



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 AM UTC

PDB ID : 6BDZ / pdb_00006bdz
Title : ADAM10 Extracellular Domain Bound by the 11G2 Fab
Authors : Seegar, T.C.M.
Deposited on : 2017-10-24
Resolution : 3.10 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

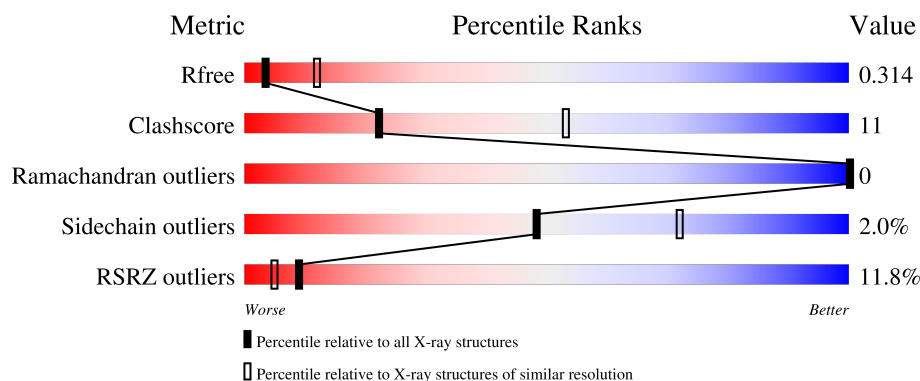
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	L	215	80% 19% .
2	H	226	2% 81% 16% .
3	A	443	21% 70% 23% 5%
4	B	4	100%
5	C	3	67% 33%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6631 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 11G2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1645	1020	279	337	9			

- Molecule 2 is a protein called 11G2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1643	1035	274	327	7			

- Molecule 3 is a protein called Disintegrin and metalloproteinase domain-containing protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	421	Total	C	N	O	S	0	0	0
			3242	1991	574	637	40			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLN	ASN	conflict	UNP O14672
A	439	GLN	ASN	conflict	UNP O14672
A	551	GLN	ASN	conflict	UNP O14672
A	655	GLY	-	expression tag	UNP O14672
A	656	GLY	-	expression tag	UNP O14672
A	657	HIS	-	expression tag	UNP O14672
A	658	HIS	-	expression tag	UNP O14672
A	659	HIS	-	expression tag	UNP O14672
A	660	HIS	-	expression tag	UNP O14672
A	661	HIS	-	expression tag	UNP O14672
A	662	HIS	-	expression tag	UNP O14672

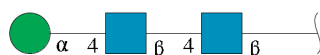
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran

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



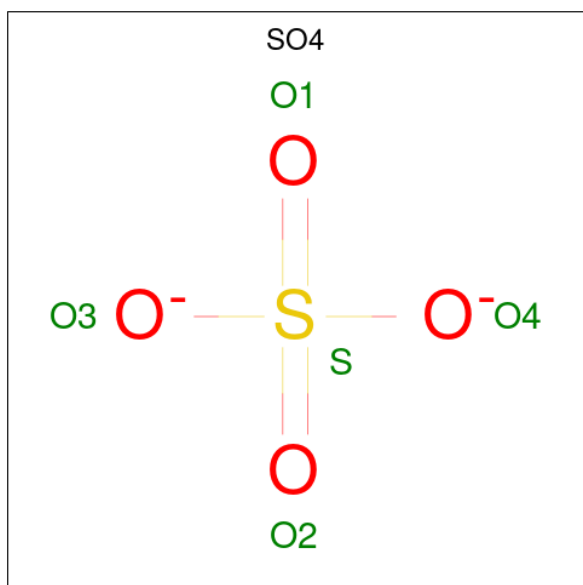
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Zn	0	0
			1	1		

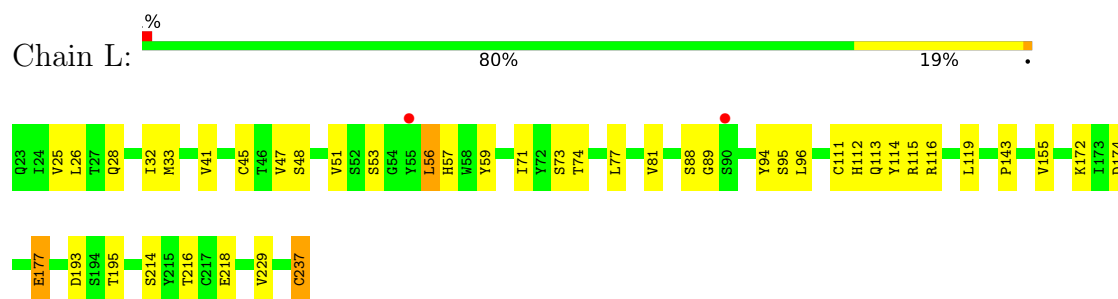
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	O	0	0
			1	1		

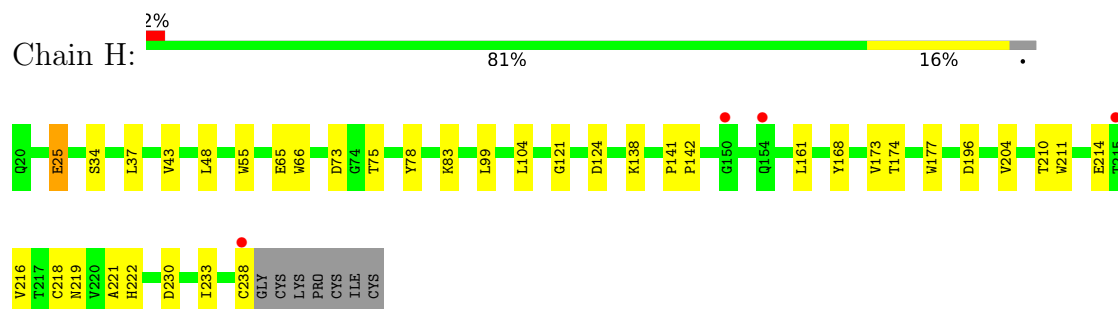
3 Residue-property plots [i](#)

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.

