



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 7PEE / pdb_00007pee
Title : Crystal structure of extracellular part of human Trop2
Authors : Pavsic, M.
Deposited on : 2021-08-09
Resolution : 2.81 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

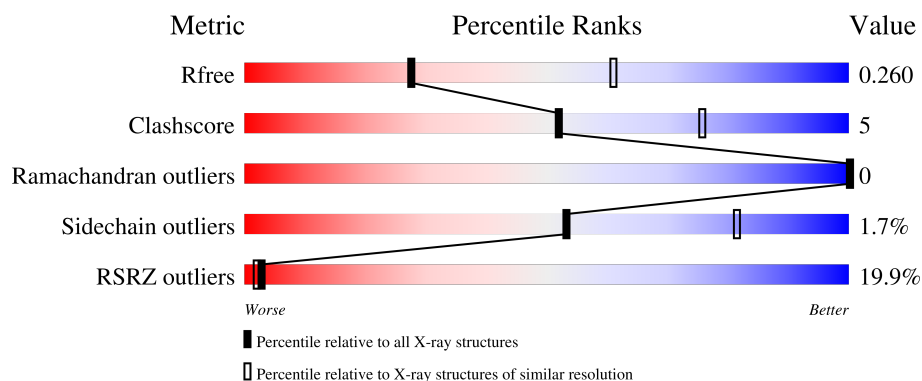
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	250	
1	B	250	
1	C	250	
1	D	250	
2	E	3	

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Mol	Chain	Length	Quality of chain
2	F	3	33% 67%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7620 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 Tumor-associated calcium signal transducer 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1866	1150	351	350	15			
1	B	238	Total	C	N	O	S	0	0	0
			1872	1153	352	352	15			
1	C	238	Total	C	N	O	S	0	0	0
			1872	1153	352	352	15			
1	D	237	Total	C	N	O	S	0	0	0
			1866	1150	351	350	15			

There are 32 discrepancies between the modelled and reference sequences:

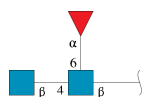
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	GLN	ASN	engineered mutation	UNP P09758
A	208	GLN	ASN	engineered mutation	UNP P09758
A	275	HIS	-	expression tag	UNP P09758
A	276	HIS	-	expression tag	UNP P09758
A	277	HIS	-	expression tag	UNP P09758
A	278	HIS	-	expression tag	UNP P09758
A	279	HIS	-	expression tag	UNP P09758
A	280	HIS	-	expression tag	UNP P09758
B	120	GLN	ASN	engineered mutation	UNP P09758
B	208	GLN	ASN	engineered mutation	UNP P09758
B	275	HIS	-	expression tag	UNP P09758
B	276	HIS	-	expression tag	UNP P09758
B	277	HIS	-	expression tag	UNP P09758
B	278	HIS	-	expression tag	UNP P09758
B	279	HIS	-	expression tag	UNP P09758
B	280	HIS	-	expression tag	UNP P09758
C	120	GLN	ASN	engineered mutation	UNP P09758
C	208	GLN	ASN	engineered mutation	UNP P09758
C	275	HIS	-	expression tag	UNP P09758
C	276	HIS	-	expression tag	UNP P09758
C	277	HIS	-	expression tag	UNP P09758

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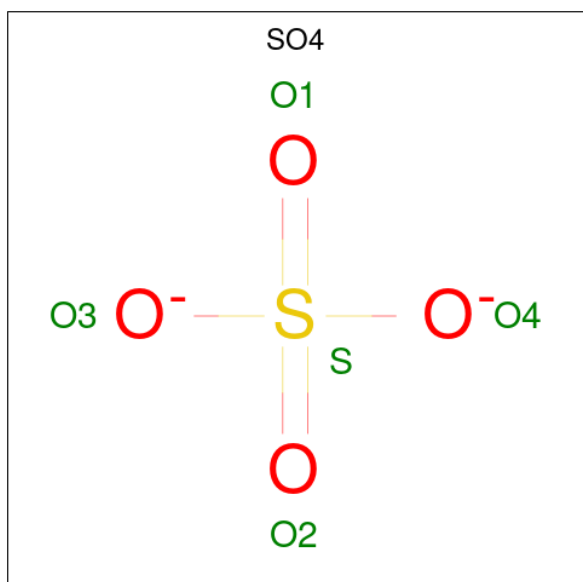
Chain	Residue	Modelled	Actual	Comment	Reference
C	278	HIS	-	expression tag	UNP P09758
C	279	HIS	-	expression tag	UNP P09758
C	280	HIS	-	expression tag	UNP P09758
D	120	GLN	ASN	engineered mutation	UNP P09758
D	208	GLN	ASN	engineered mutation	UNP P09758
D	275	HIS	-	expression tag	UNP P09758
D	276	HIS	-	expression tag	UNP P09758
D	277	HIS	-	expression tag	UNP P09758
D	278	HIS	-	expression tag	UNP P09758
D	279	HIS	-	expression tag	UNP P09758
D	280	HIS	-	expression tag	UNP P09758

