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	522	THR	3.3
1	A	495	ALA	3.2
1	B	208	ASN	3.2
1	A	617	ARG	3.2
1	B	482	THR	3.2
1	B	498	THR	3.2
1	A	329	SER	3.2
1	B	124	LEU	3.2
1	B	507	LEU	3.2
1	A	158	GLY	3.2
1	A	584	SER	3.2
1	B	511	ILE	3.2
1	A	462	HIS	3.2
1	B	178	TYR	3.2
1	B	107	GLU	3.2
1	B	500	ASN	3.2
1	A	633	THR	3.1
1	B	89	VAL	3.1
1	B	132	VAL	3.1
1	B	510	ARG	3.1
1	B	527	ILE	3.1
1	A	620	VAL	3.1
1	B	110	VAL	3.1
1	B	505	GLN	3.1
1	B	152	VAL	3.1
1	B	39	ASN	3.1
1	A	583	TYR	3.1
1	B	53	SER	3.1
1	A	594	THR	3.1
1	A	42	LEU	3.0
1	B	14	GLY	3.0
1	A	543	GLN	3.0
1	B	6	ARG	3.0
1	B	36	LYS	3.0
1	B	571	LYS	3.0
1	A	592	VAL	3.0
1	B	438	VAL	3.0
1	B	479	PRO	3.0
1	A	339	ALA	3.0
1	B	569	LYS	3.0
1	B	24	LEU	3.0
1	A	43	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	54	ILE	3.0
1	A	588	GLU	3.0
1	A	619	THR	3.0
1	A	484	VAL	3.0
1	A	325	LEU	3.0
1	A	623	SER	2.9
1	B	548	ASN	2.9
1	A	153	GLN	2.9
1	A	440	VAL	2.9
1	A	297	LEU	2.9
1	A	538	ALA	2.9
1	B	450	ILE	2.9
1	B	584	SER	2.9
1	A	482	THR	2.9
1	A	537	ASN	2.9
1	B	158	GLY	2.9
1	A	627	ARG	2.9
1	B	525	ALA	2.9
1	B	637	THR	2.9
1	A	461	GLY	2.9
1	A	580	GLU	2.9
1	B	10	GLU	2.9
1	B	122	ILE	2.9
1	A	601	GLU	2.9
1	A	45	VAL	2.8
1	A	79	VAL	2.8
1	A	430	VAL	2.8
1	B	523	SER	2.8
1	A	531	ILE	2.8
1	B	537	ASN	2.8
1	B	475	VAL	2.8
1	A	570	ALA	2.8
1	A	150	ILE	2.8
1	A	188	GLY	2.8
1	A	26	LEU	2.8
1	A	453	VAL	2.8
1	B	493	VAL	2.8
1	A	499	PHE	2.8
1	A	550	SER	2.8
1	B	433	LYS	2.8
1	A	105	GLY	2.8
1	A	503	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	549	GLY	2.8
1	B	18	GLY	2.8
1	B	386	THR	2.8
1	A	629	PRO	2.8
1	B	59	ASP	2.8
1	B	161	TYR	2.8
1	B	521	LEU	2.8
1	B	474	GLU	2.8
1	B	189	SER	2.8
1	B	516	GLY	2.7
1	A	446	PRO	2.7
1	B	163	ASP	2.7
1	B	572	ASP	2.7
1	B	176	SER	2.7
1	B	626	GLY	2.7
1	B	452	THR	2.7
1	B	434	PRO	2.7
