



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:27 PM UTC

PDB ID : 3KLS / pdb_00003kls
Title : Structure of complement C5 in complex with SSL7
Authors : Laursen, N.S.; Gordon, N.; Hermans, S.; Lorenz, N.; Jackson, N.; Wines, B.;
Spillner, E.; Christensen, J.B.; Jensen, M.; Fredslund, F.; Bjerre, M.; Sottrup-
Jensen, L.; Fraser, J.D.; Andersen, G.R.
Deposited on : 2009-11-09
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

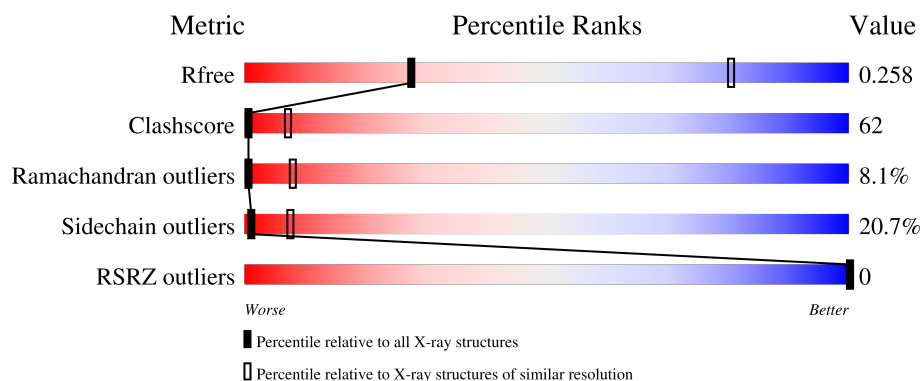
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

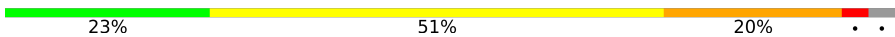
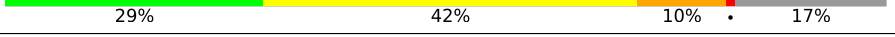
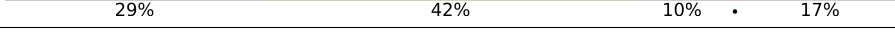
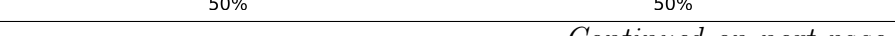
The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	1676	
1	B	1676	
2	X	231	
2	Y	231	
3	C	2	

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

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27683 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1622	Total	C	N	O	S	0	0	0
			12836	8224	2107	2452	53			
1	B	1478	Total	C	N	O	S	0	0	0
			11676	7478	1926	2226	46			

- Molecule 2 is a protein called Exotoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
2	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	35	GLY	GLU	engineered mutation	UNP Q6GJP2
Y	35	GLY	GLU	engineered mutation	UNP Q6GJP2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

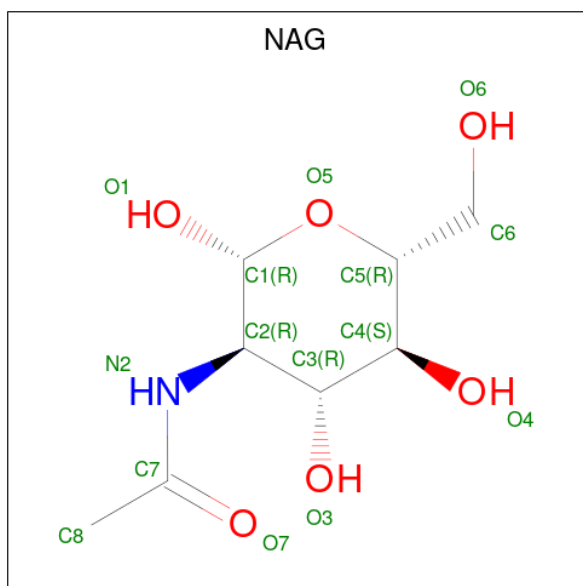


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cd	0	0
			5	5		
4	B	4	Total	Cd	0	0
			4	4		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

