



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:00 PM EDT

PDB ID : 6SOZ / pdb_00006soz
Title : Glycosylated Trypanosoma brucei transferrin receptor in complex with human transferrin
Authors : Trevor, C.; Carrington, M.; Higgins, M.K.
Deposited on : 2019-08-30
Resolution : 3.42 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:

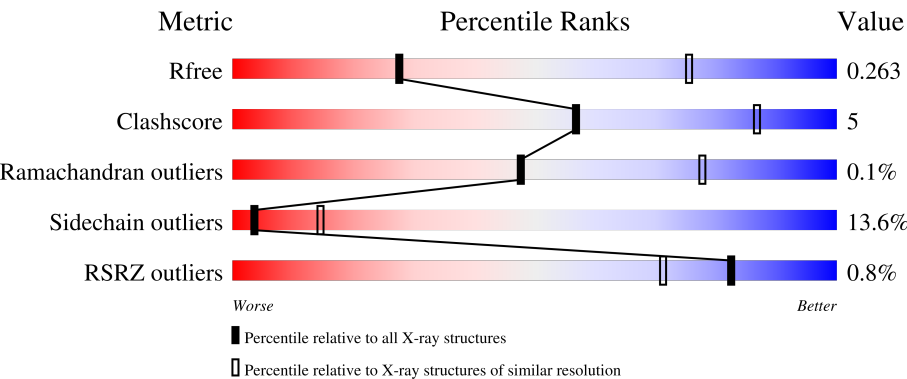
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.42 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	399	
2	B	338	
3	C	677	
4	D	3	
4	E	3	

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Mol	Chain	Length	Quality of chain
5	F	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10211 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 ESAG6, subunit of heterodimeric transferrin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2500	1554	443	492	11			

- Molecule 2 is a protein called ESAG7, subunit of heterodimeric transferrin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	320	Total	C	N	O	S	0	0	0
			2490	1561	433	484	12			

- Molecule 3 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	651	Total	C	N	O	S	0	0	0
			5058	3181	878	955	44			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	VAL	ILE	conflict	UNP P02787

- Molecule 4 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
4	D	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	E	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 5 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
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

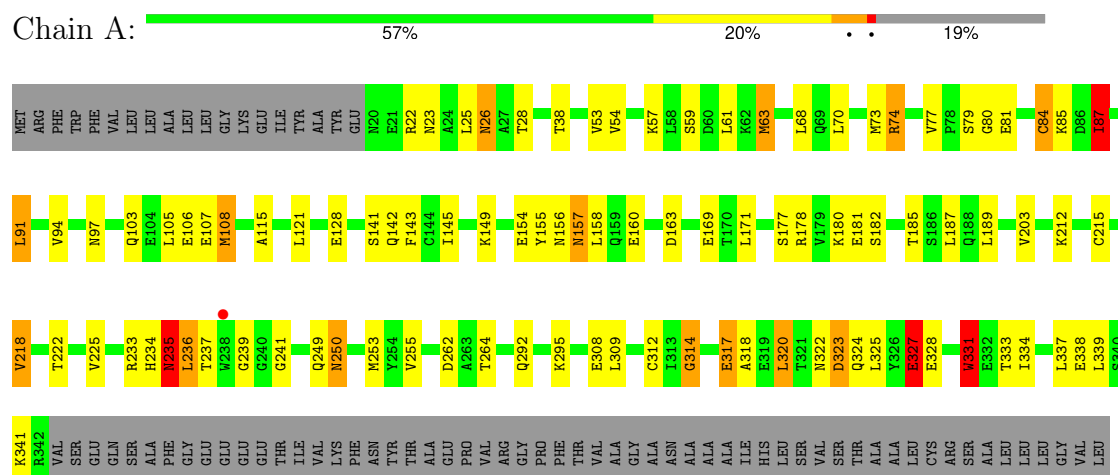
- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Fe 1	1	0

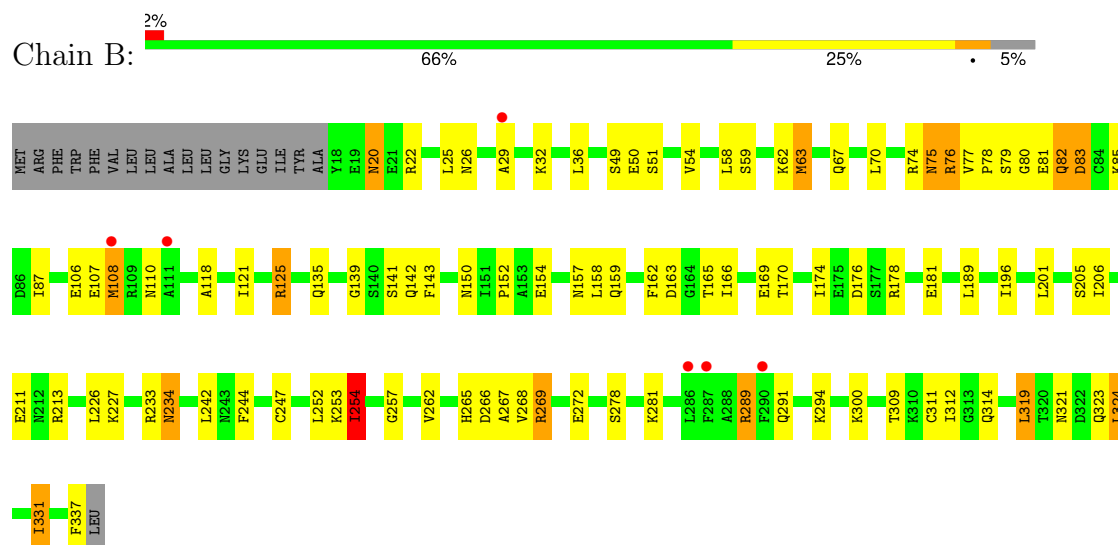
3 Residue-property plots

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.