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



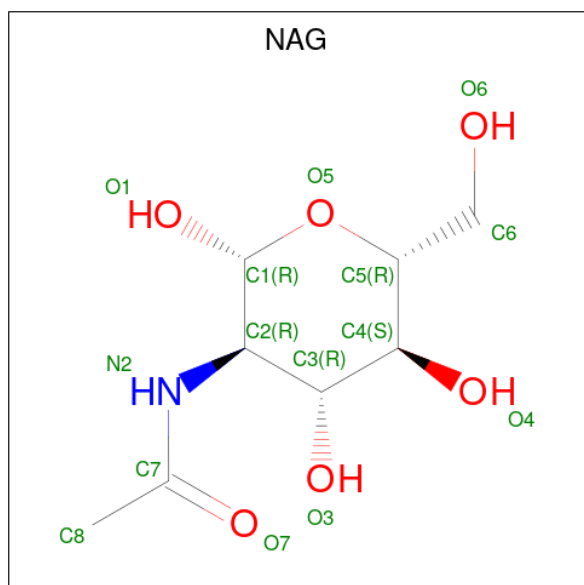
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

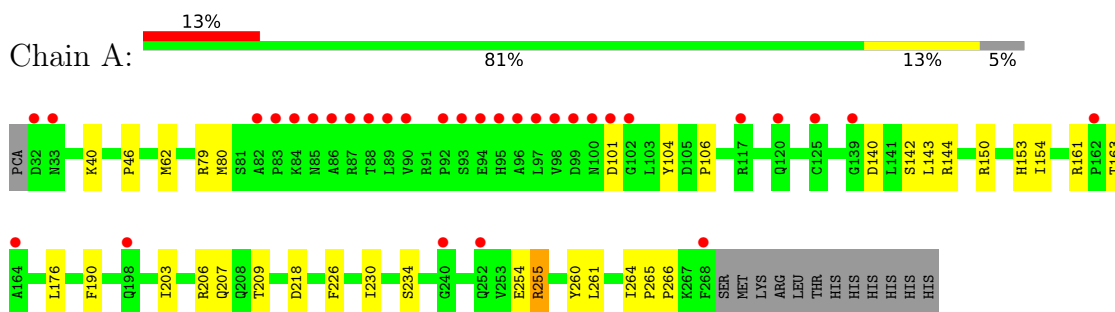
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	B	8	Total O 8 8	0	0
5	C	9	Total O 9 9	0	0
5	D	2	Total O 2 2	0	0

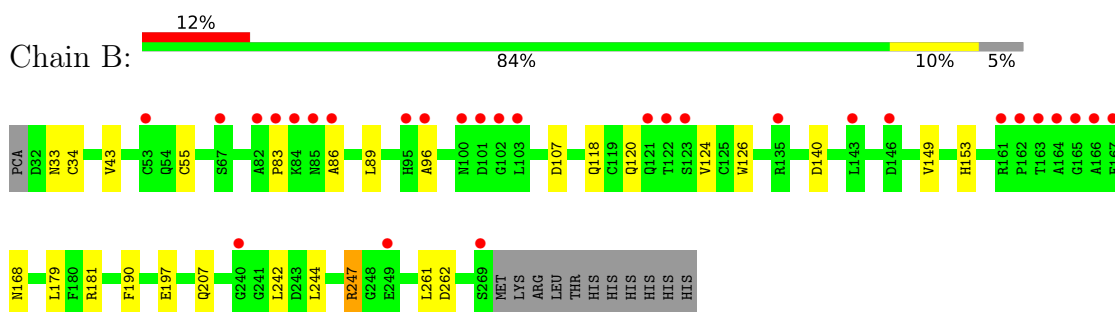
3 Residue-property plots

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.