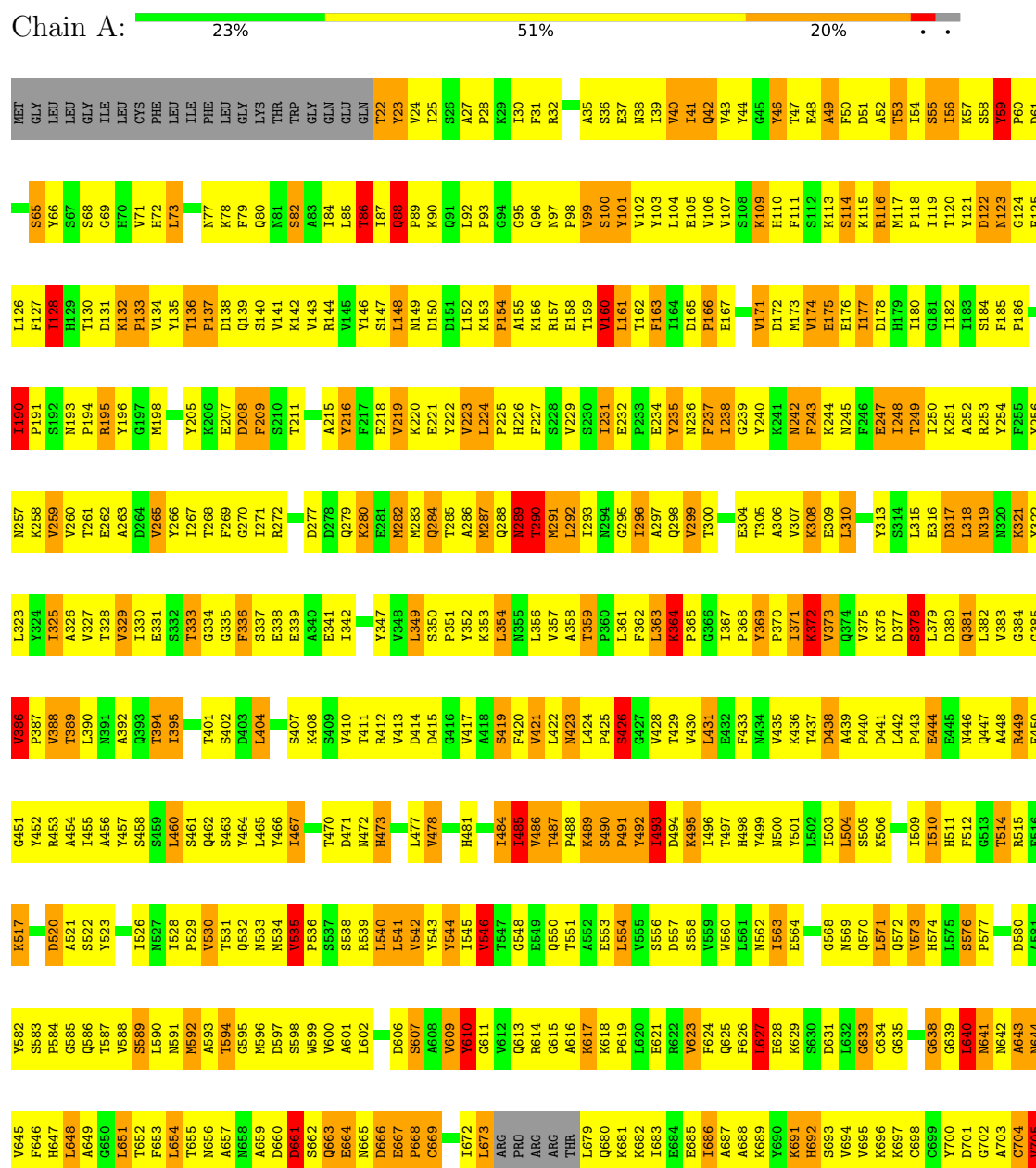


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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: Complement C5





L1673
N1674
G1675
C1676

● Molecule 1: Complement C5

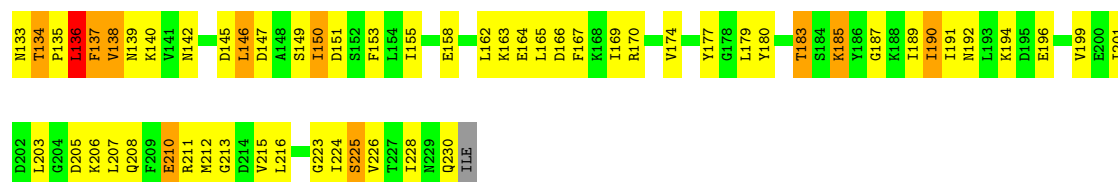
Chain B: 