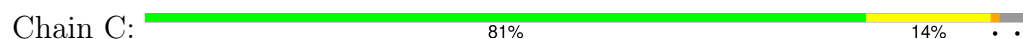
- Molecule 1: ESAG6, subunit of heterodimeric transferrin receptor

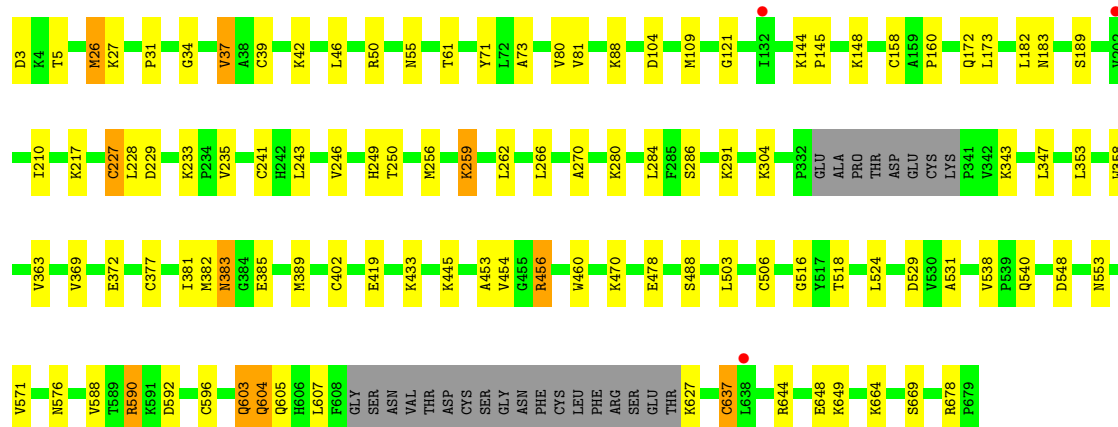


- Molecule 2: ESAG7, subunit of heterodimeric transferrin receptor



- Molecule 3: Serotransferrin





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

Chain D: 67% 33%



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

Chain E: 33% 33% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.18Å 117.87Å 134.55Å 90.00° 111.45° 90.00°	Depositor
Resolution (Å)	39.59 – 3.42 39.59 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.59-3.42) 98.9 (39.59-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.211 , 0.241 0.230 , 0.263	Depositor DCC
R_{free} test set	1239 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	154.2	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 176.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å ²)	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: FE, NAG, MAN

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	0.88	0/2535	1.55	32/3414 (0.9%)
2	B	0.88	1/2526 (0.0%)	1.59	35/3403 (1.0%)
3	C	0.84	1/5172 (0.0%)	1.37	23/6986 (0.3%)
All	All	0.86	2/10233 (0.0%)	1.47	90/13803 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	ASN	CA-CB	6.48	1.63	1.53
3	C	26	MET	SD-CE	-5.51	1.65	1.79

