



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:25 PM UTC

PDB ID : 6VG1 / pdb_00006vg1
Title : xenopus protocadherin 8.1 EC1-6
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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 ⓘ 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

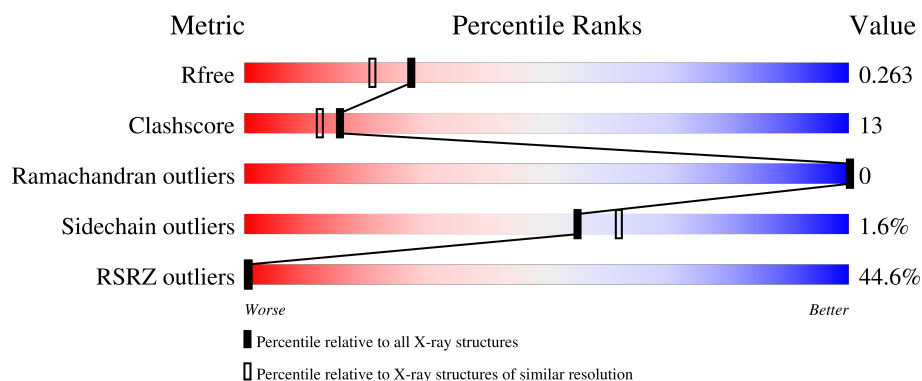
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	647	37% 74% 25%
1	B	647	52% 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.

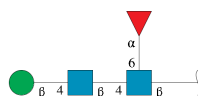
- Molecule 1 is a protein called protocadherin protein.

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

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.



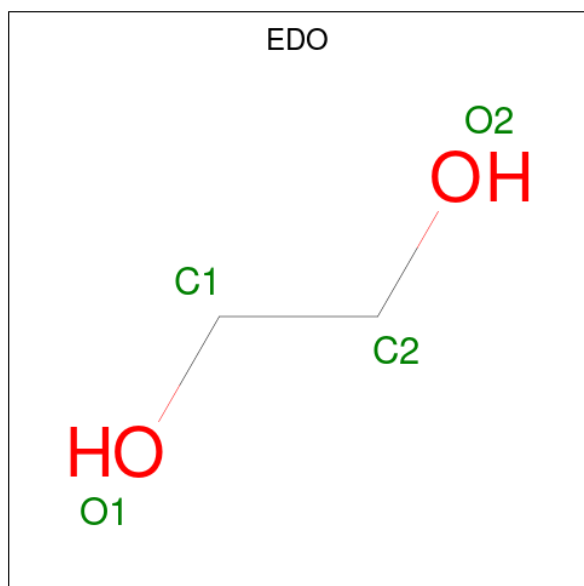
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O		0	0	0
			92	28	43	2	19				

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

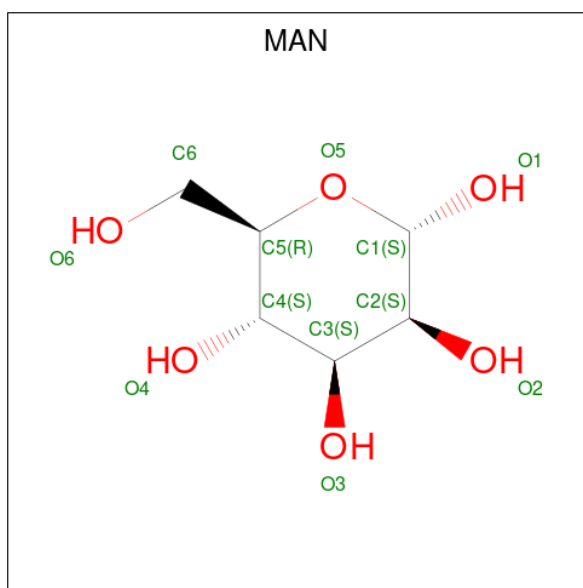
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



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 (CCD ID: 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		

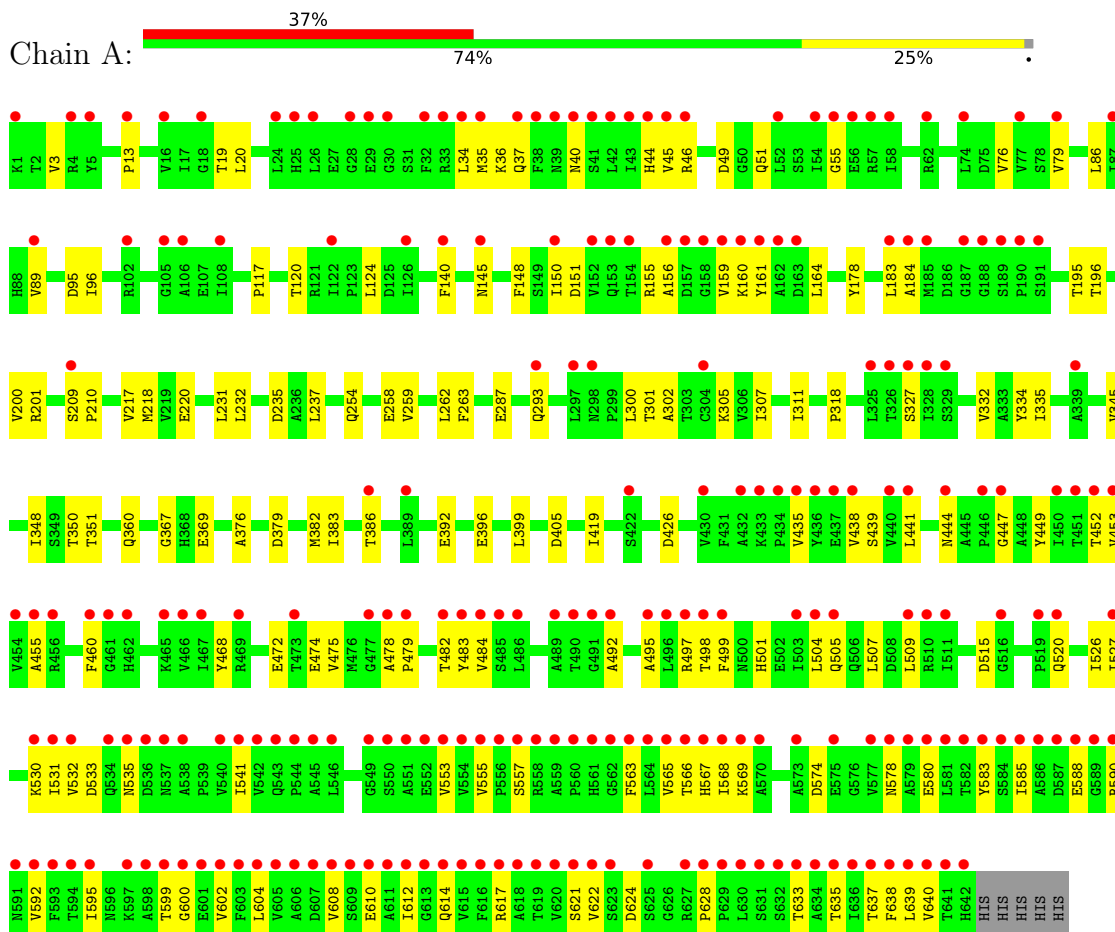
- Molecule 8 is water.