W833	R834	R835	G836	E837	Q838	I839	Q840	L841	G842	H843	T844	V845	Y846	N847	Y848	M853	Q854	F855	C856	V857	K858	M859	S860	A861	E862	E863	T867	S868	E869	S870	PRO	VAL	ILE	ASP	HIS	G810	G811	GLY	THR	LYS	SER	THR	K882	R884	R885	Q886	K887	D888	E889	S892	S893	H894	N828	L895	V896	T897	R898				
Y768	F769	P770	W773	L774	W775	E776	L777	H778	L779	W780	R781	R782	R783	R784	W785	L786	W787	F788	A789	L790	P791	S792	S793	L794	T795	T796	W797	E798	I799	Q800	S801	I802	VAL	ILE	ASP	HIS	G810	G811	GLY	THR	LYS	SER	THR	K882	R884	R885	Q886	K887	D888	E889	S892	S893	H894	N828	L895	V896	T897	R898			
G702	A703	C704	V705	N706	T707	D708	E709	T710	T711	E712	Q713	R714	A715	T716	R717	I718	S719	L720	G721	P722	Q723	C724	F728	T729	V733	A734	V735	V736	V737	L738	R739	G803	I804	ASP	THR	HIS	G810	G811	GLY	THR	LYS	SER	THR	K882	R884	R885	Q886	K887	D888	E889	S892	S893	H894	N828	L895	V896	T897	R898			
N641	N642	A643	N644	V645	F646	H647	L648	A649	G650	L651	T652	F653	L654	T655	N656	A657	N658	A659	D660	S661	Q662	Q663	E664	N665	D666	E667	P668	C669	L672	L673	ARG	PRO	ARG	ARG	THR	L679	Q680	K681	L682	K683	E684	E685	I686	A687	A688	K689	Y690	K691	H692	S693	V694	V695	L696	K697	C698	C699	Y700	D701			
G513	T514	R515	E516	K517	D520	A521	S522	Y523	I526	N527	L528	P529	V530	T531	Q532	N533	H534	V535	P536	S537	S538	L540	L541	V542	Y543	Y544	I545	V546	T547	G548	F549	Q550	T551	L552	E553	L554	V555	S556	D557	S558	V559	N560	L561	N562	I563	E564	N569	Q570	L571	Q572	V573	H574	L575	G576	P577						
Q447	A448	R449	E450	G451	Y452	R453	A454	L455	A456	Y457	S458	S459	L460	Q461	Q462	S463	Y464	L465	Y466	I467	T470	D471	N472	H473	L477	V478	H481	A482	T483	I484	V485	F486	T487	N488	L489	S490	P491	Y492	L493	D494	K495	L496	T497	H498	Y499	N500	Y501	L502	L503	Q504	S505	Q506	L509	S510	H511	F512					
V383	G384	G385	V386	P387	V388	T389	L390	N391	Q392	Q393	T394	I395	T401	S402	D403	L404	D405	P406	S407	K408	E341	I342	Y347	V348	L349	S350	P351	Y352	K353	L354	N355	L356	V357	A358	T359	P360	L361	F362	L363	K364	P365	G366	L367	P368	Y369	N370	K371	P372	V373	Q374	L375	L379	D380	Q381	L382						
N320	K321	Y322	L323	V324	K325	A326	V327	T328	A329	K330	S331	S332	T333	G334	G335	F336	S337	E338	E339	A340	E341	I342	Y347	V348	L349	S350	P351	Y352	K353	L354	N355	L356	V357	A358	T359	P360	L361	F362	L363	K364	P365	G366	L367	P368	Y369	N370	K371	P372	V373	Q374	L375	L379	D380	Q381	L382						
P255	T256	N257	K258	V259	V260	T261	E262	A263	D264	V265	Y266	T267	T268	F269	K270	L271	K272	E273	D274	D277	D278	K279	E281	N282	K283	Q284	T285	A286	H287	Q288	N289	T290	K291	L292	T293	N294	G295	T296	A297	Q298	V299	E304	T305	A306	V307	K308	E309	L310	Y313	S314	G315	E316	D317	L318	N319						
L126	F127	I128	H129	T130	D131	K132	G133	V134	H135	T136	P137	D138	Q139	S140	Q141	K142	V143	A144	V145	Y146	S147	L148	N149	D150	D151	L152	K153	P154	A155	K156	R157	E158	T159	L161	T162	F163	I164	D165	P166	E167	V171	D172	M173	V174	E175	E176	I177	D178	H179	I180	G181	T182	I183	S184	P185	P186					
D61	S65	Y66	S67	S68	S69	H70	V71	H72	L73	N77	K78	F79	Q80	K81	S82	A83	L84	L85	S86	L87	F88	P89	K90	G91	P93	Q96	N97	P98	V99	S100	Y101	Y102	Y103	L104	E105	V106	Y107	S108	K109	H110	F111	S112	K113	S114	K115	R116	M117	P118	I119	T120	S121	D122	N123	G124	F125						
MET	GLY	LEU	LEU	GLY	ILE	LEU	CYS	PHE	LEU	ILE	PHE	LEU	GLY	LYS	THR	TRP	GLY	GLN	GLU	GLN	T22	T23	T22	T23	T24	T25	S26	A27	P28	K29	I30	F31	R32	V33	G34	A35	S36	E37	I38	I39	V40	I41	Q42	V43	Y44	G45	Y46	T47	E48	A49	F50	D51	A52	T53	I54	S55	I56	K57	S58	G59	F60