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	ASN	OD1-CG-ND2	-15.63	106.97	122.60
2	B	110	ASN	CB-CG-ND2	14.99	138.88	116.40
1	A	81	GLU	N-CA-C	-13.15	96.68	113.12
2	B	26	ASN	OD1-CG-ND2	-12.98	109.62	122.60
2	B	110	ASN	CA-CB-CG	-10.29	102.31	112.60
2	B	26	ASN	CB-CG-ND2	9.19	130.18	116.40
1	A	157	ASN	N-CA-C	-7.84	99.23	110.59
1	A	314	GLY	CA-C-N	7.46	130.28	120.28
1	A	314	GLY	C-N-CA	7.46	130.28	120.28
3	C	246	VAL	N-CA-C	7.24	115.98	107.73
2	B	150	ASN	CA-CB-CG	7.16	119.76	112.60
2	B	83	ASP	N-CA-C	7.08	121.15	111.17
1	A	218	VAL	N-CA-CB	-7.06	102.89	112.28
1	A	79	SER	N-CA-C	-6.74	96.45	110.80
2	B	76	ARG	CA-C-N	6.61	127.35	122.59
2	B	76	ARG	C-N-CA	6.61	127.35	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	ILE	N-CA-CB	6.57	118.39	110.31
2	B	81	GLU	CA-C-N	6.42	131.72	122.21
2	B	81	GLU	C-N-CA	6.42	131.72	122.21
1	A	250	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	A	26	ASN	OD1-CG-ND2	6.28	128.88	122.60
2	B	77	VAL	N-CA-C	-6.13	101.56	107.76
3	C	183	ASN	CA-CB-CG	6.13	118.73	112.60
2	B	82	GLN	CA-C-N	6.06	131.42	122.82
2	B	82	GLN	C-N-CA	6.06	131.42	122.82
2	B	82	GLN	N-CA-C	-6.00	101.39	110.70
2	B	75	ASN	N-CA-C	-6.00	105.54	112.86
2	B	234	ASN	CB-CG-ND2	5.83	125.15	116.40
3	C	104	ASP	CA-CB-CG	5.82	118.42	112.60
2	B	234	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	239	GLY	N-CA-C	-5.67	102.35	112.22
1	A	87	ILE	CA-C-N	5.65	128.16	120.54
1	A	87	ILE	C-N-CA	5.65	128.16	120.54
2	B	20	ASN	CA-C-N	5.62	129.34	121.02
2	B	20	ASN	C-N-CA	5.62	129.34	121.02
3	C	34	GLY	N-CA-C	5.61	118.73	112.00
3	C	259	LYS	CA-C-N	5.58	128.07	120.54
3	C	259	LYS	C-N-CA	5.58	128.07	120.54
2	B	110	ASN	CB-CA-C	5.57	119.62	110.88
1	A	84	CYS	N-CA-C	-5.53	106.54	113.72
3	C	529	ASP	CA-CB-CG	5.50	118.10	112.60
2	B	289	ARG	CA-C-N	5.45	127.53	120.44
2	B	289	ARG	C-N-CA	5.45	127.53	120.44
1	A	235	ASN	CA-CB-CG	5.42	118.02	112.60
2	B	266	ASP	CA-C-N	5.42	128.80	121.05
2	B	266	ASP	C-N-CA	5.42	128.80	121.05
1	A	250	ASN	CB-CG-ND2	5.38	124.48	116.40
1	A	169	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	249	GLN	CA-C-N	5.35	127.71	120.38
1	A	249	GLN	C-N-CA	5.35	127.71	120.38
2	B	265	HIS	CA-C-N	5.34	127.88	120.29
2	B	265	HIS	C-N-CA	5.34	127.88	120.29
2	B	80	GLY	N-CA-C	-5.31	100.60	113.18
2	B	291	GLN	CA-C-N	5.28	127.66	120.54
2	B	291	GLN	C-N-CA	5.28	127.66	120.54
2	B	272	GLU	CB-CG-CD	5.22	121.48	112.60
3	C	604	GLN	CA-C-N	5.22	127.28	120.28
3	C	604	GLN	C-N-CA	5.22	127.28	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	GLN	CA-C-N	5.21	127.27	120.28
3	C	603	GLN	C-N-CA	5.21	127.27	120.28
2	B	163	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	155	TYR	CA-C-N	5.19	127.23	120.28
1	A	155	TYR	C-N-CA	5.19	127.23	120.28
2	B	20	ASN	CA-CB-CG	5.16	117.76	112.60
3	C	31	PRO	CA-C-N	5.15	127.44	120.38
3	C	31	PRO	C-N-CA	5.15	127.44	120.38
2	B	110	ASN	N-CA-C	-5.13	105.58	111.07
3	C	26	MET	CA-C-N	5.13	127.15	120.28
3	C	26	MET	C-N-CA	5.13	127.15	120.28
3	C	669	SER	CA-C-N	5.09	127.37	120.44
3	C	669	SER	C-N-CA	5.09	127.37	120.44
3	C	88	LYS	CA-C-N	5.08	127.35	120.44
3	C	88	LYS	C-N-CA	5.08	127.35	120.44
3	C	460	TRP	CA-C-N	5.07	127.33	120.38
3	C	460	TRP	C-N-CA	5.07	127.33	120.38
1	A	97	ASN	CA-C-N	5.07	127.07	120.28
1	A	97	ASN	C-N-CA	5.07	127.07	120.28
1	A	115	ALA	CA-C-N	5.06	127.83	120.79
1	A	115	ALA	C-N-CA	5.06	127.83	120.79
1	A	331	TRP	CA-C-N	5.06	129.24	120.58
1	A	331	TRP	C-N-CA	5.06	129.24	120.58
1	A	181	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	262	ASP	N-CA-C	5.05	117.68	111.82
1	A	322	ASN	CA-C-N	5.05	127.30	120.38
1	A	322	ASN	C-N-CA	5.05	127.30	120.38
1	A	327	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	74	ARG	CA-C-N	5.04	129.70	122.40
1	A	74	ARG	C-N-CA	5.04	129.70	122.40
3	C	518	THR	CA-C-N	5.01	125.55	119.98
3	C	518	THR	C-N-CA	5.01	125.55	119.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2500	0	2470	39	0
2	B	2490	0	2467	37	0
3	C	5058	0	4902	24	0
4	D	39	0	34	2	0
4	E	39	0	34	1	0
5	F	28	0	25	4	0
6	A	28	0	26	4	0
6	B	28	0	26	1	0
7	C	1	0	0	0	0
All	All	10211	0	9984	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (93) 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:A:233:ARG:HG3	2:B:139:GLY:H	1.47	0.77
2:B:74:ARG:HH21	2:B:331:ILE:HD11	1.50	0.77
1:A:154:GLU:H	1:A:157:ASN:HD22	1.34	0.76
1:A:94:VAL:HG21	1:A:309:LEU:HD21	1.69	0.74
2:B:233:ARG:HA	6:B:404:NAG:H62	1.68	0.74
1:A:327:GLU:OE1	1:A:328:GLU:HG3	1.87	0.74
3:C:538:VAL:HB	3:C:571:VAL:HG11	1.71	0.72
5:F:1:NAG:H62	5:F:2:NAG:H61	1.72	0.72
3:C:383:ASN:HD21	3:C:385:GLU:HG3	1.58	0.67
1:A:68:LEU:HD22	1:A:309:LEU:HD22	1.78	0.66
3:C:37:VAL:HG22	3:C:266:LEU:HD11	1.79	0.65
2:B:262:VAL:HG13	2:B:267:ALA:HB3	1.78	0.65
3:C:145:PRO:HG2	3:C:148:LYS:HB2	1.80	0.64
2:B:49:SER:HB3	4:D:2:NAG:H82	1.80	0.64
1:A:26:ASN:OD1	6:A:401:NAG:H2	1.98	0.62
1:A:77:VAL:HG13	1:A:312:CYS:HB3	1.80	0.62
3:C:381:ILE:O	3:C:590:ARG:HD3	2.00	0.62
2:B:50:GLU:HB3	2:B:294:LYS:HE2	1.81	0.62
2:B:54:VAL:HG21	2:B:108:MET:HE1	1.83	0.60
2:B:74:ARG:NH2	2:B:331:ILE:HD11	2.15	0.60
1:A:341:LYS:HZ2	2:B:75:ASN:HB2	1.66	0.60
2:B:319:LEU:HB3	2:B:324:LEU:HD12	1.83	0.60
3:C:233:LYS:HD2	3:C:241:CYS:HB2	1.86	0.58
3:C:605:GLN:HE21	3:C:637:CYS:HB2	1.69	0.58
2:B:278:SER:HA	2:B:281:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:ND2	1:A:28:THR:HG22	2.19	0.57
2:B:178:ARG:HA	2:B:181:GLU:HG2	1.86	0.56
1:A:235:ASN:OD1	6:A:405:NAG:O5	2.24	0.55
2:B:252:LEU:HG	2:B:268:VAL:HG21	1.88	0.55
3:C:358:TRP:HE1	3:C:604:GLN:NE2	2.05	0.55
1:A:320:LEU:HD23	1:A:325:LEU:HA	1.89	0.55
3:C:26:MET:HE1	3:C:270:ALA:HA	1.89	0.54
3:C:121:GLY:HA2	3:C:160:PRO:HD2	1.90	0.54
1:A:54:VAL:HG11	1:A:108:MET:HE1	1.88	0.54
1:A:237:THR:OG1	1:A:241:GLY:HA2	2.08	0.54
3:C:453:ALA:HB3	3:C:456:ARG:HG3	1.90	0.52
1:A:128:GLU:OE1	2:B:125:ARG:HD2	2.09	0.52
1:A:145:ILE:HG21	1:A:158:LEU:HD21	1.91	0.52
3:C:210:ILE:HD13	3:C:235:VAL:HG11	1.91	0.52
2:B:309:THR:HA	2:B:312:ILE:HD12	1.92	0.52
1:A:264:THR:HA	6:A:405:NAG:H83	1.92	0.52
1:A:28:THR:HG22	6:A:401:NAG:C1	2.39	0.51
2:B:67:GLN:HG3	2:B:324:LEU:HD11	1.92	0.51
3:C:158:CYS:HB2	3:C:173:LEU:HB2	1.92	0.51
1:A:236:LEU:HD22	2:B:135:GLN:HB2	1.94	0.50
2:B:234:ASN:OD1	2:B:244:PHE:O	2.28	0.50
1:A:107:GLU:HG3	4:D:1:NAG:H81	1.93	0.50
1:A:341:LYS:NZ	2:B:75:ASN:HB2	2.26	0.49
1:A:250:ASN:HB2	4:E:1:NAG:H2	1.94	0.49
2:B:118:ALA:HA	2:B:121:ILE:HD12	1.94	0.49
3:C:524:LEU:HB2	3:C:531:ALA:HB2	1.93	0.49
1:A:237:THR:H	2:B:135:GLN:HE22	1.61	0.48
1:A:25:LEU:O	1:A:145:ILE:HA	2.14	0.48
2:B:107:GLU:N	5:F:1:NAG:H82	2.30	0.47
2:B:143:PHE:CB	2:B:152:PRO:HB3	2.44	0.47
2:B:162:PHE:HD1	2:B:170:THR:HG23	1.79	0.47
1:A:108:MET:HE2	1:A:295:LYS:HA	1.97	0.46
1:A:143:PHE:O	1:A:215:CYS:HB2	2.15	0.46
1:A:236:LEU:HD22	2:B:135:GLN:CB	2.44	0.46
1:A:160:GLU:HG2	1:A:178:ARG:HH22	1.81	0.46
1:A:23:ASN:HB2	1:A:253:MET:HB2	1.97	0.45
3:C:259:LYS:HB3	3:C:262:LEU:HB3	1.97	0.45
3:C:3:ASP:OD1	3:C:5:THR:HG22	2.16	0.45
2:B:154:GLU:H	2:B:157:ASN:HD22	1.64	0.44
2:B:257:GLY:HA3	2:B:269:ARG:HG2	1.98	0.44
2:B:29:ALA:HB2	2:B:206:ILE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:CYS:SG	3:C:73:ALA:HB1	2.58	0.44
1:A:74:ARG:HD2	1:A:317:GLU:OE1	2.18	0.44
1:A:317:GLU:H	1:A:317:GLU:HG2	1.62	0.43
2:B:63:MET:HG3	2:B:321:ASN:HD22	1.83	0.43
2:B:106:GLU:OE1	5:F:1:NAG:H83	2.19	0.43
2:B:78:PRO:HD2	2:B:311:CYS:O	2.19	0.43
1:A:80:GLY:HA2	1:A:84:CYS:HB2	2.01	0.43
1:A:63:MET:HE3	1:A:63:MET:HB3	1.89	0.43
2:B:254:ILE:HG23	2:B:268:VAL:HG12	2.01	0.43
3:C:227:CYS:HB2	3:C:229:ASP:OD1	2.19	0.43
1:A:80:GLY:CA	1:A:84:CYS:HB2	2.49	0.42
2:B:36:LEU:HD22	2:B:196:ILE:HG12	2.02	0.42
3:C:644:ARG:HA	3:C:649:LYS:HB3	2.02	0.42
1:A:234:HIS:CE1	2:B:166:ILE:HB	2.55	0.41
3:C:80:VAL:HG23	3:C:81:VAL:HG23	2.03	0.41
3:C:456:ARG:NH2	3:C:516:GLY:HA2	2.35	0.41
2:B:252:LEU:HB3	2:B:254:ILE:CD1	2.50	0.41
3:C:109:MET:HE3	3:C:228:LEU:HD23	2.03	0.41
3:C:603:GLN:O	3:C:607:LEU:HG	2.19	0.41
1:A:328:GLU:HA	1:A:331:TRP:HB2	2.03	0.41
1:A:87:ILE:O	1:A:91:LEU:HB2	2.21	0.41
3:C:382:MET:SD	3:C:402:CYS:HB3	2.61	0.41
1:A:314:GLY:O	1:A:318:ALA:HB2	2.21	0.41
1:A:73:MET:HE1	1:A:333:THR:HA	2.03	0.40
1:A:323:ASP:O	1:A:327:GLU:HB3	2.21	0.40
2:B:165:THR:O	2:B:170:THR:HG21	2.21	0.40
5:F:1:NAG:H62	5:F:2:NAG:C6	2.48	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	321/399 (80%)	306 (95%)	15 (5%)	0	100	100
2	B	318/338 (94%)	297 (93%)	21 (7%)	0	100	100
3	C	645/677 (95%)	609 (94%)	35 (5%)	1 (0%)	43	71
All	All	1284/1414 (91%)	1212 (94%)	71 (6%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	363	VAL