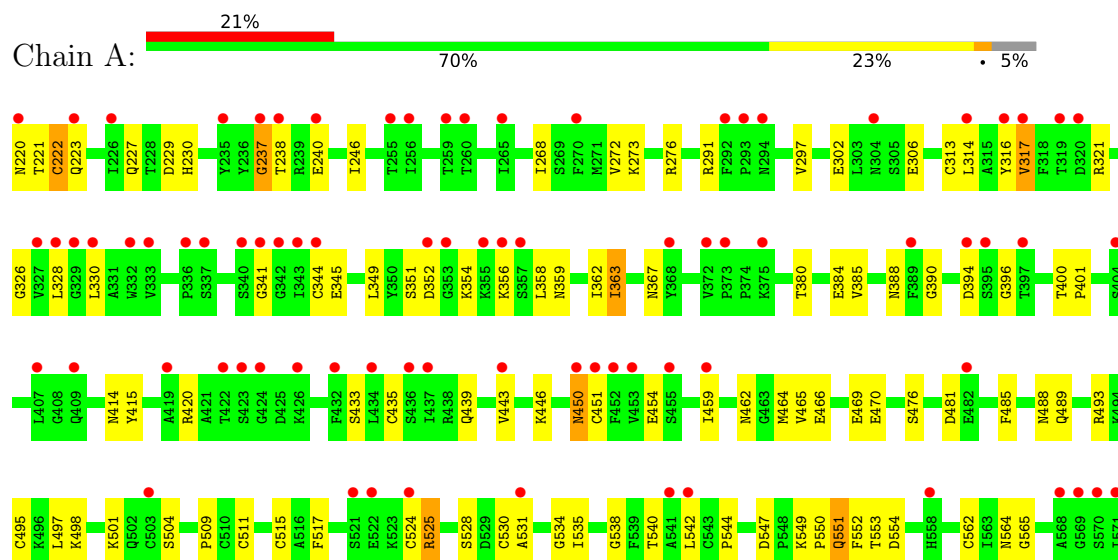
• Molecule 1: 11G2 Fab Light Chain

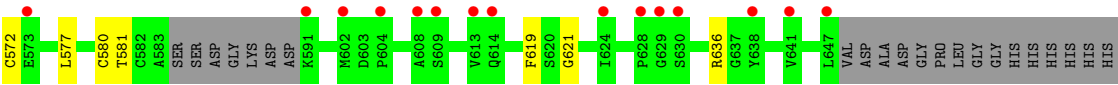


• Molecule 2: 11G2 Fab Heavy Chain



• Molecule 3: Disintegrin and metalloproteinase domain-containing protein 10





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



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.23Å 97.58Å 262.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.10 48.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.79-3.10) 84.0 (48.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.261 , 0.317 0.262 , 0.314	Depositor DCC
R_{free} test set	1895 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6631	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZN, NAG, CA, SO4

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	L	0.28	0/1682	0.37	0/2282
2	H	0.08	0/1684	0.28	0/2305
3	A	0.14	0/3307	0.46	6/4454 (0.1%)
All	All	0.18	0/6673	0.40	6/9041 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	237	GLY	N-CA-C	11.15	131.23	114.61
3	A	547	ASP	CA-C-N	6.00	125.91	119.85
3	A	547	ASP	C-N-CA	6.00	125.91	119.85
3	A	349	LEU	N-CA-C	5.24	116.80	111.14
3	A	237	GLY	CA-C-N	5.12	130.55	121.80
3	A	237	GLY	C-N-CA	5.12	130.55	121.80

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	L	1645	0	1575	37	0
2	H	1643	0	1612	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3242	0	3060	82	0
4	B	49	0	43	3	0
5	C	39	0	34	0	0
6	L	10	0	0	1	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6631	0	6324	137	1

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 11.