- Molecule 2: Exotoxin 1

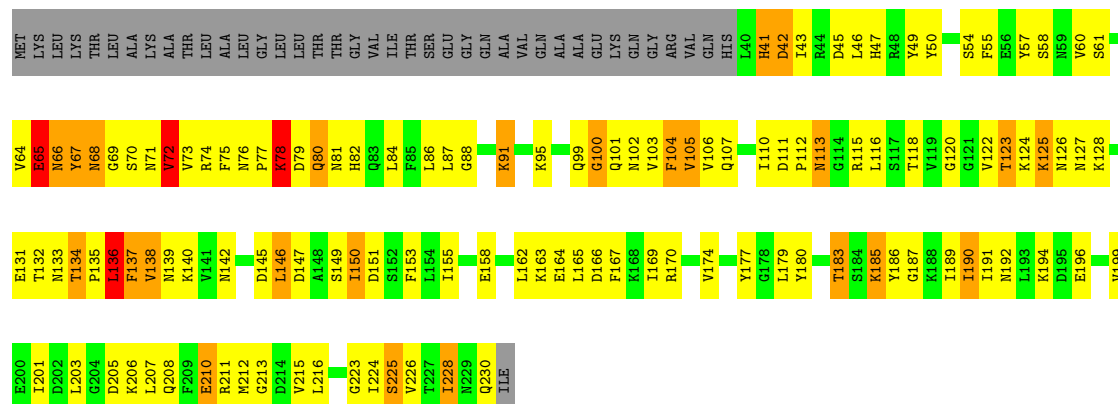
Chain X: 29% 42% 10% 17%

V64	E65	E66	Y67	N68	G69	S70	M71	V72	V73	R74	F75	M76	P77	K78	D79	Q80	N81	H82	Q83	L84	L86	L87	G88		K91		Q99	G100	Q101	M102	V103	F104	V105	V106	Q107		I110	D111	P112	M113	G114	R115	L116	S117	T118	V119	G120	G121	T123	K124	K125	M126	M127	K128		E131	V132			
MET	LYS	LEU	LYS	THR	LEU	ALA	LYS	THR	LEU	ALA	ALA	GLY	LEU	LEU	THR	THR	GLY	VAL	ILE	THR	SER	GLU	GLY	GLN	ALA	VAL	GLN	GLN	ALA	ALA	GLU	LYS	GLN	GLY	ARG	VAL	GLN	HIS	L40	H41	D42	L43	H44	D45	L46	H47	H48	Y49	Y50		S54	F55	E56	Y57	S58	N59	V60	S61		V62



• Molecule 2: Exotoxin 1

Chain Y: 29% 42% 10% 17%



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

Chain C: 50% 50%



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

Chain D: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	143.88Å 143.88Å 241.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.05 – 3.60 29.05 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.05-3.60) 99.6 (29.05-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.198 , 0.263 0.193 , 0.258	Depositor DCC
R_{free} test set	3224 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	111.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 158.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.410 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27683	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	5/13111 (0.0%)	1.20	97/17784 (0.5%)
1	B	0.77	6/11928 (0.1%)	1.21	78/16183 (0.5%)
2	X	0.46	0/1560	0.90	3/2096 (0.1%)
2	Y	0.46	1/1560 (0.1%)	0.91	4/2096 (0.2%)
All	All	0.73	12/28159 (0.0%)	1.17	182/38159 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1313	ILE	CA-CB	-6.39	1.47	1.54
1	A	238	ILE	CA-CB	-6.34	1.46	1.54
1	A	1313	ILE	CA-CB	-5.89	1.48	1.54
1	B	1218	VAL	CA-CB	-5.59	1.47	1.55
1	B	1056	ILE	CA-CB	5.36	1.61	1.54

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1003	LEU	CA-C-N	14.89	135.08	119.90
1	B	1003	LEU	C-N-CA	14.89	135.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	LEU	CA-C-N	14.87	135.07	119.90
1	A	1003	LEU	C-N-CA	14.87	135.07	119.90
1	A	1634	ARG	N-CA-C	14.19	122.37	108.75

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1179	THR	Peptide
1	A	1633	PHE	Peptide
1	A	1635	TYR	Peptide
1	A	651	LEU	Peptide
1	B	651	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12836	0	12796	1677	1
1	B	11676	0	11649	1490	1
2	X	1539	0	1530	160	0
2	Y	1539	0	1530	161	0
3	C	28	0	25	3	0
3	D	28	0	25	2	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
All	All	27683	0	27581	3439	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 62.