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	268/327 (82%)	220 (82%)	48 (18%)	2	7
2	B	268/283 (95%)	224 (84%)	44 (16%)	2	10
3	C	547/570 (96%)	492 (90%)	55 (10%)	7	25
All	All	1083/1180 (92%)	936 (86%)	147 (14%)	3	14

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	38	THR
1	A	53	VAL
1	A	57	LYS
1	A	59	SER
1	A	61	LEU
1	A	63	MET
1	A	70	LEU
1	A	85	LYS
1	A	87	ILE
1	A	91	LEU
1	A	103	GLN

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	106	GLU
1	A	108	MET
1	A	121	LEU
1	A	141	SER
1	A	142	GLN
1	A	149	LYS
1	A	156	ASN
1	A	163	ASP
1	A	171	LEU
1	A	177	SER
1	A	180	LYS
1	A	182	SER
1	A	185	THR
1	A	187	LEU
1	A	189	LEU
1	A	203	VAL
1	A	212	LYS
1	A	218	VAL
1	A	222	THR
1	A	225	VAL
1	A	235	ASN
1	A	236	LEU
1	A	255	VAL
1	A	292	GLN
1	A	308	GLU
1	A	317	GLU
1	A	320	LEU
1	A	323	ASP
1	A	324	GLN
1	A	327	GLU
1	A	331	TRP
1	A	334	ILE
1	A	337	LEU
1	A	338	GLU
1	A	339	LEU
2	B	20	ASN
2	B	22	ARG
2	B	25	LEU
2	B	32	LYS
2	B	51	SER
2	B	58	LEU

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Mol	Chain	Res	Type
2	B	59	SER
2	B	62	LYS
2	B	63	MET
2	B	70	LEU
2	B	76	ARG
2	B	79	SER
2	B	82	GLN
2	B	83	ASP
2	B	85	LYS
2	B	87	ILE
2	B	108	MET
2	B	125	ARG
2	B	141	SER
2	B	142	GLN
2	B	158	LEU
2	B	159	GLN
2	B	169	GLU
2	B	174	ILE
2	B	176	ASP
2	B	189	LEU
2	B	201	LEU
2	B	205	SER
2	B	211	GLU
2	B	213	ARG
2	B	226	LEU
2	B	227	LYS
2	B	242	LEU
2	B	253	LYS
2	B	254	ILE
2	B	269	ARG
2	B	289	ARG
2	B	300	LYS
2	B	314	GLN
2	B	319	LEU
2	B	323	GLN
2	B	324	LEU
2	B	331	ILE
2	B	337	PHE
3	C	27	LYS
3	C	37	VAL
3	C	39	CYS
3	C	42	LYS

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Mol	Chain	Res	Type
3	C	46	LEU
3	C	50	ARG
3	C	55	ASN
3	C	61	THR
3	C	71	TYR
3	C	144	LYS
3	C	172	GLN
3	C	182	LEU
3	C	189	SER
3	C	217	LYS
3	C	227	CYS
3	C	243	LEU
3	C	249	HIS
3	C	250	THR
3	C	256	MET
3	C	280	LYS
3	C	284	LEU
3	C	286	SER
3	C	291	LYS
3	C	304	LYS
3	C	343	LYS
3	C	347	LEU
3	C	353	LEU
3	C	369	VAL
3	C	372	GLU
3	C	377	CYS
3	C	383	ASN
3	C	389	MET
3	C	419	GLU
3	C	433	LYS
3	C	445	LYS
3	C	454	VAL
3	C	456	ARG
3	C	470	LYS
3	C	478	GLU
3	C	488	SER
3	C	503	LEU
3	C	506	CYS
3	C	540	GLN
3	C	548	ASP
3	C	553	ASN
3	C	576	ASN