All (137) 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)
3:A:344:CYS:CB	3:A:451:CYS:SG	2.32	1.17
3:A:344:CYS:SG	3:A:451:CYS:SG	1.35	1.17
1:L:28:GLN:HG2	1:L:45:CYS:SG	1.91	1.11
3:A:549:LYS:HB3	3:A:550:PRO:CD	1.84	1.06
3:A:551:GLN:OE1	3:A:564:ASN:ND2	2.01	0.94
3:A:549:LYS:HB3	3:A:550:PRO:HD3	1.50	0.93
3:A:549:LYS:CB	3:A:550:PRO:CD	2.54	0.85
3:A:341:GLY:H	3:A:345:GLU:HG3	1.39	0.85
1:L:33:MET:HE1	1:L:41:VAL:HB	1.56	0.84
3:A:306:GLU:OE2	3:A:354:LYS:HD3	1.81	0.81
3:A:237:GLY:O	3:A:238:THR:HG23	1.81	0.80
1:L:193:ASP:OD2	1:L:195:THR:OG1	1.99	0.80
3:A:549:LYS:HB3	3:A:550:PRO:HD2	1.65	0.77
1:L:25:VAL:HG22	1:L:48:SER:HB3	1.69	0.73
1:L:53:SER:O	1:L:74:THR:HG23	1.88	0.73
2:H:219:ASN:ND2	2:H:230:ASP:OD2	2.20	0.72
3:A:344:CYS:SG	3:A:451:CYS:CB	2.75	0.72
1:L:33:MET:CE	1:L:41:VAL:HB	2.21	0.71
3:A:540:THR:HG23	3:A:542:LEU:H	1.56	0.70
3:A:344:CYS:CA	3:A:451:CYS:SG	2.80	0.69
3:A:485:PHE:HB3	3:A:489:GLN:HG3	1.73	0.69
2:H:37:LEU:HB2	2:H:104:LEU:HD11	1.74	0.69
3:A:435:CYS:O	3:A:439:GLN:NE2	2.27	0.68
3:A:552:PHE:N	3:A:562:CYS:O	2.28	0.67
2:H:141:PRO:HA	2:H:222:HIS:HD2	1.60	0.66
2:H:73:ASP:OD2	3:A:498:LYS:NZ	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:GLN:CG	1:L:45:CYS:SG	2.78	0.65
3:A:328:LEU:HD21	3:A:367:ASN:HB2	1.80	0.63
3:A:390:GLY:HA3	3:A:443:VAL:HG21	1.81	0.63
2:H:78:TYR:HB2	2:H:83:LYS:HG2	1.81	0.62
2:H:73:ASP:OD1	2:H:75:THR:OG1	2.17	0.62
2:H:174:THR:HB	2:H:221:ALA:HB3	1.81	0.61
1:L:113:GLN:HE21	1:L:116:ARG:H	1.47	0.61
3:A:240:GLU:OE2	3:A:509:PRO:HB3	2.00	0.60
1:L:115:ARG:NH1	3:A:470:GLU:OE2	2.34	0.60
3:A:525:ARG:HB3	3:A:534:GLY:H	1.66	0.59
3:A:549:LYS:CB	3:A:550:PRO:HD2	2.28	0.59
3:A:580:CYS:SG	3:A:581:THR:N	2.76	0.58
3:A:344:CYS:HA	3:A:451:CYS:SG	2.43	0.58
1:L:116:ARG:NH1	6:L:301:SO4:O4	2.37	0.57
3:A:420:ARG:NH1	3:A:636:ARG:HG2	2.19	0.57
2:H:25:GLU:N	2:H:25:GLU:OE2	2.37	0.57
2:H:65:GLU:OE2	4:B:1:NAG:H4	2.05	0.56
3:A:237:GLY:O	3:A:238:THR:CG2	2.51	0.56
3:A:345:GLU:O	3:A:359:ASN:ND2	2.38	0.56
3:A:223:GLN:N	3:A:313:CYS:SG	2.79	0.56
1:L:114:TYR:HB3	3:A:493:ARG:HH12	1.70	0.56
1:L:114:TYR:HB3	3:A:493:ARG:NH1	2.20	0.56
3:A:227:GLN:HG2	3:A:276:ARG:HB3	1.87	0.56
3:A:351:SER:O	3:A:352:ASP:HB3	2.07	0.56
3:A:420:ARG:HH11	3:A:636:ARG:HG2	1.71	0.55
3:A:222:CYS:C	3:A:313:CYS:SG	2.89	0.55
3:A:481:ASP:OD2	3:A:504:SER:OG	2.25	0.55
3:A:229:ASP:OD2	3:A:321:ARG:NH2	2.41	0.54
2:H:216:VAL:HG12	2:H:233:ILE:HD13	1.90	0.53
3:A:509:PRO:HG2	3:A:524:CYS:SG	2.48	0.53
3:A:302:GLU:HG3	3:A:356:LYS:NZ	2.25	0.52
1:L:172:LYS:HB2	1:L:216:THR:HB	1.92	0.52
3:A:450:ASN:HD22	3:A:450:ASN:N	2.08	0.52
3:A:476:SER:N	3:A:488:ASN:OD1	2.43	0.51
3:A:314:LEU:HD23	3:A:359:ASN:HB2	1.92	0.51
3:A:553:THR:CG2	3:A:554:ASP:N	2.73	0.51
1:L:113:GLN:NE2	1:L:116:ARG:H	2.09	0.51
1:L:89:GLY:HA3	1:L:94:TYR:HA	1.93	0.51
3:A:385:VAL:HA	3:A:388:ASN:HD22	1.76	0.50
3:A:363:ILE:HD11	3:A:380:THR:HG22	1.92	0.50
3:A:415:TYR:CG	3:A:433:SER:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:THR:HG23	2:H:214:GLU:HG3	1.94	0.49