The worst 5 of 3439 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:1279:ARG:HG3	1:B:1284:PHE:CB	1.60	1.32
1:B:1488:LEU:HD12	1:B:1488:LEU:O	1.31	1.30
1:A:1279:ARG:HG3	1:A:1284:PHE:CB	1.60	1.29
1:A:1486:GLY:O	1:A:1487:PHE:CD2	1.86	1.27
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.04	1.15

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)
1:A:955:ARG:NH2	1:B:434:ASN:OD1[3_454]	2.19	0.01

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	1612/1676 (96%)	1199 (74%)	273 (17%)	140 (9%)	0	7
1	B	1468/1676 (88%)	1126 (77%)	224 (15%)	118 (8%)	1	8
2	X	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	1	13
2	Y	189/231 (82%)	150 (79%)	29 (15%)	10 (5%)	1	14
All	All	3458/3814 (91%)	2625 (76%)	554 (16%)	279 (8%)	1	8

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	TYR
1	A	59	TYR
1	A	97	ASN
1	A	209	PHE
1	A	243	PHE

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	1438/1484 (97%)	1130 (79%)	308 (21%)	1	7
1	B	1311/1484 (88%)	1017 (78%)	294 (22%)	1	6
2	X	175/205 (85%)	155 (89%)	20 (11%)	5	26
2	Y	175/205 (85%)	155 (89%)	20 (11%)	5	26
All	All	3099/3378 (92%)	2457 (79%)	642 (21%)	1	7

5 of 642 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	776	GLU
1	B	1303	LEU
1	B	859	MET
1	B	758	LEU
1	B	1027	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	80	GLN
1	B	572	GLN
2	Y	59	ASN
1	B	110	HIS
1	B	393	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

4 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$
3	NAG	C	1	3,1	14,14,15	0.57	0	17,19,21	1.44	2 (11%)
3	NAG	C	2	3	14,14,15	0.43	0	17,19,21	1.08	1 (5%)
3	NAG	D	1	3,1	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
3	NAG	D	2	3	14,14,15	0.39	0	17,19,21	1.01	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	3.79	117.27	112.19
3	C	1	NAG	C2-N2-C7	-3.60	118.08	122.90
3	C	2	NAG	C1-O5-C5	3.54	116.93	112.19
3	D	2	NAG	C1-O5-C5	3.39	116.73	112.19
3	D	1	NAG	C3-C4-C5	-2.64	105.44	110.23