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Mol	Chain	Res	Type
3	C	588	VAL
3	C	590	ARG
3	C	592	ASP
3	C	596	CYS
3	C	627	LYS
3	C	637	CYS
3	C	648	GLU
3	C	664	LYS
3	C	678	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	69	GLN
1	A	103	GLN
1	A	157	ASN
1	A	234	HIS
1	A	335	ASN
2	B	69	GLN
2	B	82	GLN
2	B	150	ASN
2	B	157	ASN
2	B	190	HIS
2	B	321	ASN
2	B	323	GLN
3	C	55	ASN
3	C	108	GLN
3	C	172	GLN
3	C	222	GLN
3	C	289	HIS
3	C	383	ASN
3	C	417	ASN
3	C	540	GLN
3	C	546	ASN
3	C	584	ASN
3	C	604	GLN
3	C	605	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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.37	0	17,19,21	0.73	0
4	NAG	D	2	4	14,14,15	0.31	0	17,19,21	0.94	1 (5%)
4	MAN	D	3	4	11,11,12	0.39	0	15,15,17	1.09	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	0.75	0
4	MAN	E	3	4	11,11,12	0.49	0	15,15,17	1.10	1 (6%)
5	NAG	F	1	5,2	14,14,15	0.42	0	17,19,21	1.38	2 (11%)
5	NAG	F	2	5	14,14,15	0.56	0	17,19,21	1.84	4 (23%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	NAG	C1-O5-C5	5.56	119.63	112.19
5	F	1	NAG	C1-O5-C5	-4.18	106.59	112.19
4	D	2	NAG	O5-C1-C2	-3.51	105.86	111.29
4	D	3	MAN	C1-O5-C5	3.50	116.87	112.19
4	E	3	MAN	C1-O5-C5	3.44	116.79	112.19
5	F	2	NAG	C2-N2-C7	3.27	127.28	122.90
5	F	2	NAG	C1-C2-N2	3.08	115.28	110.43
4	E	1	NAG	C1-O5-C5	-2.65	108.64	112.19
5	F	1	NAG	O3-C3-C2	2.29	114.16	109.40
5	F	2	NAG	O5-C1-C2	2.05	114.47	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	3	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	3	MAN	C4-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
5	F	2	NAG	C3-C2-N2-C7
5	F	1	NAG	C8-C7-N2-C2
5	F	2	NAG	C1-C2-N2-C7
5	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

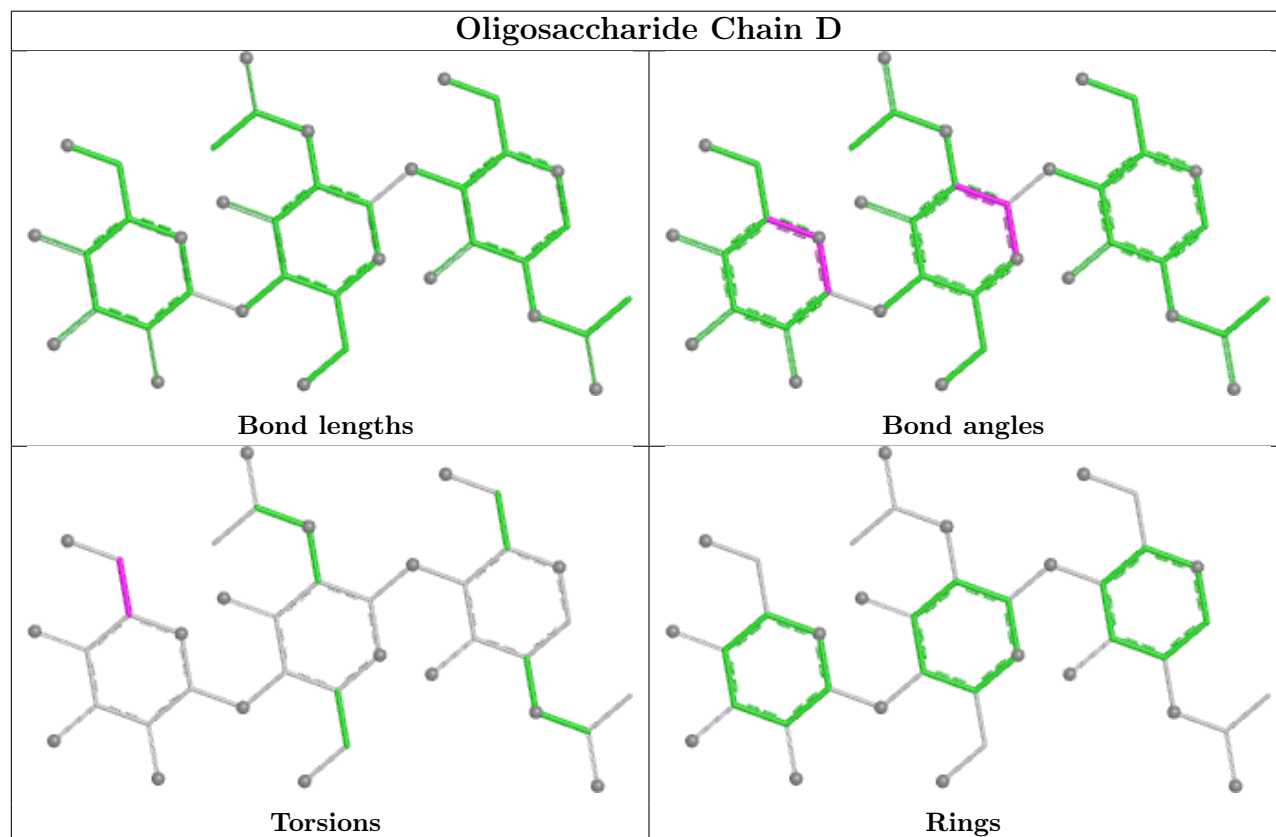
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0