3:A:553:THR:HG22	3:A:554:ASP:N	2.26	0.49
2:H:124:ASP:OD1	2:H:124:ASP:N	2.41	0.49
3:A:462:ASN:ND2	3:A:466:GLU:OE2	2.28	0.49
3:A:469:GLU:HB2	3:A:495:CYS:HB3	1.95	0.49
1:L:177:GLU:H	1:L:177:GLU:CD	2.19	0.49
3:A:454:GLU:CD	3:A:454:GLU:H	2.20	0.49
1:L:53:SER:O	1:L:74:THR:CG2	2.61	0.48
1:L:174:ASP:HA	1:L:214:SER:HG	1.78	0.48
4:B:1:NAG:H62	4:B:2:NAG:N2	2.29	0.48
3:A:572:CYS:HB3	3:A:577:LEU:HB2	1.94	0.48
2:H:43:VAL:HG21	2:H:48:LEU:HD21	1.94	0.47
3:A:351:SER:O	3:A:352:ASP:CB	2.62	0.47
1:L:71:ILE:HD12	1:L:77:LEU:HD23	1.96	0.47
3:A:535:ILE:O	3:A:544:PRO:HG3	2.15	0.47
3:A:221:THR:OG1	3:A:454:GLU:O	2.25	0.47
3:A:230:HIS:CE1	3:A:291:ARG:HA	2.50	0.47
3:A:220:ASN:HA	3:A:268:ILE:HA	1.97	0.47
2:H:210:THR:O	2:H:214:GLU:N	2.40	0.47
1:L:218:GLU:HG3	1:L:229:VAL:HG22	1.97	0.46
1:L:59:TYR:HE1	1:L:112:HIS:HB3	1.79	0.46
1:L:114:TYR:CD1	1:L:119:LEU:HD12	2.51	0.46
3:A:297:VAL:HG22	3:A:330:LEU:HD22	1.98	0.46
2:H:55:TRP:CG	2:H:99:LEU:HD13	2.50	0.46
1:L:26:LEU:HG	1:L:47:VAL:HG12	1.98	0.46
1:L:119:LEU:HD22	2:H:66:TRP:CD1	2.51	0.46
2:H:142:PRO:HD3	2:H:222:HIS:CD2	2.51	0.46
3:A:317:VAL:HG13	3:A:362:ILE:HG22	1.98	0.46
2:H:75:THR:OG1	3:A:498:LYS:NZ	2.48	0.45
1:L:71:ILE:HG13	1:L:96:LEU:HD13	1.98	0.45
1:L:71:ILE:CD1	1:L:77:LEU:CD2	2.95	0.45
3:A:272:VAL:HG13	3:A:462:ASN:HD22	1.81	0.45
3:A:619:PHE:C	3:A:621:GLY:H	2.26	0.44
1:L:115:ARG:HH12	3:A:470:GLU:CD	2.26	0.44
2:H:121:GLY:HA3	3:A:493:ARG:HH11	1.83	0.44
3:A:273:LYS:HA	3:A:459:ILE:HD11	1.99	0.44
3:A:384:GLU:O	3:A:388:ASN:ND2	2.51	0.44
1:L:71:ILE:CD1	1:L:77:LEU:HD23	2.48	0.44
3:A:246:ILE:HG13	3:A:464:MET:HE2	1.99	0.43
3:A:517:PHE:HB3	3:A:538:GLY:HA2	2.00	0.43
4:B:3:MAN:H62	4:B:4:MAN:H2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:138:LYS:HA	2:H:138:LYS:HD2	1.84	0.43
2:H:161:LEU:O	2:H:204:VAL:N	2.40	0.43
1:L:71:ILE:HD12	1:L:77:LEU:CD2	2.48	0.43
2:H:142:PRO:HB3	2:H:168:TYR:HB3	2.00	0.43
3:A:341:GLY:HA2	3:A:358:LEU:HB3	2.00	0.43
1:L:88:SER:O	1:L:95:SER:N	2.44	0.43
3:A:401:PRO:HD2	3:A:414:ASN:HA	2.01	0.43
3:A:530:CYS:O	3:A:565:GLY:HA2	2.19	0.43
1:L:26:LEU:HD23	1:L:111:CYS:SG	2.59	0.43
2:H:177:TRP:CZ3	2:H:218:CYS:HB3	2.54	0.43
3:A:230:HIS:HE1	3:A:291:ARG:HA	1.84	0.42
1:L:51:VAL:HA	1:L:116:ARG:HH22	1.85	0.42
3:A:316:TYR:OH	3:A:388:ASN:ND2	2.53	0.42
1:L:143:PRO:HD3	1:L:155:VAL:HG22	2.01	0.42
3:A:394:ASP:OD2	3:A:415:TYR:HB2	2.20	0.42
1:L:57:HIS:CD2	1:L:73:SER:H	2.38	0.42
3:A:237:GLY:C	3:A:238:THR:HG23	2.42	0.42
3:A:501:LYS:HB3	3:A:515:CYS:HB3	2.01	0.42
3:A:396:GLY:O	3:A:400:THR:OG1	2.22	0.41
1:L:119:LEU:HB3	2:H:66:TRP:CD2	2.55	0.41
3:A:528:SER:HB3	3:A:531:ALA:HB3	2.02	0.41
3:A:446:LYS:HE2	3:A:446:LYS:HA	2.02	0.41
3:A:326:GLY:HA2	3:A:367:ASN:OD1	2.21	0.41
2:H:161:LEU:HD11	2:H:211:TRP:CG	2.55	0.41
3:A:420:ARG:HD3	3:A:636:ARG:HA	2.03	0.40
1:L:237:CYS:HA	2:H:238:CYS:HB3	2.03	0.40
1:L:56:LEU:HD22	1:L:94:TYR:CG	2.56	0.40
3:A:497:LEU:HD12	3:A:497:LEU:HA	1.96	0.40
2:H:75:THR:CB	3:A:498:LYS:HZ2	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:SER:OG	2:H:196:ASP:OD2[4_565]	2.19	0.01