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

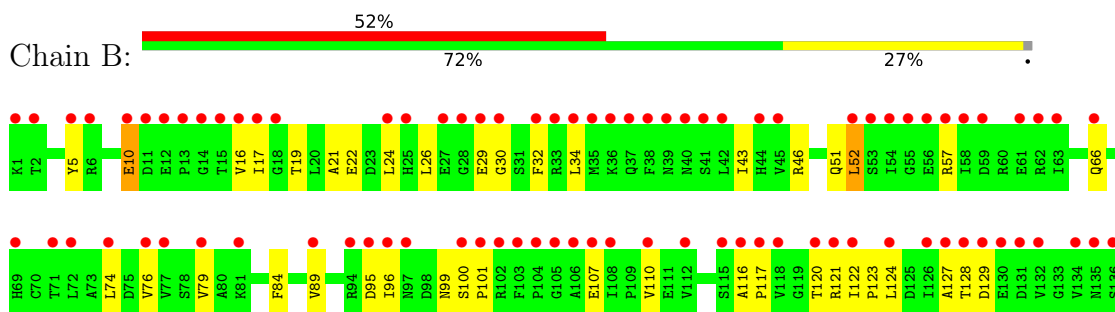
3 Residue-property plots

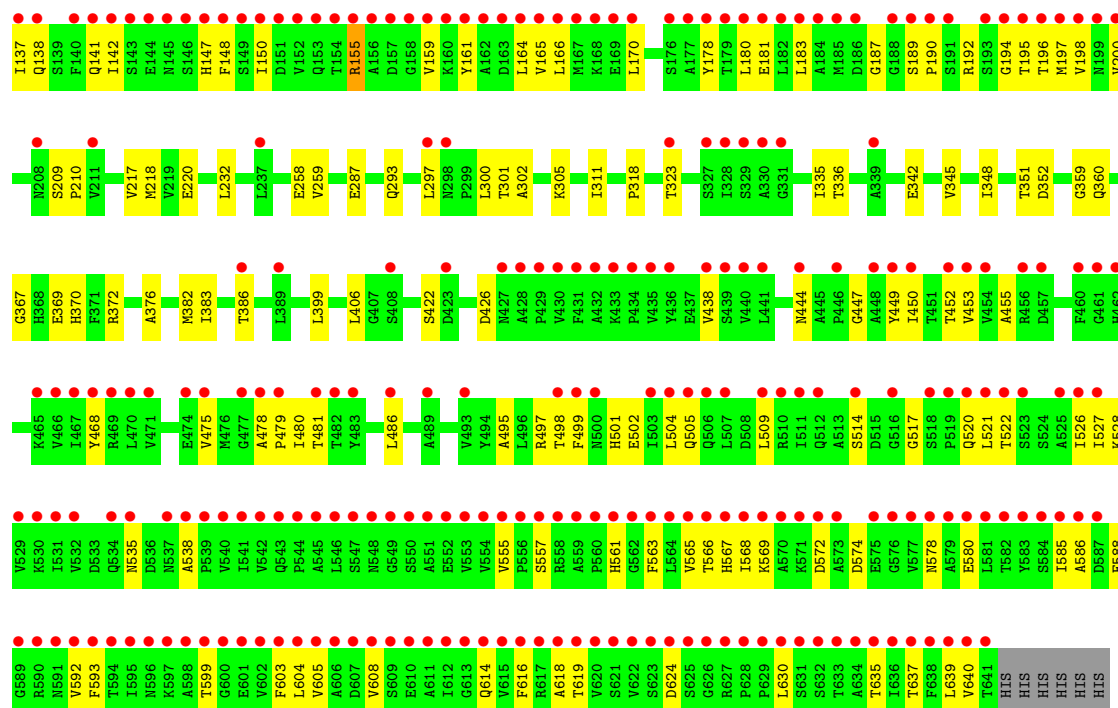
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: protocadherin protein





• 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: 25% 25% 50%



• 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: 50% 25% 25%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (1.36%)	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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.24	0/5010	0.46	0/6823
1	B	0.22	0/5005	0.44	0/6816
All	All	0.23	0/10015	0.45	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

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	121	0
1	B	4921	4770	4828	143	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	263	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 (263) 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	0.93
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:B:574:ASP:CG	1:B:578:ASN:OD1	2.37	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PHE:CE2	1:B:200:VAL:HG11	2.31	0.66
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: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:A:574:ASP:CG	1:A:578:ASN:OD1	2.40	0.62
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: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:B:370:HIS:C	1:B:386:THR:HG22	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ILE:O	1:A:585:ILE:HG23	2.07	0.54
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: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:183:LEU:C	1:A:183:LEU:HD12	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:HG23	1:B:323:THR:O	2.15	0.47
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: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:B:502:GLU:H	1:B:502:GLU:CD	2.23	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:A:254:GLN:CD	1:B:123:PRO:HG2	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG23	1:A:79:VAL:O	2.17	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:A:35:MET:HE1	1:A:86:LEU:HD11	2.00	0.42
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: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:B:183:LEU:HD12	1:B:183:LEU:C	2.46	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:254:GLN:CD	1:A:254:GLN:N	2.78	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:A:405:ASP:C	1:A:405:ASP:OD1	2.64	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 ⓘ