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

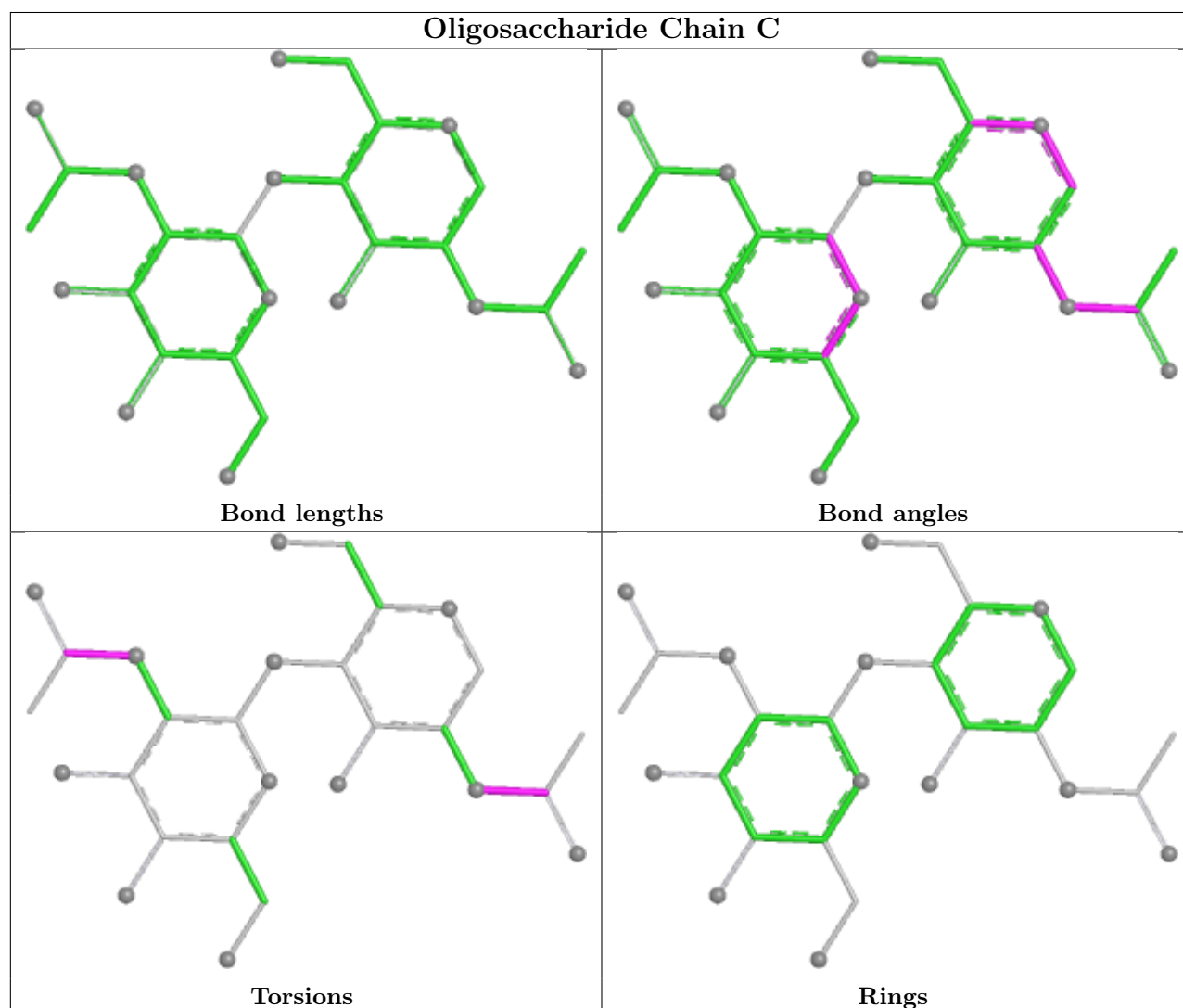
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2

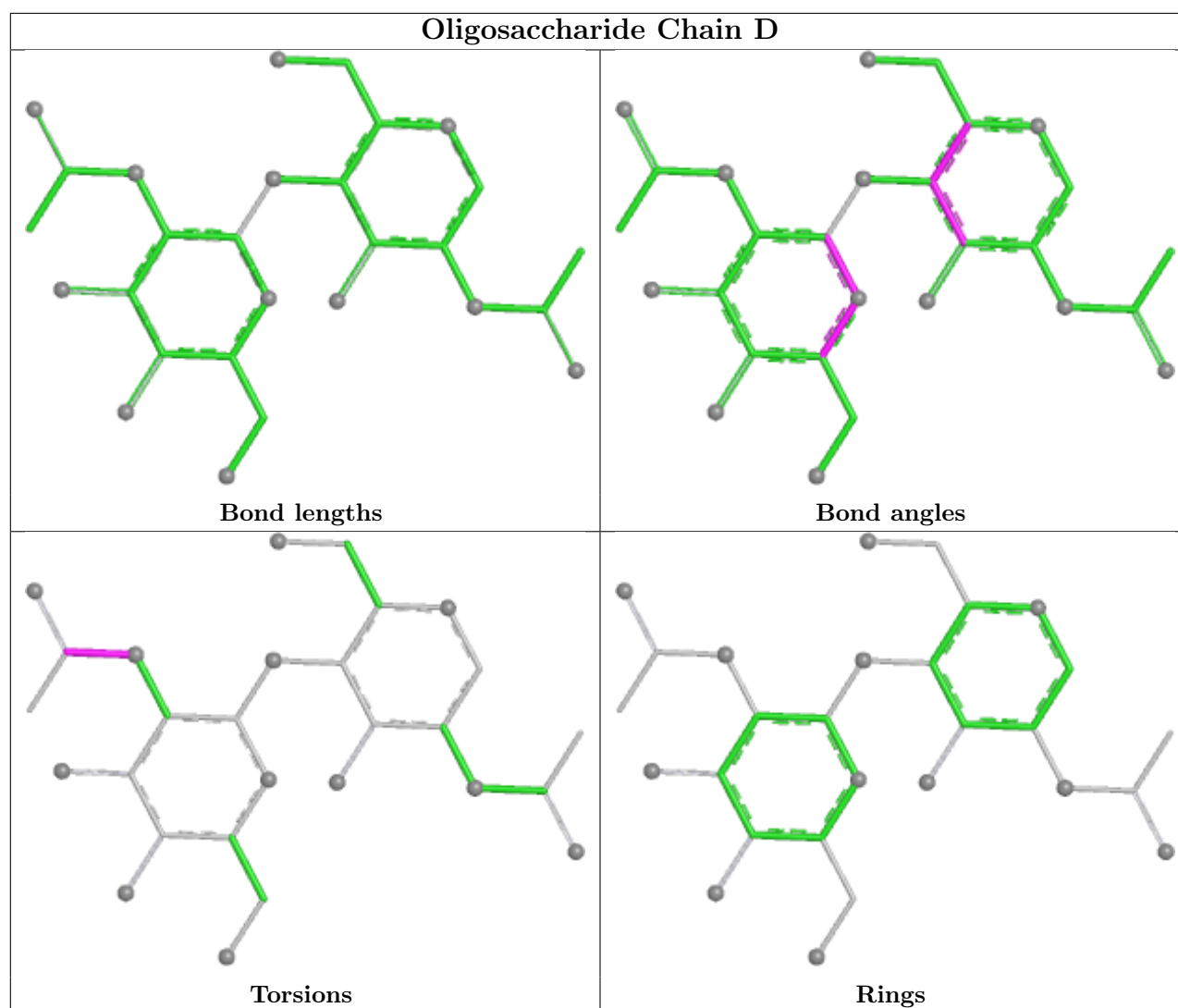
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	3	0
3	D	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 11 ligands modelled in this entry, 9 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	$\# Z > 2$
5	NAG	B	1681	1	14,14,15	0.75	0	17,19,21	1.16	1 (5%)
5	NAG	A	1682	1	14,14,15	0.69	0	17,19,21	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1681	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1682	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1681	NAG	C1-O5-C5	2.24	115.19	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1682	NAG	C8-C7-N2-C2
5	A	1682	NAG	O7-C7-N2-C2
5	B	1681	NAG	C8-C7-N2-C2
5	B	1681	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1622/1676 (96%)	-0.87	0 100 100	60, 136, 275, 372	0
1	B	1478/1676 (88%)	-0.90	0 100 100	61, 129, 232, 340	0
2	X	191/231 (82%)	-0.90	0 100 100	150, 242, 308, 342	0
2	Y	191/231 (82%)	-0.85	0 100 100	149, 242, 308, 342	0
All	All	3482/3814 (91%)	-0.89	0 100 100	60, 140, 279, 372	0