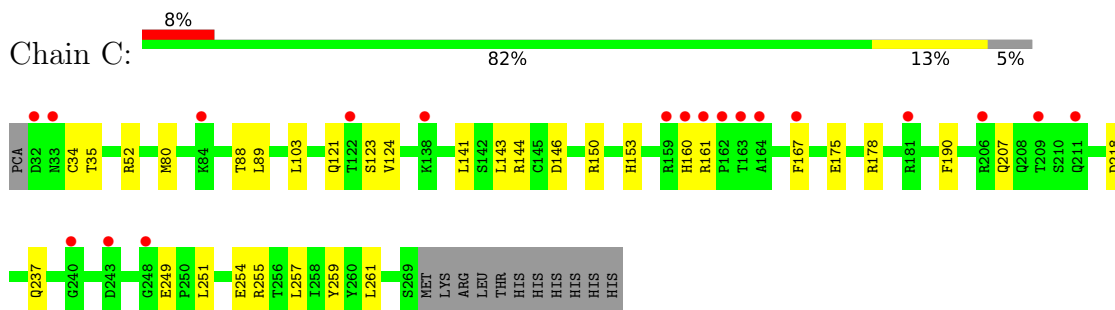
- Molecule 1: Tumor-associated calcium signal transducer 2



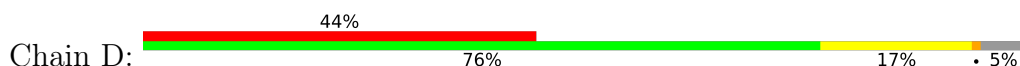
- Molecule 1: Tumor-associated calcium signal transducer 2

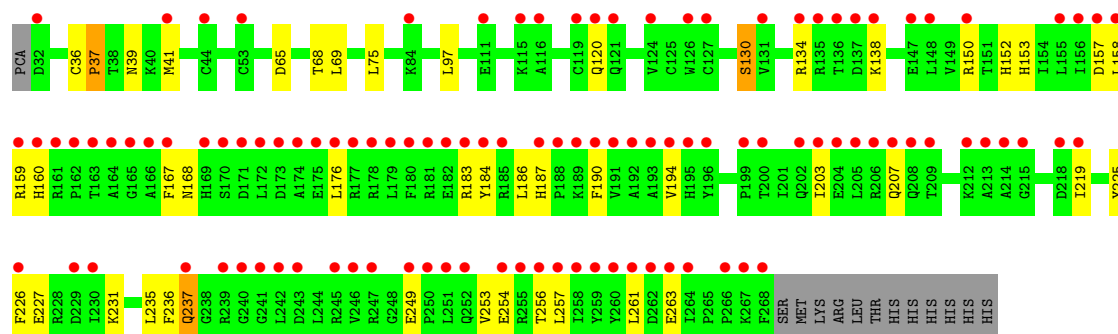


- Molecule 1: Tumor-associated calcium signal transducer 2



- Molecule 1: Tumor-associated calcium signal transducer 2





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

Chain E: 33% 67%



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

Chain F: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.08Å 145.08Å 217.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.37 – 2.81 48.37 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.37-2.81) 99.6 (48.37-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.240 , 0.263 0.238 , 0.260	Depositor DCC
R_{free} test set	2867 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: FUC, SO4, 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	0.37	0/1901	0.58	2/2568 (0.1%)
1	B	0.47	0/1907	0.72	0/2576
1	C	0.44	1/1907 (0.1%)	0.69	0/2576
1	D	0.54	2/1901 (0.1%)	0.79	0/2568
All	All	0.46	3/7616 (0.0%)	0.70	2/10288 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	PHE	C-N	6.27	1.42	1.33
1	C	52	ARG	C-N	6.16	1.42	1.33
1	D	237	GLN	C-N	5.85	1.42	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PRO	N-CA-CB	-5.98	98.07	102.25
1	A	101	ASP	N-CA-C	-5.58	106.42	113.23