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	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 ⓘ

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%)	539 (98%)	10 (2%)	51	58
1	B	549/555 (99%)	541 (98%)	8 (2%)	57	64
All	All	1098/1110 (99%)	1080 (98%)	18 (2%)	55	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	45	VAL
1	A	151	ASP
1	A	160	LYS
1	A	201	ARG
1	A	218	MET
1	A	237	LEU
1	A	262	LEU
1	A	396	GLU
1	A	460	PHE
1	B	10	GLU
1	B	52	LEU
1	B	155	ARG
1	B	218	MET
1	B	297	LEU

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Mol	Chain	Res	Type
1	B	426	ASP
1	B	497	ARG
1	B	521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	44	HIS
1	A	83	GLN
1	A	208	ASN
1	A	277	GLN
1	A	567	HIS
1	B	147	HIS
1	B	175	GLN
1	B	229	HIS
1	B	277	GLN
1	B	316	ASN
1	B	368	HIS
1	B	444	ASN
1	B	506	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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(°)	Ideal(°)
2	C	4	FUC	O2-C2-C1	5.76	122.41	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

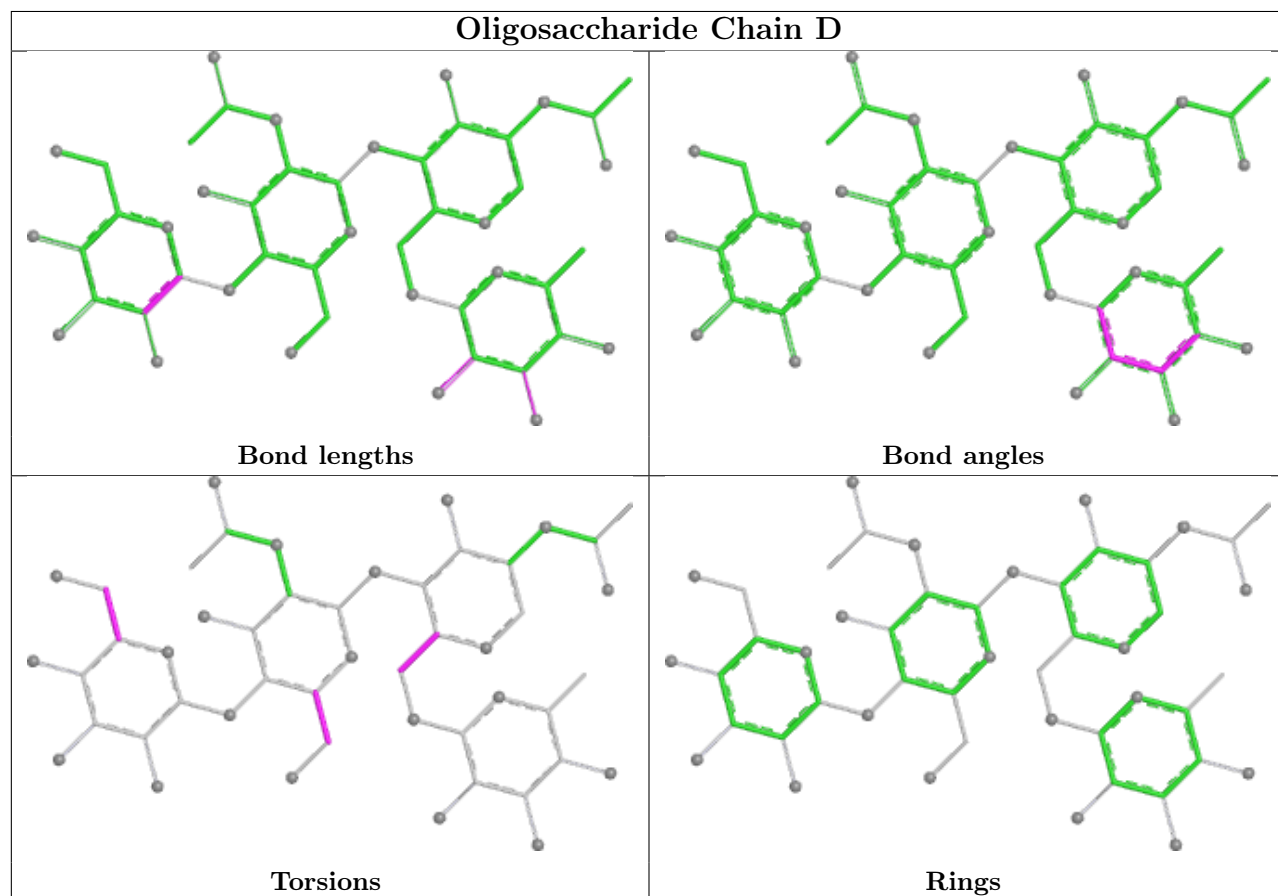
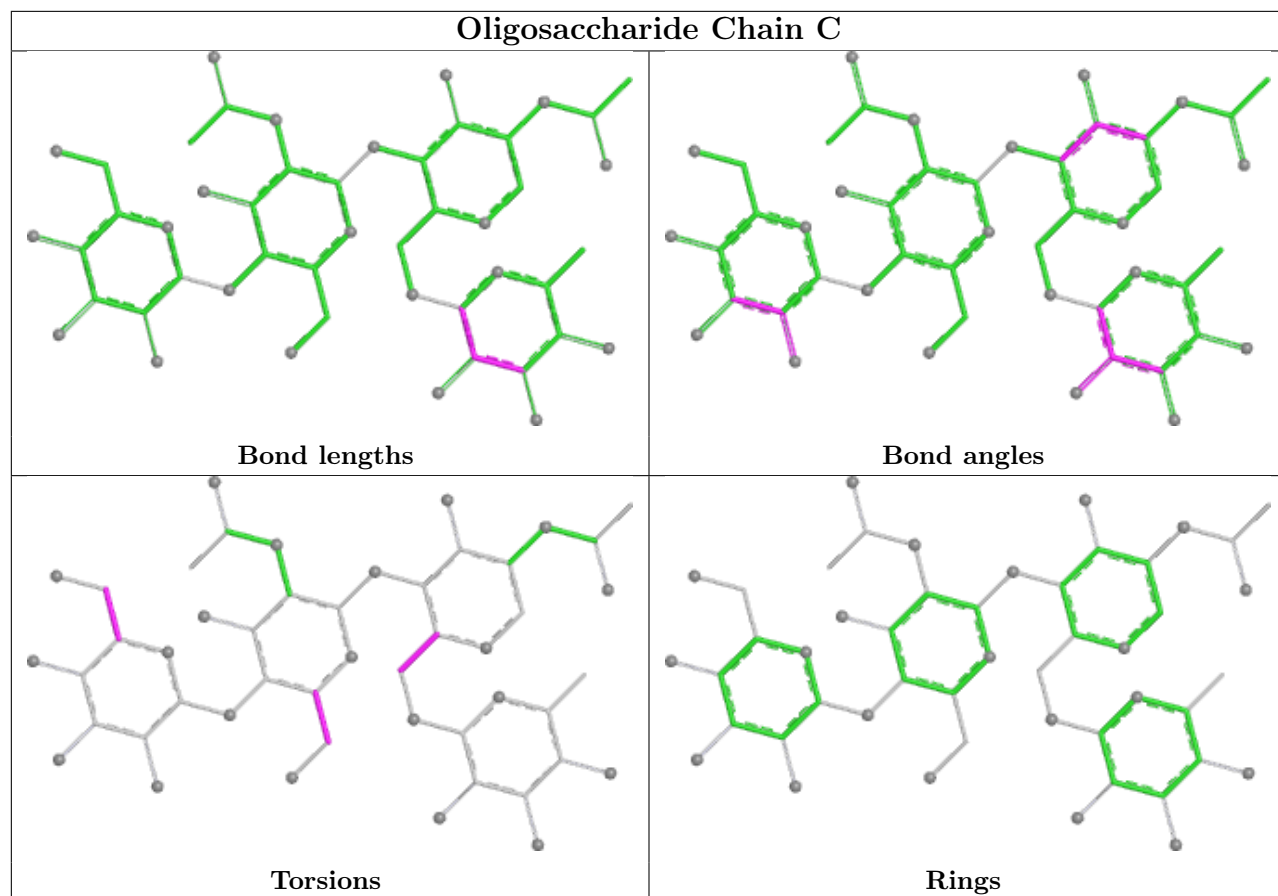
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