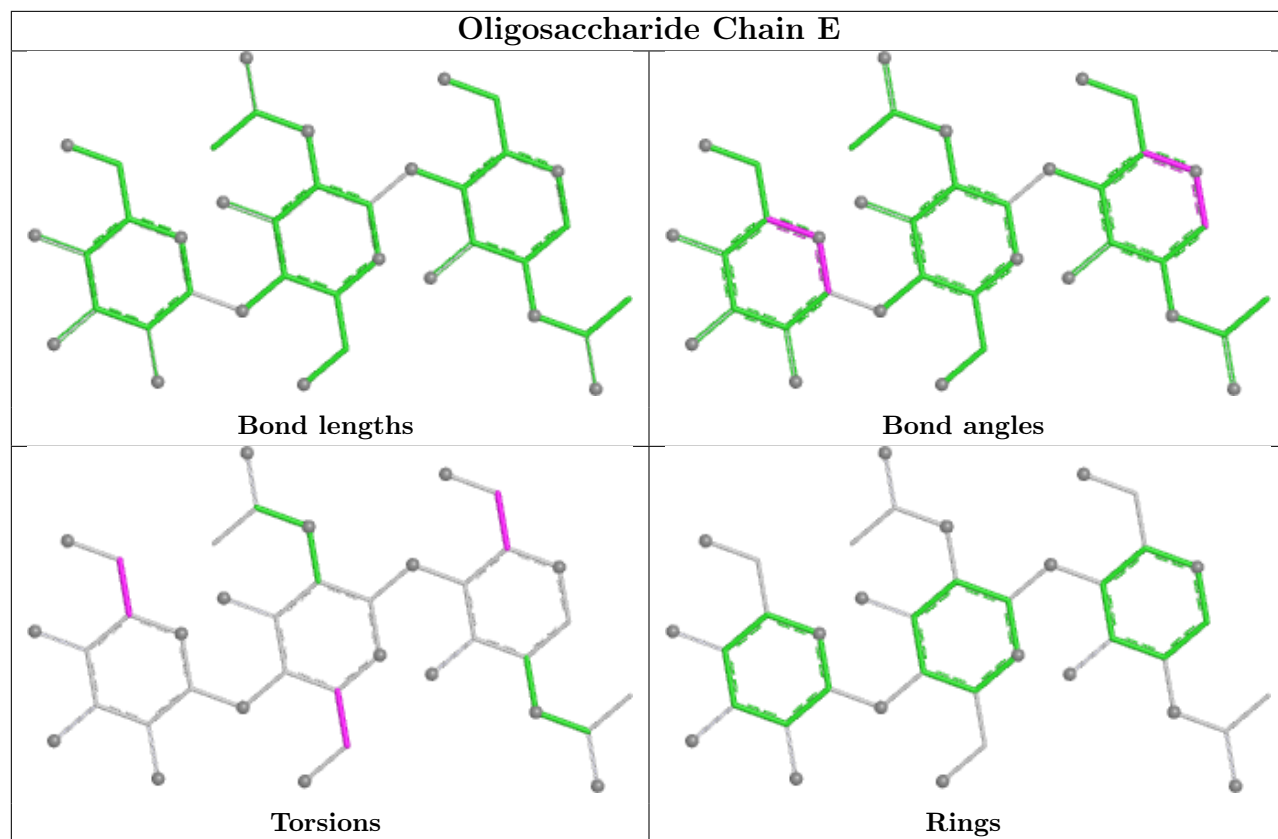
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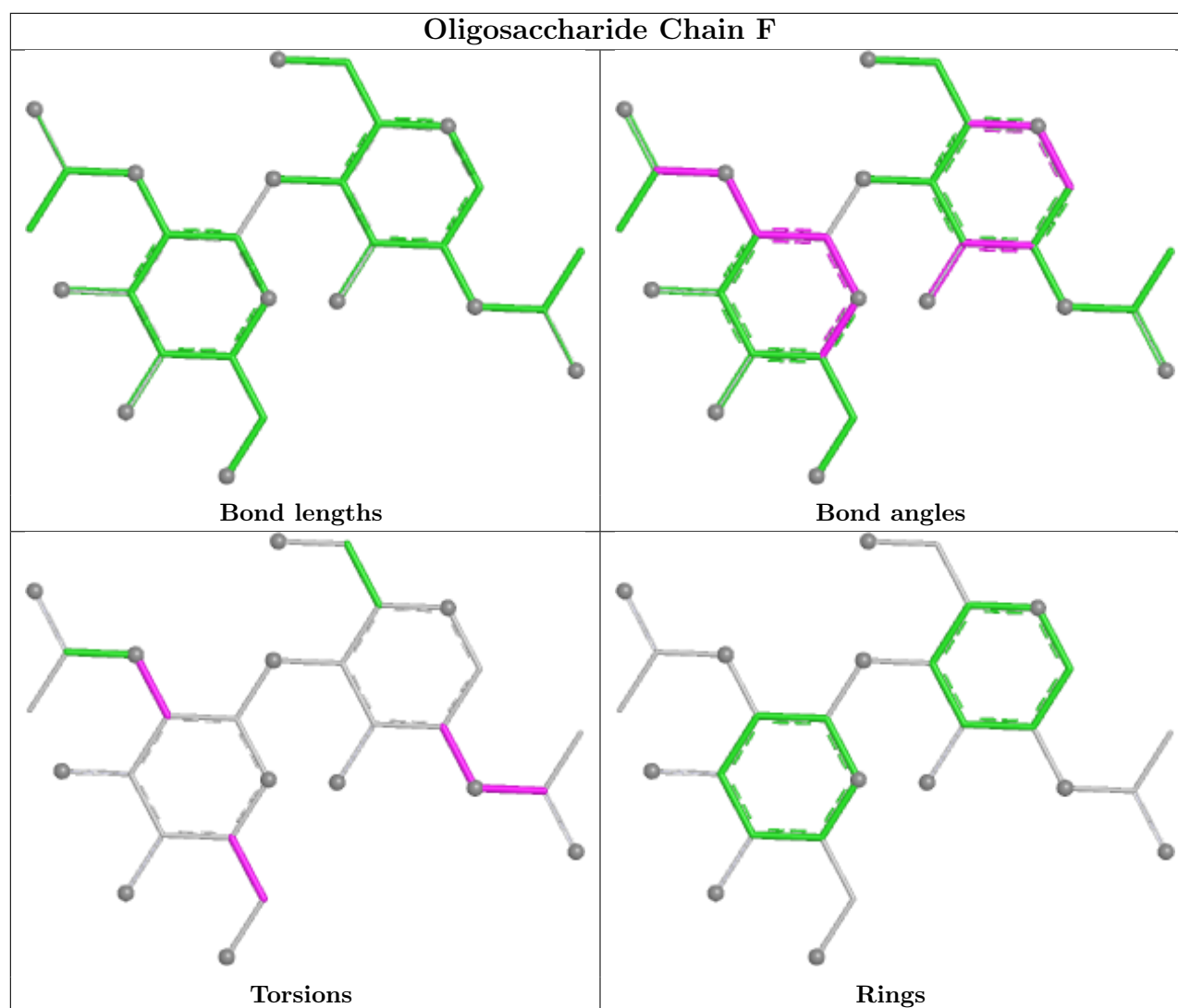
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	1	0
5	F	2	NAG	2	0
4	D	1	NAG	1	0
5	F	1	NAG	4	0