There are no RSRZ outliers to report.

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](#)

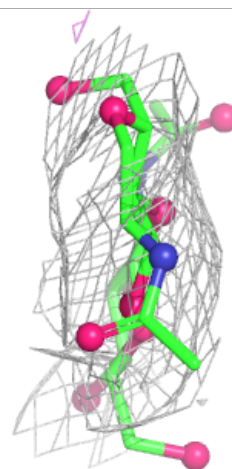
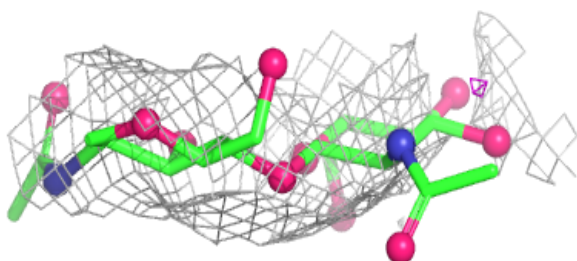
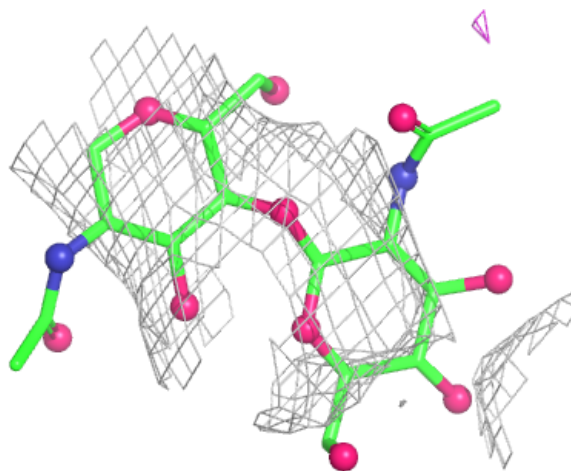
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