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.



5.6 Ligand geometry

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
6	MAN	A	723	1	11,11,12	1.01	0	15,15,17	1.35	3 (20%)
6	MAN	B	722	1	11,11,12	1.27	1 (9%)	15,15,17	1.10	1 (6%)
3	EDO	A	705	-	3,3,3	0.46	0	2,2,2	0.60	0
3	EDO	B	724	-	3,3,3	0.46	0	2,2,2	0.49	0
6	MAN	A	722	1	11,11,12	0.90	0	15,15,17	1.11	1 (6%)
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
6	MAN	A	723	1	-	2/2/19/22	0/1/1/1
6	MAN	B	722	1	-	0/2/19/22	0/1/1/1
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	B	724	-	-	1/1/1/1	-
6	MAN	A	722	1	-	0/2/19/22	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(°)	Ideal(°)
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
6	A	723	MAN	1	0
6	B	722	MAN	2	0
3	A	705	EDO	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

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	642/647 (99%)	1.77	237 (36%) 1 1	12, 65, 130, 196	0
1	B	641/647 (99%)	2.45	335 (52%) 0 0	21, 81, 156, 231	0
All	All	1283/1294 (99%)	2.11	572 (44%) 0 1	12, 72, 145, 231	0

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	PHE	10.5
1	A	616	PHE	8.8
1	B	556	PRO	8.8
1	B	555	VAL	8.6
1	A	38	PHE	8.3
1	B	568	ILE	8.3
1	B	605	VAL	8.3
1	B	598	ALA	8.0
1	A	642	HIS	7.9
1	A	618	ALA	7.9
1	B	622	VAL	7.8
1	B	554	VAL	7.8
1	B	595	ILE	7.8
1	A	546	LEU	7.6
1	A	563	PHE	7.6
1	B	581	LEU	7.5
1	B	563	PHE	7.5
1	B	545	ALA	7.5
1	B	560	PRO	7.5
1	A	586	ALA	7.4
1	A	582	THR	7.4
1	B	621	SER	7.3
1	B	564	LEU	7.2
1	B	641	THR	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	540	VAL	7.1
1	B	577	VAL	7.1
1	B	612	ILE	7.0
1	B	592	VAL	6.8
1	A	159	VAL	6.7
1	B	615	VAL	6.6
1	A	602	VAL	6.6
1	B	602	VAL	6.6
1	B	38	PHE	6.5
1	B	618	ALA	6.4
1	A	636	ILE	6.4
1	B	559	ALA	6.4
1	A	615	VAL	6.4
1	B	583	TYR	6.3
1	B	638	PHE	6.3
1	B	142	ILE	6.2
1	A	554	VAL	6.2
1	B	118	VAL	6.1
1	B	440	VAL	6.1
1	A	162	ALA	6.1
1	B	566	THR	6.1
1	B	611	ALA	6.1
1	B	127	ALA	6.0
1	B	608	VAL	6.0
1	B	603	PHE	6.0
1	B	96	ILE	6.0
1	B	585	ILE	6.0
1	B	606	ALA	5.9
1	A	603	PHE	5.9
1	B	436	TYR	5.9
1	B	546	LEU	5.9
1	B	147	HIS	5.9
1	B	185	MET	5.9
1	B	150	ILE	5.9
1	B	541	ILE	5.8
1	B	607	ASP	5.8
1	B	553	VAL	5.8
1	B	193	SER	5.8
1	A	585	ILE	5.7
1	B	636	ILE	5.7
1	B	146	SER	5.7
1	B	625	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	5.7
1	B	632	SER	5.6
1	B	594	THR	5.6
1	B	177	ALA	5.6
1	B	557	SER	5.5
1	B	168	LYS	5.4
1	B	558	ARG	5.3
1	B	580	GLU	5.3
1	A	555	VAL	5.3
1	B	593	PHE	5.3
1	B	184	ALA	5.3
1	A	564	LEU	5.3
1	A	640	VAL	5.3
1	B	565	VAL	5.3
1	B	619	THR	5.3
1	B	532	VAL	5.2
1	A	126	ILE	5.2
1	B	620	VAL	5.2
1	A	606	ALA	5.2
1	B	183	LEU	5.1
1	B	478	ALA	5.1
1	A	535	ASN	5.1
1	B	519	PRO	5.0
1	B	582	THR	5.0
1	B	148	PHE	5.0
1	B	570	ALA	5.0
1	B	52	LEU	5.0
1	A	608	VAL	5.0
1	B	126	ILE	5.0
1	B	630	LEU	5.0
1	B	639	LEU	5.0
1	A	587	ASP	4.9
1	B	586	ALA	4.9
1	A	604	LEU	4.9
1	A	630	LEU	4.9
1	B	34	LEU	4.9
1	B	330	ALA	4.9
1	B	634	ALA	4.9
1	B	44	HIS	4.8
1	A	632	SER	4.8
1	B	600	GLY	4.8
1	B	33	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	599	THR	4.8
1	B	190	PRO	4.8
1	B	561	HIS	4.8
1	B	1	LYS	4.8
1	B	597	LYS	4.8
1	A	578	ASN	4.8
1	B	58	ILE	4.8
1	B	591	ASN	4.8
1	A	589	GLY	4.8
1	B	567	HIS	4.8
1	A	553	VAL	4.8
1	B	149	SER	4.8
1	A	559	ALA	4.8
1	B	499	PHE	4.7
1	B	456	ARG	4.7
1	A	599	THR	4.7
1	A	591	ASN	4.7
1	B	198	VAL	4.7
1	B	441	LEU	4.7
1	A	605	VAL	4.6
1	B	237	LEU	4.6
1	B	134	VAL	4.6
1	B	166	LEU	4.6
1	B	180	LEU	4.6
1	A	612	ILE	4.5
1	B	16	VAL	4.5
1	B	587	ASP	4.5
1	A	452	THR	4.5
1	A	37	GLN	4.5
1	B	529	VAL	4.5
1	B	575	GLU	4.5
1	B	143	SER	4.4
1	A	595	ILE	4.4
1	A	160	LYS	4.4
1	B	140	PHE	4.4
1	A	556	PRO	4.4
1	B	604	LEU	4.4
1	A	1	LYS	4.4
1	A	566	THR	4.4
1	B	40	ASN	4.4
1	B	162	ALA	4.4
1	A	189	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	596	ASN	4.4
1	B	156	ALA	4.4
1	B	100	SER	4.4
1	A	597	LYS	4.4
1	B	633	THR	4.3
1	A	560	PRO	4.3
1	A	558	ARG	4.3
1	B	576	GLY	4.3
1	B	613	GLY	4.3
1	B	37	GLN	4.3
1	B	520	GLN	4.3
1	A	625	SER	4.3
1	B	55	GLY	4.3
1	A	641	THR	4.3
1	A	611	ALA	4.3
1	B	165	VAL	4.3
1	A	456	ARG	4.3
1	A	467	ILE	4.3
1	B	578	ASN	4.3
1	A	519	PRO	4.3
1	A	638	PHE	4.2
1	A	152	VAL	4.2
1	B	182	LEU	4.2
1	B	181	GLU	4.2
1	B	628	PRO	4.2
1	A	634	ALA	4.2
1	B	477	GLY	4.2
1	B	579	ALA	4.2
1	A	577	VAL	4.2
1	B	467	ILE	4.1
1	B	551	ALA	4.1
1	A	24	LEU	4.1
1	B	562	GLY	4.1
1	B	329	SER	4.1
1	A	622	VAL	4.1
1	B	503	ILE	4.1
1	B	573	ALA	4.1
1	A	460	PHE	4.1
1	B	635	THR	4.1
1	A	609	SER	4.1
1	B	539	PRO	4.1
1	A	25	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	154	THR	4.0
1	B	160	LYS	4.0
1	B	129	ASP	4.0
1	B	45	VAL	4.0
1	A	593	PHE	4.0
1	A	562	GLY	4.0
1	B	194	GLY	4.0
1	B	102	ARG	3.9
1	B	518	SER	3.9
1	A	157	ASP	3.9
1	B	30	GLY	3.9
1	A	598	ALA	3.9
1	B	609	SER	3.9
1	B	164	LEU	3.9
1	A	544	PRO	3.9
1	B	197	MET	3.9
1	A	469	ARG	3.9
1	B	590	ARG	3.9
1	B	526	ILE	3.9
1	B	623	SER	3.9
1	B	104	PRO	3.9
1	B	69	HIS	3.8
1	A	52	LEU	3.8
1	A	635	THR	3.8
1	B	589	GLY	3.8
1	B	141	GLN	3.8
1	B	170	LEU	3.8
1	B	179	THR	3.8
1	B	144	GLU	3.8
1	B	108	ILE	3.8
1	A	567	HIS	3.8
1	B	297	LEU	3.8
1	B	629	PRO	3.8
1	B	601	GLU	3.8
1	B	610	GLU	3.8
1	B	41	SER	3.7
1	B	448	ALA	3.7
1	B	614	GLN	3.7
1	B	453	VAL	3.7
1	A	607	ASP	3.7
1	B	42	LEU	3.7
1	B	117	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	511	ILE	3.7
1	A	489	ALA	3.7
1	B	535	ASN	3.7
1	A	532	VAL	3.7
1	A	540	VAL	3.7
1	B	542	VAL	3.7
1	B	640	VAL	3.7
1	B	531	ILE	3.7
1	A	57	ARG	3.7
1	B	449	TYR	3.7
1	A	614	GLN	3.6
1	B	167	MET	3.6
1	B	462	HIS	3.6
1	A	190	PRO	3.6
1	A	628	PRO	3.6
1	A	328	ILE	3.6
1	A	579	ALA	3.6
1	B	538	ALA	3.6
1	A	581	LEU	3.6
1	A	610	GLU	3.6
1	A	161	TYR	3.6