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	NAG	B	404	2	14,14,15	0.44	0	17,19,21	1.10	2 (11%)
6	NAG	B	401	2	14,14,15	0.51	0	17,19,21	2.03	3 (17%)
6	NAG	A	401	1	14,14,15	0.37	0	17,19,21	1.39	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	405	1	14,14,15	0.32	0	17,19,21	1.53	4 (23%)

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	NAG	B	404	2	-	3/6/23/26	0/1/1/1
6	NAG	B	401	2	-	5/6/23/26	0/1/1/1
6	NAG	A	401	1	-	5/6/23/26	0/1/1/1
6	NAG	A	405	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	401	NAG	C1-O5-C5	6.58	121.01	112.19
6	B	401	NAG	C1-C2-N2	3.54	116.02	110.43
6	A	401	NAG	C1-C2-N2	3.44	115.86	110.43
6	A	405	NAG	C1-O5-C5	3.40	116.74	112.19
6	B	404	NAG	C1-C2-N2	-3.27	105.28	110.43
6	A	401	NAG	C1-O5-C5	3.06	116.29	112.19
6	A	405	NAG	O5-C1-C2	-3.05	106.56	111.29
6	B	404	NAG	O5-C1-C2	2.69	115.45	111.29
6	A	401	NAG	C2-N2-C7	2.61	126.40	122.90
6	A	405	NAG	C2-N2-C7	2.61	126.39	122.90
6	A	405	NAG	C1-C2-N2	2.39	114.20	110.43
6	B	401	NAG	O5-C1-C2	2.07	114.50	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C1-C2-N2-C7
6	A	405	NAG	C8-C7-N2-C2
6	A	405	NAG	O7-C7-N2-C2
6	B	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C8-C7-N2-C2
6	B	401	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	405	NAG	O5-C5-C6-O6
6	B	404	NAG	C8-C7-N2-C2
6	B	401	NAG	C1-C2-N2-C7
6	A	401	NAG	O7-C7-N2-C2
6	B	401	NAG	O7-C7-N2-C2
6	A	405	NAG	C3-C2-N2-C7
6	B	401	NAG	C3-C2-N2-C7
6	B	404	NAG	C3-C2-N2-C7
6	A	401	NAG	C4-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6
6	B	404	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	404	NAG	1	0
6	A	401	NAG	2	0
6	A	405	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/399 (80%)	-0.86	1 (0%) 90 84	132, 192, 240, 256	0
2	B	320/338 (94%)	-0.67	6 (1%) 66 51	123, 183, 234, 256	0
3	C	651/677 (96%)	-0.71	3 (0%) 87 78	158, 240, 292, 296	0
All	All	1294/1414 (91%)	-0.74	10 (0%) 82 71	123, 216, 288, 296	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	287	PHE	4.1
3	C	202	VAL	3.7
2	B	111	ALA	3.6
2	B	286	LEU	3.2
3	C	638	LEU	3.1
2	B	290	PHE	2.8
3	C	132	ILE	2.8
2	B	108	MET	2.4
2	B	29	ALA	2.4
1	A	238	TRP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

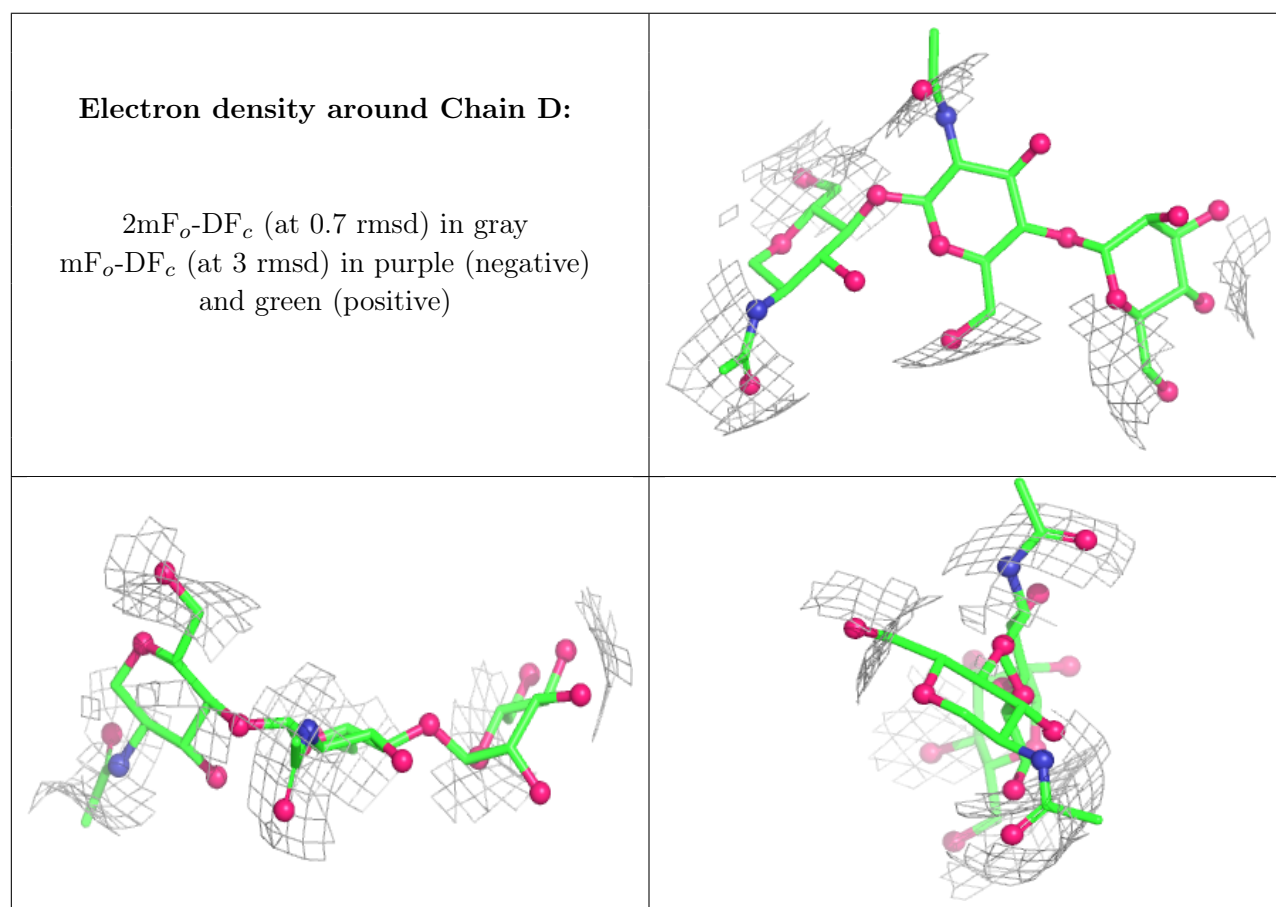
There are no non-standard protein/DNA/RNA residues in this entry.

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.