1	A	40	ASN	2.7
1	B	514	SER	2.7
1	B	77	VAL	2.7
1	B	471	VAL	2.7
1	B	103	PHE	2.7
1	B	136	SER	2.7
1	B	439	SER	2.7
1	B	509	LEU	2.7
1	B	121	ARG	2.7
1	B	2	THR	2.7
1	B	196	THR	2.7
1	B	470	LEU	2.6
1	B	486	LEU	2.6
1	B	25	HIS	2.6
1	B	15	THR	2.6
1	B	389	LEU	2.6
1	B	504	LEU	2.6
1	A	552	GLU	2.6
1	A	326	THR	2.6
1	B	460	PHE	2.6
1	B	138	GLN	2.6
1	B	29	GLU	2.6
1	B	432	ALA	2.6
1	A	436	TYR	2.6
1	B	5	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	536	ASP	2.6
1	A	450	ILE	2.6
1	B	298	ASN	2.6
1	B	57	ARG	2.6
1	B	631	SER	2.6
1	A	74	LEU	2.6
1	A	573	ALA	2.5
1	A	154	THR	2.5
1	A	102	ARG	2.5
1	B	62	ARG	2.5
1	B	469	ARG	2.5
1	A	55	GLY	2.5
1	B	105	GLY	2.5
1	A	16	VAL	2.5
1	A	637	THR	2.5
1	B	534	GLN	2.5
1	A	621	SER	2.5
1	A	34	LEU	2.5
1	A	389	LEU	2.5
1	B	157	ASP	2.5
1	A	551	ALA	2.5
1	B	106	ALA	2.5
1	B	195	THR	2.5
1	B	211	VAL	2.5
1	B	617	ARG	2.5
1	A	561	HIS	2.5
1	B	95	ASP	2.5
1	A	29	GLU	2.4
1	B	74	LEU	2.4
1	B	159	VAL	2.4
1	B	435	VAL	2.4
1	A	527	ILE	2.4
1	A	541	ILE	2.4
1	A	497	ARG	2.4
1	B	153	GLN	2.4
1	A	106	ALA	2.4
1	B	339	ALA	2.4
1	A	490	THR	2.4
1	B	120	THR	2.4
1	B	454	VAL	2.4
1	B	466	VAL	2.4
1	B	547	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	431	PHE	2.4
1	B	624	ASP	2.4
1	A	156	ALA	2.4
1	B	323	THR	2.4
1	A	438	VAL	2.4
1	A	28	GLY	2.4
1	A	447	GLY	2.4
1	B	63	ILE	2.4
1	B	137	ILE	2.4
1	A	575	GLU	2.3
1	A	569	LYS	2.3
1	A	434	PRO	2.3
1	B	115	SER	2.3
1	B	200	VAL	2.3
1	B	12	GLU	2.3
1	B	444	ASN	2.3
1	A	89	VAL	2.3
1	B	76	VAL	2.3
1	B	506	GLN	2.3
1	B	130	GLU	2.3
1	A	58	ILE	2.3
1	B	483	TYR	2.3
1	A	509	LEU	2.3
1	A	639	LEU	2.3
1	B	71	THR	2.3
1	B	101	PRO	2.3
1	A	516	GLY	2.3
1	A	465	LYS	2.3
1	B	199	ASN	2.3
1	A	386	THR	2.3
1	A	473	THR	2.3
1	A	13	PRO	2.2
1	B	27	GLU	2.2
1	A	77	VAL	2.2
1	A	54	ILE	2.2
1	A	534	GLN	2.2
1	B	128	THR	2.2
1	A	492	ALA	2.2