1	B	56	GLU	3.5
1	B	544	PRO	3.5
1	A	600	GLY	3.5
1	B	461	GLY	3.5
1	A	542	VAL	3.5
1	A	565	VAL	3.5
1	A	613	GLY	3.5
1	A	483	TYR	3.5
1	A	44	HIS	3.5
1	A	479	PRO	3.4
1	A	33	ARG	3.4
1	A	590	ARG	3.4
1	B	543	GLN	3.4
1	A	39	ASN	3.4
1	B	145	ASN	3.4
1	A	495	ALA	3.4
1	B	327	SER	3.4
1	B	522	THR	3.4
1	A	158	GLY	3.4
1	B	11	ASP	3.4
1	B	627	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	433	LYS	3.4
1	B	124	LEU	3.4
1	B	507	LEU	3.4
1	B	208	ASN	3.4
1	B	482	THR	3.4
1	B	498	THR	3.4
1	A	56	GLU	3.4
1	B	178	TYR	3.3
1	B	530	LYS	3.3
1	A	329	SER	3.3
1	B	511	ILE	3.3
1	A	584	SER	3.3
1	B	89	VAL	3.3
1	B	132	VAL	3.3
1	A	462	HIS	3.3
1	A	617	ARG	3.3
1	A	633	THR	3.3
1	A	620	VAL	3.3
1	B	110	VAL	3.3
1	B	527	ILE	3.3
1	B	500	ASN	3.3
1	B	152	VAL	3.2
1	A	583	TYR	3.2
1	B	14	GLY	3.2
1	B	107	GLU	3.2
1	A	42	LEU	3.2
1	A	594	THR	3.2
1	B	510	ARG	3.2
1	B	39	ASN	3.2
1	A	592	VAL	3.2
1	B	438	VAL	3.2
1	A	339	ALA	3.2
1	B	505	GLN	3.2
1	B	53	SER	3.2
1	B	479	PRO	3.2
1	B	24	LEU	3.1
1	A	543	GLN	3.1
1	A	484	VAL	3.1
1	A	43	ILE	3.1
1	A	325	LEU	3.1
1	B	54	ILE	3.1
1	A	619	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	6	ARG	3.1
1	A	440	VAL	3.1
1	A	538	ALA	3.1
1	A	297	LEU	3.1
1	B	36	LYS	3.1
1	B	571	LYS	3.1
1	B	158	GLY	3.1
1	B	525	ALA	3.1
1	B	569	LYS	3.1
1	B	450	ILE	3.1
1	A	623	SER	3.1
1	A	461	GLY	3.0
1	A	482	THR	3.0
1	B	548	ASN	3.0
1	A	588	GLU	3.0
1	A	153	GLN	3.0
1	B	584	SER	3.0
1	A	537	ASN	3.0
1	B	637	THR	3.0
1	A	45	VAL	3.0
1	A	79	VAL	3.0
1	A	430	VAL	3.0
1	B	122	ILE	3.0
1	A	570	ALA	3.0
1	A	627	ARG	3.0
1	B	475	VAL	3.0
1	A	188	GLY	3.0
1	A	531	ILE	3.0
1	A	499	PHE	3.0
1	A	580	GLU	2.9
1	B	10	GLU	2.9
1	B	523	SER	2.9
1	A	26	LEU	2.9
1	B	537	ASN	2.9
1	A	453	VAL	2.9
1	B	493	VAL	2.9
1	A	105	GLY	2.9
1	A	549	GLY	2.9
1	B	18	GLY	2.9
1	A	150	ILE	2.9
1	B	161	TYR	2.9
1	A	601	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	2.9
1	B	516	GLY	2.9
1	A	503	ILE	2.9
1	B	386	THR	2.9
1	A	629	PRO	2.9
1	A	550	SER	2.9
1	B	626	GLY	2.9
1	A	446	PRO	2.9
1	B	103	PHE	2.9
1	B	189	SER	2.9
1	B	59	ASP	2.8
1	B	77	VAL	2.8
1	B	471	VAL	2.8
1	B	452	THR	2.8
1	B	434	PRO	2.8
1	B	433	LYS	2.8
1	B	176	SER	2.8
1	B	163	ASP	2.8
1	B	572	ASP	2.8
1	B	509	LEU	2.8
1	B	474	GLU	2.8
1	A	40	ASN	2.8
1	B	514	SER	2.8
1	B	470	LEU	2.8
1	B	486	LEU	2.8
1	B	2	THR	2.8
1	B	196	THR	2.8
1	B	136	SER	2.8
1	B	439	SER	2.8
1	B	460	PHE	2.8
1	B	389	LEU	2.8
1	B	504	LEU	2.8
1	B	15	THR	2.8
1	B	25	HIS	2.7
1	B	432	ALA	2.7
1	A	436	TYR	2.7
1	B	5	TYR	2.7
1	A	326	THR	2.7
1	B	121	ARG	2.7
1	A	573	ALA	2.7
1	A	74	LEU	2.7
1	A	450	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	55	GLY	2.7
1	B	105	GLY	2.7
1	B	138	GLN	2.7
1	A	154	THR	2.7
1	A	552	GLU	2.7
1	B	298	ASN	2.7
1	A	16	VAL	2.7
1	B	631	SER	2.7
1	A	536	ASP	2.7
1	A	551	ALA	2.6
1	B	29	GLU	2.6
1	B	106	ALA	2.6
1	A	34	LEU	2.6
1	A	389	LEU	2.6
1	A	637	THR	2.6
1	B	211	VAL	2.6
1	B	57	ARG	2.6
1	B	195	THR	2.6
1	A	621	SER	2.6
1	A	102	ARG	2.6
1	B	62	ARG	2.6
1	B	469	ARG	2.6
1	B	534	GLN	2.6
1	A	561	HIS	2.6
1	B	74	LEU	2.6
1	B	157	ASP	2.6
1	B	159	VAL	2.6
1	B	435	VAL	2.6
1	A	106	ALA	2.6
1	B	339	ALA	2.6
1	B	95	ASP	2.6
1	B	617	ARG	2.6
1	B	431	PHE	2.5
1	A	527	ILE	2.5
1	A	541	ILE	2.5
1	B	454	VAL	2.5
1	B	466	VAL	2.5
1	A	156	ALA	2.5
1	A	490	THR	2.5
1	B	120	THR	2.5
1	A	29	GLU	2.5
1	A	28	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	438	VAL	2.5
1	A	447	GLY	2.5
1	B	153	GLN	2.5
1	B	323	THR	2.5
1	B	547	SER	2.5
1	A	497	ARG	2.5
1	B	63	ILE	2.5
1	B	137	ILE	2.5
1	B	200	VAL	2.5
1	B	624	ASP	2.5
1	A	434	PRO	2.5
1	A	89	VAL	2.4
1	B	76	VAL	2.4
1	B	483	TYR	2.4
1	B	115	SER	2.4
1	A	509	LEU	2.4
1	A	639	LEU	2.4
1	A	516	GLY	2.4
1	B	444	ASN	2.4
1	A	58	ILE	2.4
1	A	575	GLU	2.4
1	B	71	THR	2.4
1	B	101	PRO	2.4
1	A	569	LYS	2.4
1	B	12	GLU	2.4
1	B	506	GLN	2.4
1	A	77	VAL	2.4
1	A	386	THR	2.4
1	A	473	THR	2.4
1	A	13	PRO	2.4
1	A	492	ALA	2.4
1	B	130	GLU	2.4
1	B	188	GLY	2.4
1	B	199	ASN	2.4
1	A	54	ILE	2.4
1	A	454	VAL	2.4
1	B	128	THR	2.4
1	A	465	LYS	2.3
1	B	191	SER	2.3
1	A	498	THR	2.3
1	B	27	GLU	2.3
1	A	534	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	545	ALA	2.3
1	B	489	ALA	2.3
1	B	79	VAL	2.3
1	B	552	GLU	2.3
1	B	72	LEU	2.3
1	B	549	GLY	2.3
1	A	437	GLU	2.3
1	B	550	SER	2.3
1	A	122	ILE	2.3
1	A	435	VAL	2.3
1	B	430	VAL	2.3
1	A	432	ALA	2.3
1	A	478	ALA	2.3
1	B	428	ALA	2.3
1	B	457	ASP	2.3
1	A	491	GLY	2.3
1	A	496	LEU	2.3
1	A	191	SER	2.2
1	B	408	SER	2.2
1	A	530	LYS	2.2
1	B	465	LYS	2.2
1	A	520	GLN	2.2
1	B	66	GLN	2.2
1	A	140	PHE	2.2
1	B	32	PHE	2.2
1	A	87	ILE	2.2
1	A	145	ASN	2.2
1	A	298	ASN	2.2
1	B	429	PRO	2.2
1	A	185	MET	2.2
1	B	131	ASP	2.2
1	B	28	GLY	2.2
1	B	169	GLU	2.2
1	A	209	SER	2.2
1	B	81	LYS	2.2
1	B	446	PRO	2.2
1	B	186	ASP	2.2
1	B	328	ILE	2.2
1	A	477	GLY	2.2
1	A	455	ALA	2.2
1	A	41	SER	2.2
1	A	485	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	557	SER	2.2
1	B	135	ASN	2.2
1	B	35	MET	2.2
1	B	481	THR	2.2
1	B	112	VAL	2.1
1	A	4	ARG	2.1
1	A	62	ARG	2.1
1	A	304	CYS	2.1
1	A	422	SER	2.1
1	A	163	ASP	2.1
1	B	13	PRO	2.1
1	A	108	ILE	2.1
1	A	466	VAL	2.1
1	A	46	ARG	2.1
1	A	441	LEU	2.1
1	A	504	LEU	2.1
1	B	61	GLU	2.1
1	A	5	TYR	2.1
1	B	468	TYR	2.1
1	B	94	ARG	2.1
1	A	32	PHE	2.1
1	A	183	LEU	2.1
1	A	486	LEU	2.1
1	B	427	ASN	2.1
1	B	423	ASP	2.1
1	B	512	GLN	2.1
1	A	510	ARG	2.1
1	B	155	ARG	2.1
1	A	18	GLY	2.1
1	B	331	GLY	2.1
1	B	116	ALA	2.1
1	A	35	MET	2.0
1	A	444	ASN	2.0
1	B	97	ASN	2.0
1	A	505	GLN	2.0
1	A	451	THR	2.0
1	B	17	ILE	2.0
1	A	327	SER	2.0
1	A	631	SER	2.0
1	A	184	ALA	2.0
1	A	293	GLN	2.0
1	B	151	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	30	GLY	2.0
1	A	187	GLY	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](#)