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	L	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
2	H	217/226 (96%)	208 (96%)	9 (4%)	0	100	100
3	A	417/443 (94%)	393 (94%)	24 (6%)	0	100	100
All	All	847/884 (96%)	805 (95%)	42 (5%)	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	L	188/188 (100%)	183 (97%)	5 (3%)	39	67
2	H	190/196 (97%)	188 (99%)	2 (1%)	65	78
3	A	366/383 (96%)	358 (98%)	8 (2%)	45	71
All	All	744/767 (97%)	729 (98%)	15 (2%)	48	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	32	ILE
1	L	56	LEU
1	L	81	VAL
1	L	177	GLU
1	L	237	CYS

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Mol	Chain	Res	Type
2	H	25	GLU
2	H	173	VAL
3	A	222	CYS
3	A	317	VAL
3	A	363	ILE
3	A	450	ASN
3	A	465	VAL
3	A	511	CYS
3	A	525	ARG
3	A	551	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	76	ASN
1	L	112	HIS
1	L	113	GLN
1	L	161	ASN
1	L	168	ASN
1	L	180	ASN
1	L	212	HIS
2	H	20	GLN
2	H	35	GLN
2	H	102	ASN
2	H	128	GLN
2	H	222	HIS
3	A	220	ASN
3	A	227	GLN
3	A	245	GLN
3	A	359	ASN
3	A	378	HIS
3	A	388	ASN
3	A	406	ASN
3	A	409	GLN
3	A	439	GLN
3	A	450	ASN
3	A	467	GLN
3	A	558	HIS
3	A	564	ASN
3	A	614	GLN
3	A	627	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 ⓘ

7 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$
4	NAG	B	1	2,4	13,13,15	0.64	0	16,17,21	1.56	1 (6%)
4	NAG	B	2	4	14,14,15	0.27	0	17,19,21	0.79	1 (5%)
4	MAN	B	3	4	11,11,12	1.17	1 (9%)	15,15,17	1.80	2 (13%)
4	MAN	B	4	4	11,11,12	0.70	1 (9%)	15,15,17	1.16	2 (13%)
5	NAG	C	1	5,3	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	C	2	5	14,14,15	0.31	0	17,19,21	0.64	0
5	MAN	C	3	5	11,11,12	0.68	0	15,15,17	0.93	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	2,4	-	2/5/22/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	MAN	B	3	4	-	1/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
5	NAG	C	1	5,3	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	C	3	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3	MAN	C1-C2	2.73	1.58	1.52
4	B	4	MAN	C1-C2	2.09	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	MAN	C1-O5-C5	6.03	120.27	112.19
4	B	1	NAG	C7-N2-C2	5.73	123.16	114.43
4	B	4	MAN	C1-O5-C5	3.42	116.77	112.19
4	B	2	NAG	C1-O5-C5	2.44	115.46	112.19
5	C	3	MAN	O2-C2-C3	-2.25	105.49	110.15
4	B	3	MAN	O2-C2-C3	-2.18	105.64	110.15
4	B	4	MAN	O2-C2-C3	-2.07	105.87	110.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