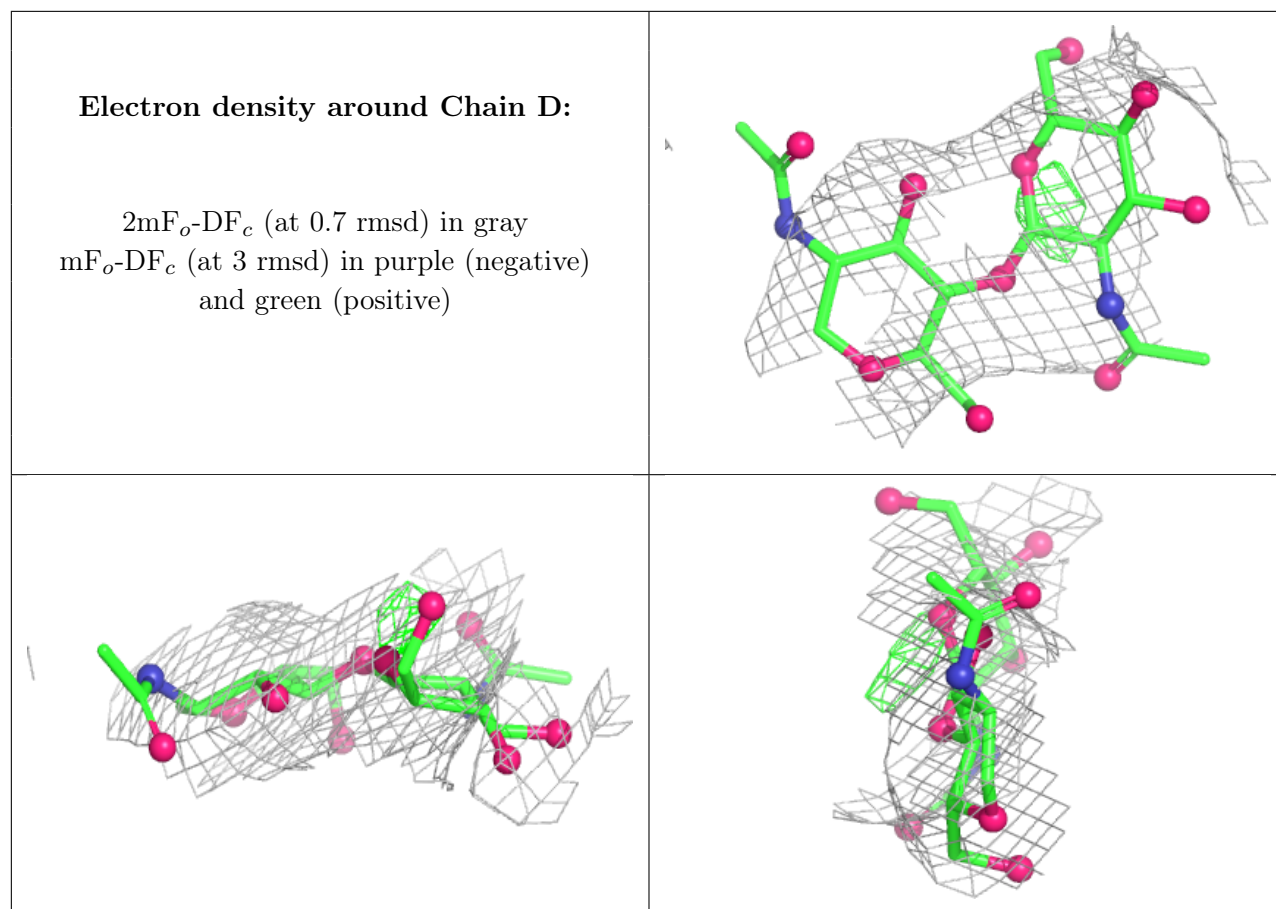
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	304,306,310,312	0
3	NAG	C	2	14/15	-	-	302,303,305,305	0
3	NAG	D	1	14/15	-	-	315,318,321,323	0
3	NAG	D	2	14/15	-	-	309,312,314,314	0

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($\text{\AA}^2$)	Q<0.9
5	NAG	A	1682	14/15	0.93	0.08	285,301,311,313	0
5	NAG	B	1681	14/15	0.94	0.06	268,294,323,333	0
4	CD	A	1679	1/1	0.96	0.05	270,270,270,270	0
4	CD	B	1678	1/1	0.97	0.05	271,271,271,271	0
4	CD	B	1680	1/1	0.98	0.03	252,252,252,252	0
4	CD	A	1680	1/1	0.98	0.04	241,241,241,241	0
4	CD	A	1678	1/1	0.98	0.04	261,261,261,261	0
4	CD	B	1679	1/1	0.99	0.06	240,240,240,240	0
4	CD	A	1681	1/1	0.99	0.04	263,263,263,263	0
4	CD	B	1677	1/1	0.99	0.03	255,255,255,255	0
4	CD	A	1677	1/1	0.99	0.03	137,137,137,137	1

6.5 Other polymers [i](#)

There are no such residues in this entry.