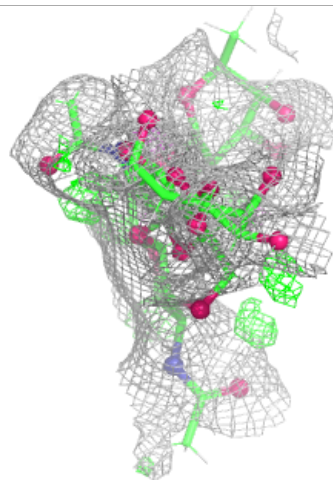
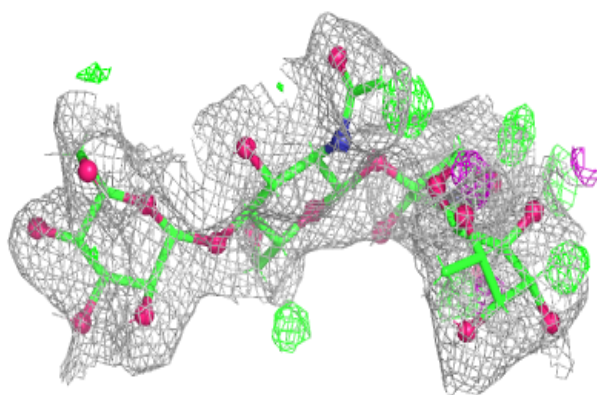
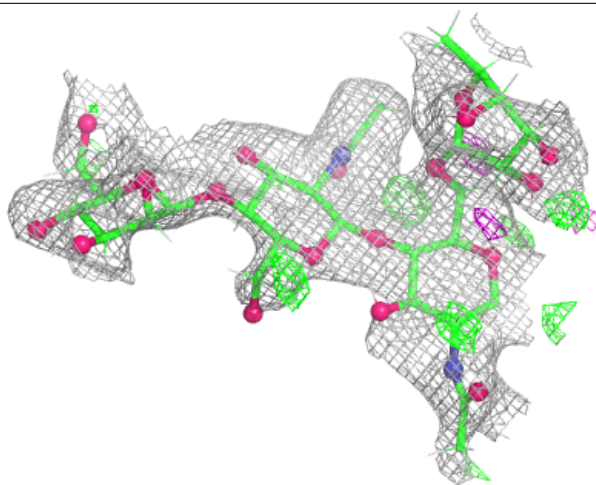
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