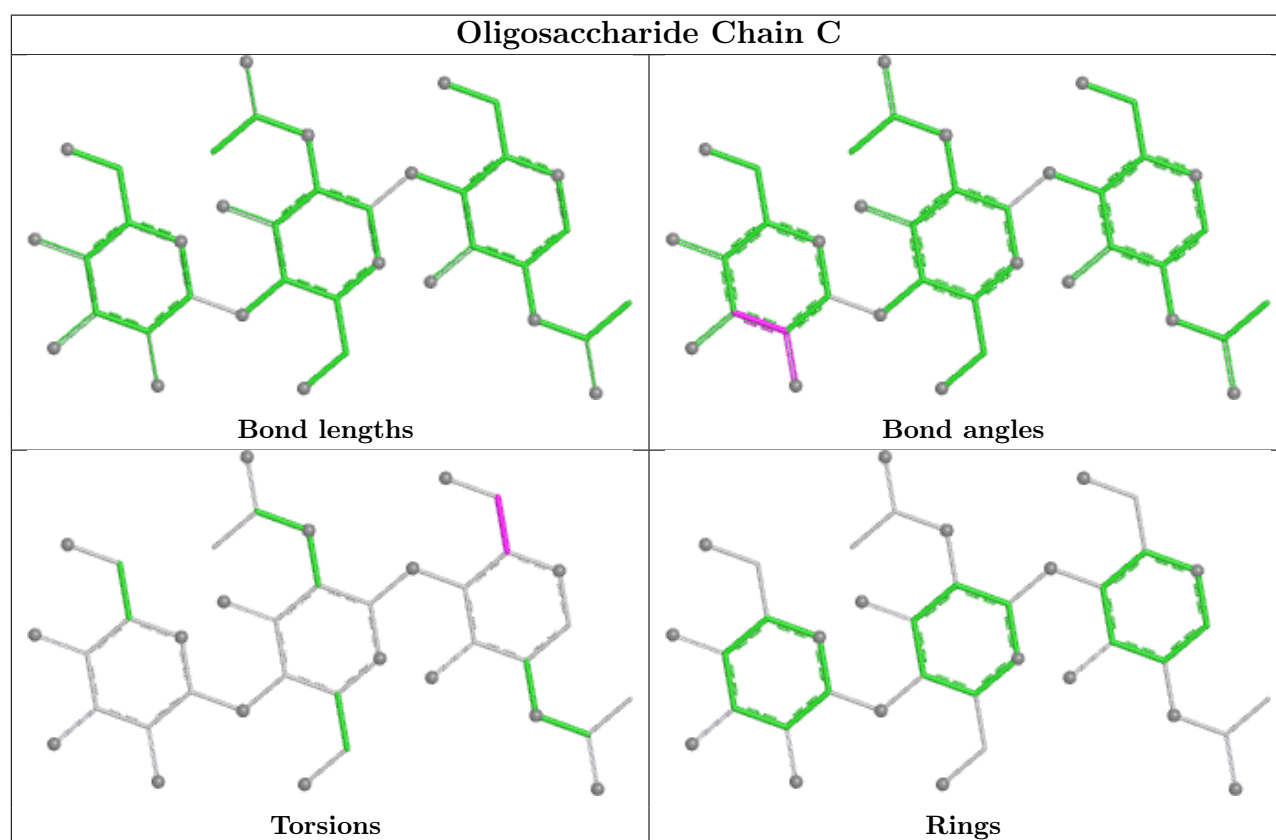
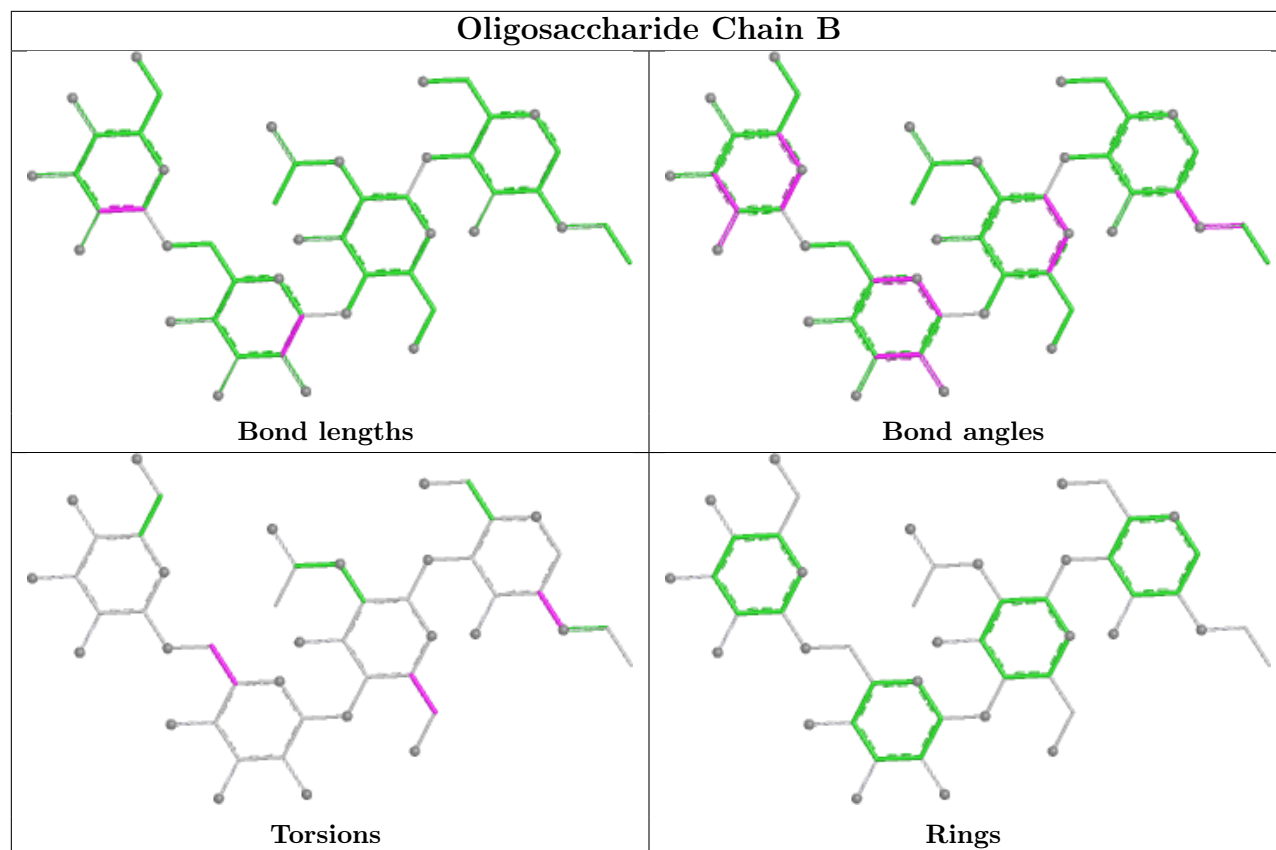
Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C1-C2-N2-C7
4	B	3	MAN	C4-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	MAN	1	0
4	B	2	NAG	1	0
4	B	3	MAN	1	0
4	B	1	NAG	2	0