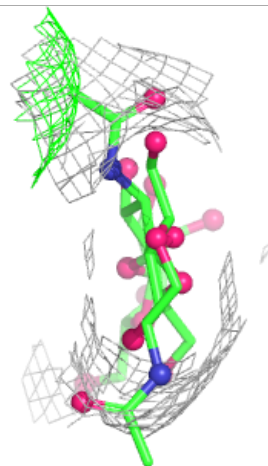
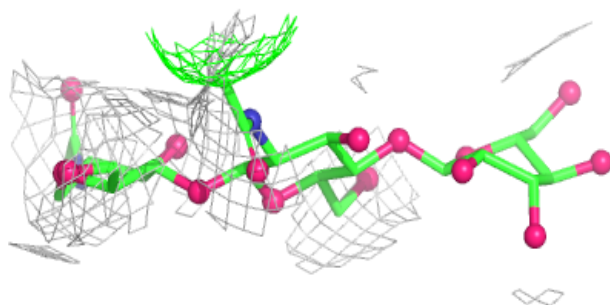
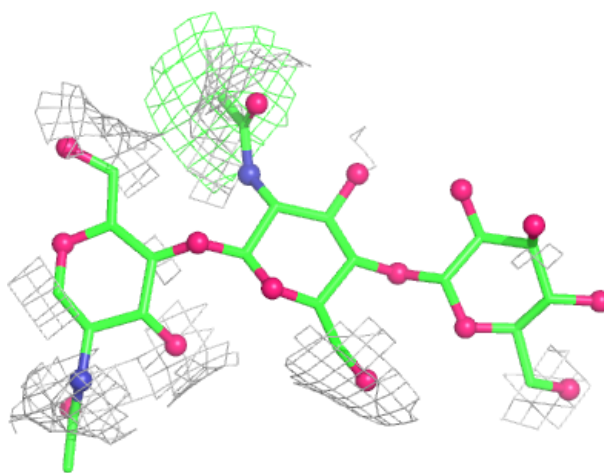
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	E	3	11/12	0.48	0.06	239,240,242,242	0
4	MAN	D	3	11/12	0.49	0.06	264,266,268,268	0
5	NAG	F	2	14/15	0.68	0.08	202,213,226,229	0
4	NAG	E	2	14/15	0.75	0.05	231,235,238,240	0
5	NAG	F	1	14/15	0.77	0.09	168,174,180,191	0
4	NAG	D	2	14/15	0.87	0.06	248,252,256,260	0
4	NAG	E	1	14/15	0.90	0.06	210,222,224,229	0
4	NAG	D	1	14/15	0.94	0.05	198,211,222,235	0

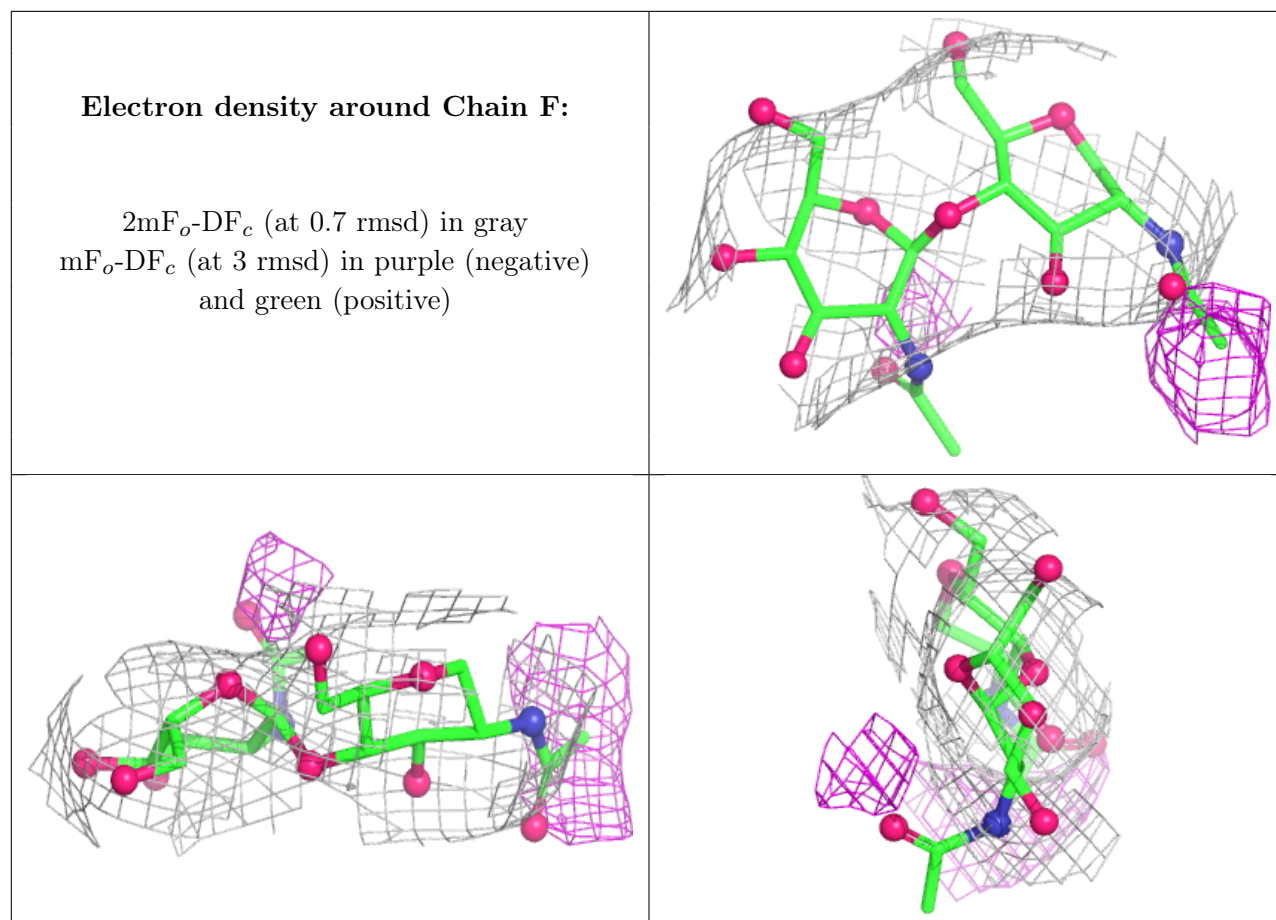
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	405	14/15	0.43	0.09	228,231,236,236	0
6	NAG	B	401	14/15	0.45	0.09	198,214,222,223	0
6	NAG	A	401	14/15	0.69	0.08	215,220,223,224	0
6	NAG	B	404	14/15	0.73	0.07	171,180,195,196	0
7	FE	C	701	1/1	-	-	265,265,265,265	1

6.5 Other polymers [i](#)

There are no such residues in this entry.