1	B	552	GLU	2.2
1	B	191	SER	2.2
1	B	188	GLY	2.2
1	A	454	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	GLU	2.2
1	A	498	THR	2.2
1	A	545	ALA	2.2
1	B	489	ALA	2.2
1	B	550	SER	2.2
1	A	530	LYS	2.2
1	B	457	ASP	2.2
1	B	465	LYS	2.2
1	B	79	VAL	2.2
1	A	122	ILE	2.1
1	B	72	LEU	2.1
1	A	191	SER	2.1
1	B	408	SER	2.1
1	B	549	GLY	2.1
1	A	520	GLN	2.1
1	B	66	GLN	2.1
1	A	435	VAL	2.1
1	B	430	VAL	2.1
1	B	169	GLU	2.1
1	A	496	LEU	2.1
1	B	81	LYS	2.1
1	B	131	ASP	2.1
1	A	432	ALA	2.1
1	A	478	ALA	2.1
1	B	428	ALA	2.1
1	A	491	GLY	2.1
1	A	145	ASN	2.1
1	A	185	MET	2.1
1	A	298	ASN	2.1
1	A	87	ILE	2.1
1	A	209	SER	2.1
1	B	186	ASP	2.1
1	B	429	PRO	2.1
1	A	4	ARG	2.1
1	A	62	ARG	2.1
1	A	41	SER	2.1
1	A	485	SER	2.1
1	A	557	SER	2.1
1	A	140	PHE	2.1
1	B	32	PHE	2.1
1	B	328	ILE	2.1
1	B	35	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	28	GLY	2.0
1	B	135	ASN	2.0
1	B	446	PRO	2.0
1	A	46	ARG	2.0
1	A	163	ASP	2.0
1	A	422	SER	2.0
1	B	481	THR	2.0
1	A	477	GLY	2.0
1	B	61	GLU	2.0
1	A	455	ALA	2.0
1	B	94	ARG	2.0
1	A	304	CYS	2.0
1	B	112	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)

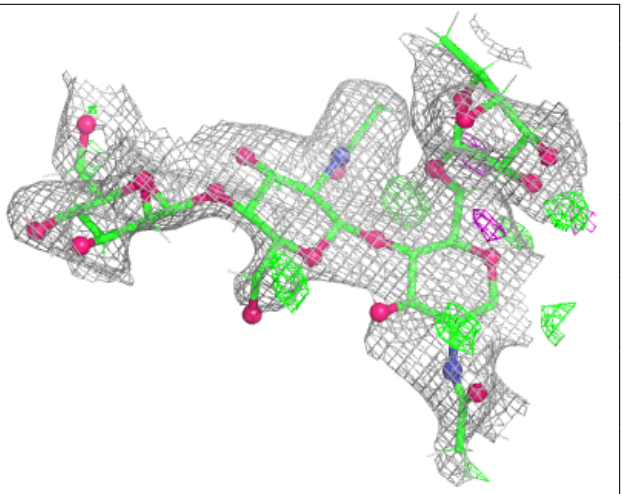
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

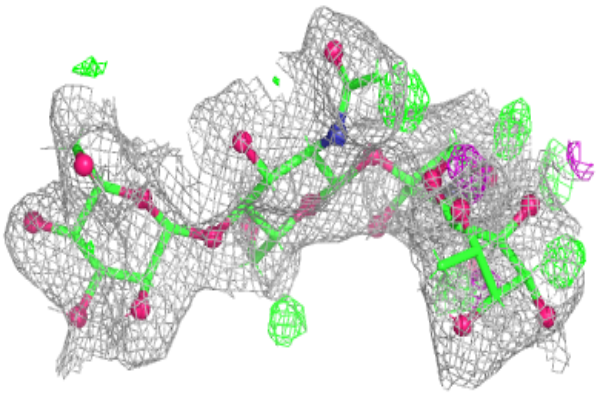
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	C	3	11/12	0.55	0.17	75,105,115,135	0
2	BMA	D	3	11/12	0.68	0.16	58,83,100,104	0
2	FUC	D	4	10/11	0.70	0.22	43,76,96,115	0
2	NAG	D	2	14/15	0.73	0.18	57,83,113,141	0
2	NAG	D	1	14/15	0.74	0.19	36,72,104,114	0
2	NAG	C	2	14/15	0.78	0.17	42,73,106,128	0
2	FUC	C	4	10/11	0.82	0.21	45,72,105,127	0
2	NAG	C	1	14/15	0.87	0.17	31,56,88,95	0

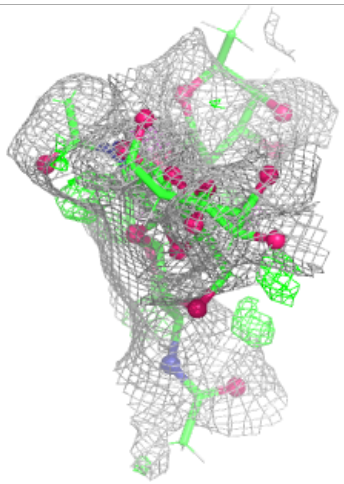
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

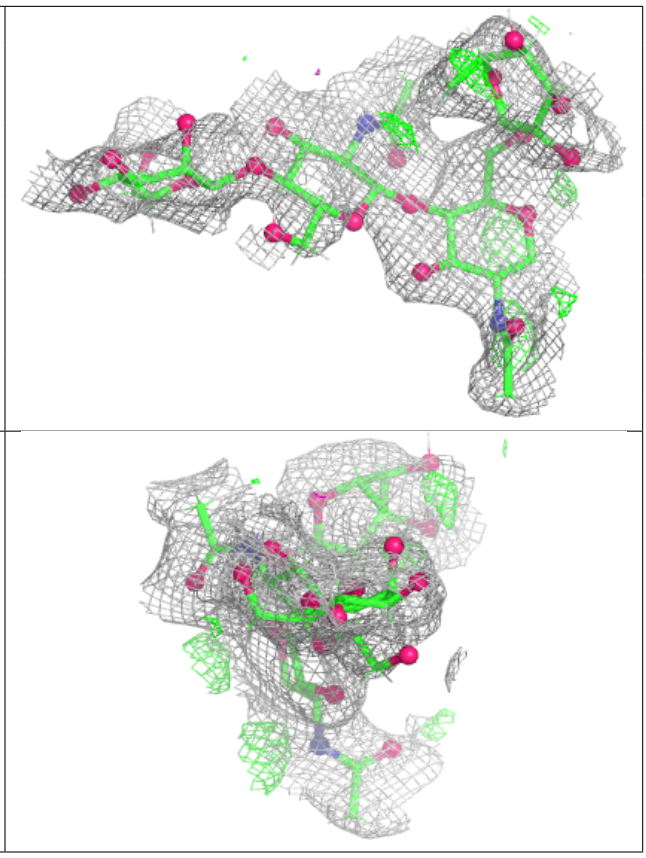






Electron density around Chain D:

$2mF_o$-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
6	MAN	B	722	11/12	0.52	0.26	64,110,135,158	0
6	MAN	B	721	11/12	0.60	0.19	66,94,131,142	0
6	MAN	A	722	11/12	0.67	0.18	49,82,99,109	0
6	MAN	A	723	11/12	0.69	0.22	56,81,104,132	0
4	CA	B	719	1/1	0.78	0.17	154,154,154,154	0
4	CA	B	706	1/1	0.86	0.12	92,92,92,92	0
3	EDO	B	724	4/4	0.86	0.17	42,65,79,88	0
4	CA	B	705	1/1	0.88	0.11	75,75,75,75	0
5	CL	B	720	1/1	0.88	0.25	69,69,69,69	0
4	CA	B	707	1/1	0.89	0.13	122,122,122,122	0
4	CA	B	714	1/1	0.90	0.11	62,62,62,62	0
5	CL	A	721	1/1	0.91	0.15	43,43,43,43	0
4	CA	B	708	1/1	0.91	0.12	74,74,74,74	0
3	EDO	A	705	4/4	0.93	0.14	25,57,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	B	718	1/1	0.94	0.10	88,88,88,88	0
4	CA	A	719	1/1	0.95	0.07	91,91,91,91	0
4	CA	B	712	1/1	0.95	0.16	52,52,52,52	0
4	CA	A	718	1/1	0.95	0.08	69,69,69,69	0
4	CA	B	717	1/1	0.95	0.09	83,83,83,83	0
7	NA	B	723	1/1	0.95	0.10	46,46,46,46	0
4	CA	A	707	1/1	0.96	0.08	58,58,58,58	0
4	CA	A	715	1/1	0.96	0.05	44,44,44,44	0
4	CA	B	710	1/1	0.97	0.04	32,32,32,32	0
4	CA	A	716	1/1	0.97	0.05	52,52,52,52	0
4	CA	B	713	1/1	0.97	0.08	38,38,38,38	0
4	CA	A	717	1/1	0.97	0.07	62,62,62,62	0
4	CA	B	715	1/1	0.97	0.05	44,44,44,44	0
4	CA	B	716	1/1	0.97	0.05	59,59,59,59	0
4	CA	A	714	1/1	0.97	0.09	29,29,29,29	0
4	CA	A	711	1/1	0.97	0.04	34,34,34,34	0
4	CA	A	709	1/1	0.98	0.04	21,21,21,21	0
4	CA	B	709	1/1	0.98	0.07	47,47,47,47	0
4	CA	A	720	1/1	0.98	0.05	48,48,48,48	0
4	CA	A	706	1/1	0.98	0.08	56,56,56,56	0
4	CA	A	712	1/1	0.98	0.05	33,33,33,33	0
4	CA	A	708	1/1	0.98	0.04	56,56,56,56	0
7	NA	A	724	1/1	0.99	0.02	14,14,14,14	0
4	CA	A	710	1/1	0.99	0.02	23,23,23,23	0
4	CA	A	713	1/1	1.00	0.01	18,18,18,18	0
4	CA	B	711	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.