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



5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	L	302	-	4,4,4	0.24	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	301	SO4	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	L	215/215 (100%)	0.32	2 (0%) 81 63	22, 43, 83, 123	0
2	H	219/226 (96%)	0.34	4 (1%) 67 47	17, 38, 70, 124	0
3	A	421/443 (95%)	1.50	95 (22%) 2 1	33, 111, 159, 201	0
All	All	855/884 (96%)	0.91	101 (11%) 9 5	17, 67, 147, 201	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	259	THR	4.0
3	A	332	TRP	4.0
3	A	521	SER	3.9
3	A	451	CYS	3.9
3	A	260	THR	3.8
3	A	352	ASP	3.8
3	A	356	LYS	3.7
3	A	614	GLN	3.7
3	A	340	SER	3.6
3	A	608	ALA	3.6
3	A	357	SER	3.5
3	A	423	SER	3.5
3	A	569	GLY	3.5
3	A	292	PHE	3.5
3	A	256	ILE	3.5
3	A	304	ASN	3.4
3	A	342	GLY	3.3
3	A	541	ALA	3.2
3	A	328	LEU	3.1
3	A	437	ILE	3.1
3	A	407	LEU	3.1
3	A	255	THR	3.0
3	A	452	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	A	422	THR	3.0
3	A	336	PRO	3.0
3	A	265	ILE	2.9
3	A	409	GLN	2.8
3	A	424	GLY	2.8
3	A	432	PHE	2.8
3	A	330	LEU	2.8
3	A	372	VAL	2.8
3	A	397	THR	2.8
3	A	419	ALA	2.8
3	A	426	LYS	2.8
3	A	226	ILE	2.7
3	A	629	GLY	2.7
3	A	453	VAL	2.7
3	A	343	ILE	2.7
3	A	482	GLU	2.6
3	A	344	CYS	2.6
3	A	317	VAL	2.6
3	A	647	LEU	2.6
2	H	150	GLY	2.6
3	A	404	SER	2.6
3	A	237	GLY	2.6
3	A	455	SER	2.6
3	A	558	HIS	2.6
3	A	320	ASP	2.6
3	A	353	GLY	2.6
3	A	337	SER	2.6
3	A	235	TYR	2.5
3	A	443	VAL	2.5
3	A	613	VAL	2.5
3	A	293	PRO	2.5
3	A	375	LYS	2.5
3	A	373	PRO	2.4
2	H	215	THR	2.4
3	A	223	GLN	2.4
3	A	542	LEU	2.4
3	A	395	SER	2.4
3	A	568	ALA	2.4
3	A	327	VAL	2.4
3	A	319	THR	2.3
3	A	503	CYS	2.3
3	A	450	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	240	GLU	2.3
3	A	434	LEU	2.3
3	A	571	ILE	2.3
3	A	630	SER	2.3
3	A	316	TYR	2.3
3	A	641	VAL	2.3
3	A	624	ILE	2.2
3	A	531	ALA	2.2
3	A	220	ASN	2.2
3	A	573	GLU	2.2
3	A	355	LYS	2.2
3	A	368	TYR	2.2
3	A	609	SER	2.2
2	H	154	GLN	2.2
2	H	238	CYS	2.2
3	A	638	TYR	2.2
3	A	570	SER	2.2
3	A	591	LYS	2.2
3	A	314	LEU	2.1
3	A	524	CYS	2.1
3	A	436	SER	2.1
3	A	238	THR	2.1
3	A	628	PRO	2.1
3	A	389	PHE	2.1
3	A	341	GLY	2.1
3	A	604	PRO	2.1
1	L	90	SER	2.1
3	A	270	PHE	2.1
3	A	459	ILE	2.0
3	A	602	MET	2.0
3	A	394	ASP	2.0
3	A	329	GLY	2.0
3	A	522	GLU	2.0
3	A	333	VAL	2.0
3	A	294	ASN	2.0
1	L	55	TYR	2.0

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

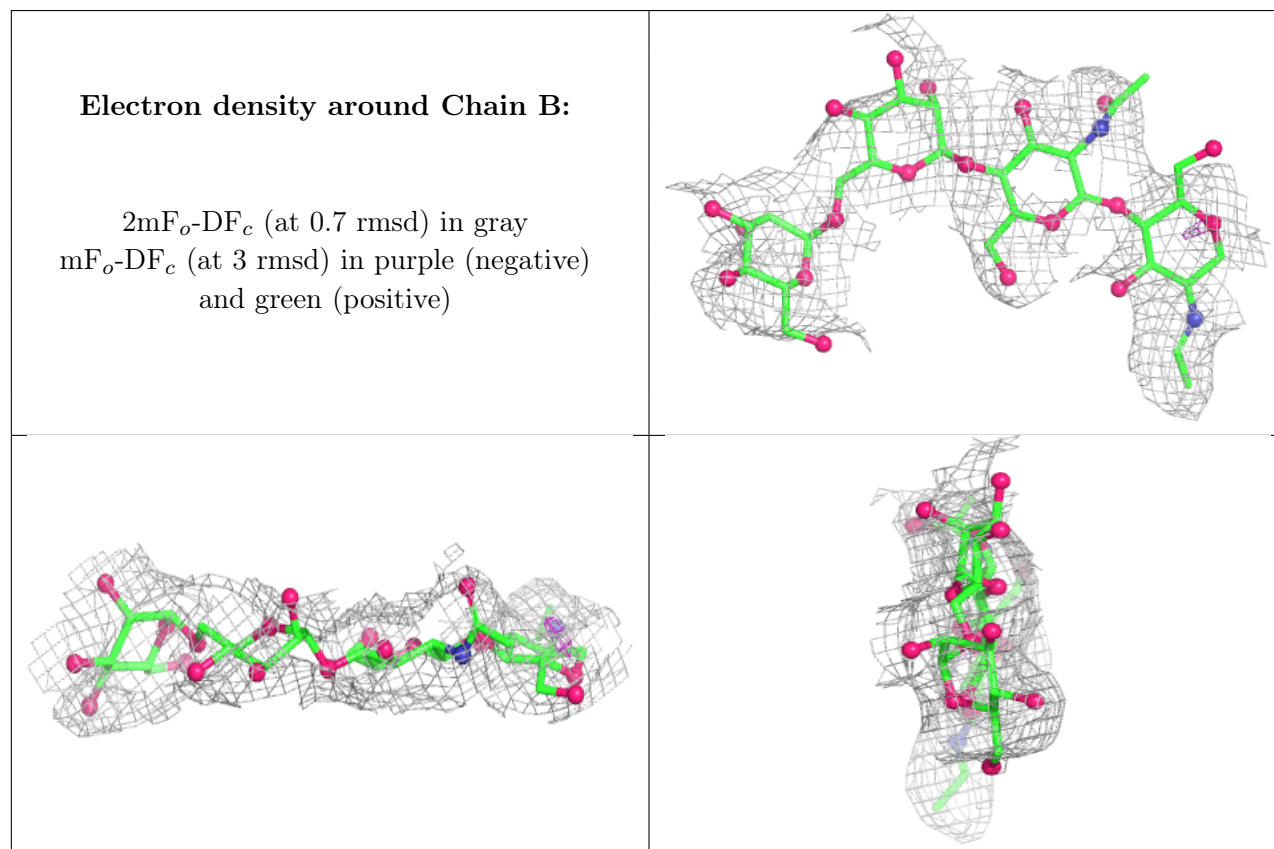
There are no non-standard protein/DNA/RNA residues in this entry.