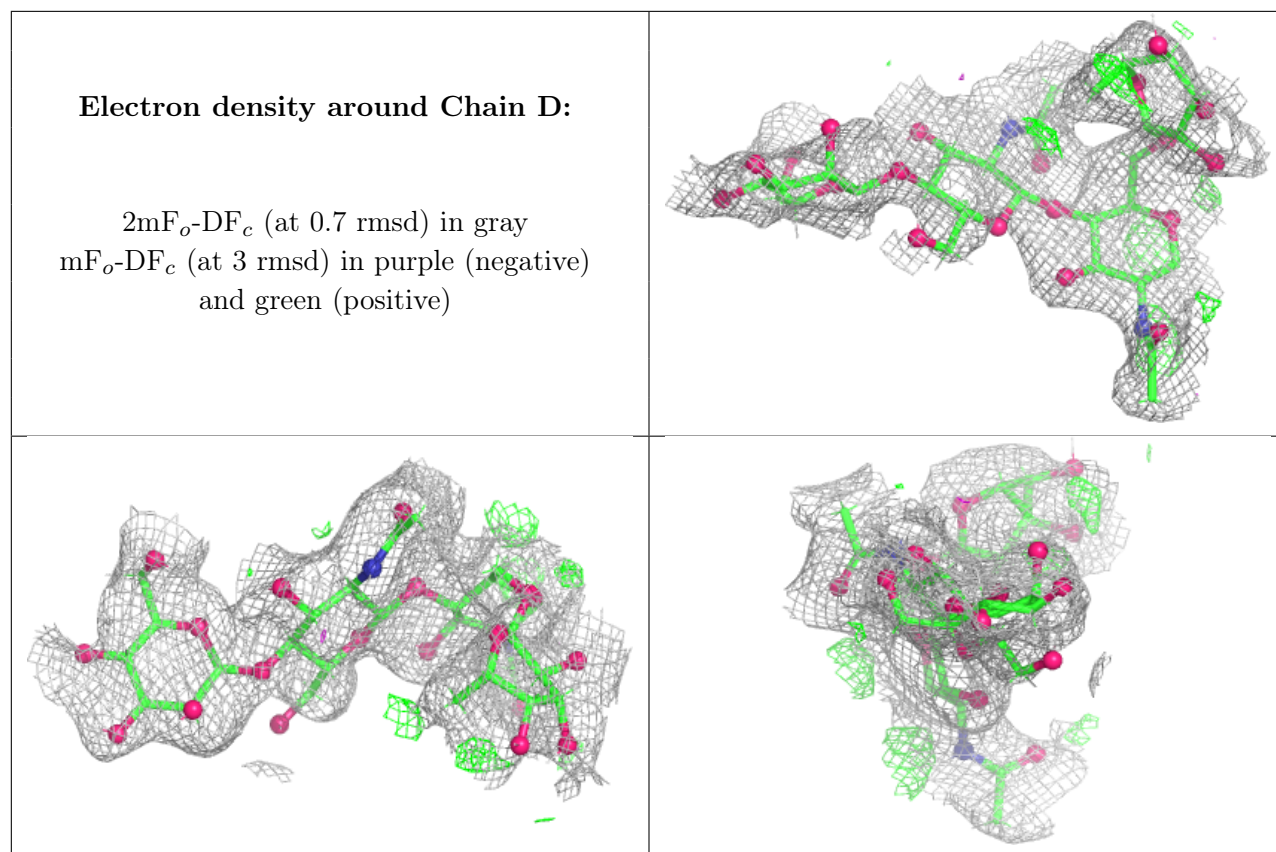
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.55	0.17	75,105,115,135	0
2	BMA	D	3	11/12	0.68	0.16	58,83,100,104	0
2	FUC	D	4	10/11	0.70	0.22	43,76,96,115	0
2	NAG	D	2	14/15	0.73	0.18	57,83,113,141	0
2	NAG	D	1	14/15	0.74	0.19	36,72,104,114	0
2	NAG	C	2	14/15	0.78	0.17	42,73,106,128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