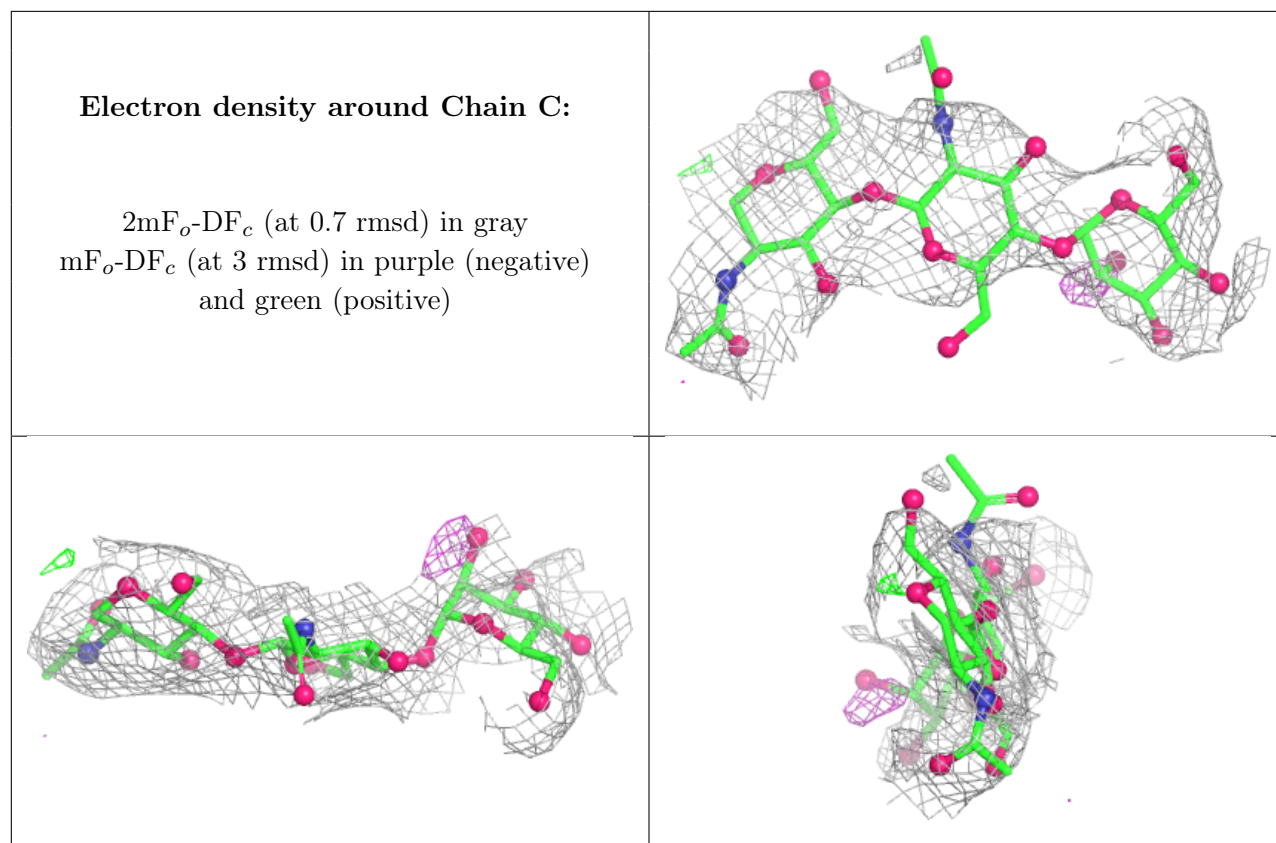
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1	13/15	-	-	21,34,52,61	0
4	NAG	B	2	14/15	-	-	38,62,76,97	0
4	MAN	B	3	11/12	-	-	76,100,112,118	0
4	MAN	B	4	11/12	-	-	82,89,102,111	0
5	NAG	C	1	14/15	-	-	72,81,105,110	0
5	NAG	C	2	14/15	-	-	84,95,106,115	0
5	MAN	C	3	11/12	-	-	64,106,125,131	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ZN	A	702	1/1	0.05	0.24	749,749,749,749	0
6	SO4	L	302	5/5	0.86	0.15	67,67,76,89	0
6	SO4	L	301	5/5	0.86	0.14	37,55,73,89	0
7	CA	A	701	1/1	0.92	0.07	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.