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	0.80	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	0.89	0.10	62,62,62,62	0
5	CL	A	721	1/1	0.90	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($\text{\AA}^2$)	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	0.08	83,83,83,83	0
7	NA	B	723	1/1	0.95	0.10	46,46,46,46	0
4	CA	A	715	1/1	0.96	0.05	44,44,44,44	0
4	CA	B	715	1/1	0.96	0.05	44,44,44,44	0
4	CA	A	707	1/1	0.96	0.08	58,58,58,58	0
4	CA	B	713	1/1	0.97	0.07	38,38,38,38	0
4	CA	A	717	1/1	0.97	0.07	62,62,62,62	0
4	CA	A	714	1/1	0.97	0.09	29,29,29,29	0
4	CA	B	716	1/1	0.97	0.05	59,59,59,59	0
4	CA	A	711	1/1	0.97	0.04	34,34,34,34	0
4	CA	B	710	1/1	0.97	0.03	32,32,32,32	0
4	CA	A	716	1/1	0.97	0.05	52,52,52,52	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	720	1/1	0.98	0.05	48,48,48,48	0
4	CA	B	709	1/1	0.98	0.07	47,47,47,47	0
4	CA	A	708	1/1	0.98	0.04	56,56,56,56	0
4	CA	A	709	1/1	0.99	0.04	21,21,21,21	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.