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	1866	0	1827	18	0
1	B	1872	0	1832	16	0
1	C	1872	0	1832	19	0
1	D	1866	0	1827	31	0
2	E	38	0	34	0	0
2	F	38	0	34	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	11	0	0	1	0
5	B	8	0	0	1	0
5	C	9	0	0	0	0
5	D	2	0	0	0	0
All	All	7620	0	7412	77	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 (77) 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:D:186:LEU:HD21	1:D:219:ILE:HG22	1.67	0.74
1:D:160:HIS:HA	1:D:253:VAL:HA	1.73	0.68
1:A:153:HIS:HB3	1:A:261:LEU:HB3	1.78	0.65
1:D:75:LEU:HD13	1:D:235:LEU:HD13	1.80	0.63
1:B:179:LEU:HD11	1:B:242:LEU:HD11	1.84	0.59
1:C:153:HIS:HB3	1:C:261:LEU:HB3	1.85	0.57
1:D:36:CYS:HB3	1:D:39:ASN:O	2.06	0.55
1:A:226:PHE:CZ	1:A:230:ILE:HD11	2.40	0.55
1:D:65:ASP:HB3	1:D:68:THR:HG22	1.89	0.55
1:C:150:ARG:NH1	1:C:218:ASP:OD2	2.38	0.55
1:D:37:PRO:HA	1:D:237:GLN:HB2	1.88	0.55
1:D:152:HIS:CD2	1:D:263:GLU:HG3	2.43	0.54
1:C:255:ARG:C	1:C:255:ARG:HD2	2.33	0.53
1:B:242:LEU:HD21	1:B:244:LEU:HD22	1.92	0.52
1:C:160:HIS:ND1	1:C:251:LEU:HD11	2.26	0.50
1:D:134:ARG:HE	1:D:138:LYS:HE3	1.76	0.50
1:C:141:LEU:O	1:C:144:ARG:NH1	2.45	0.49
1:A:154:ILE:HG12	1:A:260:TYR:HD1	1.77	0.49
1:B:83:PRO:HD3	1:C:255:ARG:HH22	1.77	0.49
1:D:227:GLU:O	1:D:231:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:LEU:HD22	1:D:256:THR:HG23	1.94	0.48
1:A:150:ARG:NH1	1:A:218:ASP:OD2	2.29	0.48
1:A:79:ARG:HG2	1:A:80:MET:HE2	1.94	0.47
1:B:120:GLN:O	1:B:124:VAL:HG22	2.14	0.47
1:A:143:LEU:HD12	1:A:144:ARG:N	2.30	0.47
1:D:159:ARG:NH2	1:D:254:GLU:OE1	2.32	0.47
1:D:256:THR:O	1:D:257:LEU:HD23	2.14	0.47
1:B:124:VAL:HG23	1:B:126:TRP:HZ3	1.80	0.47
1:D:194:VAL:HG13	1:D:203:ILE:HG12	1.97	0.47
1:A:140:ASP:OD1	1:A:142:SER:OG	2.27	0.47
1:D:190:PHE:CE1	1:D:207:GLN:HG3	2.50	0.46
1:C:146:ASP:OD1	1:C:146:ASP:N	2.49	0.46
1:A:206:ARG:HD2	5:A:405:HOH:O	2.16	0.46
1:A:161:ARG:HG3	1:A:254:GLU:OE2	2.16	0.46
1:B:107:ASP:H	1:B:118:GLN:HE22	1.62	0.46
1:B:153:HIS:HB3	1:B:261:LEU:HB3	1.97	0.46
1:B:197:GLU:HG3	1:C:89:LEU:HG	1.97	0.45
1:C:190:PHE:CE1	1:C:207:GLN:HG3	2.52	0.45
1:D:158:LEU:CD2	1:D:256:THR:HG23	2.46	0.45
1:C:175:GLU:OE2	1:C:178:ARG:NH2	2.48	0.45
1:C:121:GLN:HB2	1:C:124:VAL:HG23	1.98	0.45
1:A:264:ILE:HG23	1:A:265:PRO:HD2	1.99	0.45
1:B:86:ALA:HB1	1:B:89:LEU:HB2	2.00	0.44
1:C:35:THR:HB	1:C:237:GLN:HE22	1.82	0.44
1:A:79:ARG:O	1:D:159:ARG:NH1	2.50	0.44
1:B:149:VAL:HG12	1:B:262:ASP:HB3	1.99	0.44
1:B:181:ARG:HD2	5:B:402:HOH:O	2.18	0.44
1:B:190:PHE:CE1	1:B:207:GLN:HG3	2.53	0.44
1:C:123:SER:HA	1:C:141:LEU:CD2	2.47	0.44
1:D:152:HIS:HD2	1:D:263:GLU:HG3	1.82	0.44
1:B:197:GLU:OE2	1:C:88:THR:HB	2.17	0.43
1:C:80:MET:HE1	1:C:103:LEU:HD13	2.00	0.43
1:C:143:LEU:O	1:C:144:ARG:HD3	2.18	0.43
1:B:96:ALA:HB1	1:C:259:TYR:HB3	1.99	0.43
1:D:153:HIS:HB3	1:D:261:LEU:HB3	2.00	0.43
1:D:167:PHE:CE1	1:D:249:GLU:HB3	2.54	0.43
1:D:130:SER:HB3	1:D:150:ARG:HA	2.01	0.43
1:D:176:LEU:HD13	1:D:203:ILE:HD11	2.01	0.42
1:A:255:ARG:HG3	1:D:41:MET:HE1	2.01	0.42
1:C:161:ARG:HD2	1:C:254:GLU:OE2	2.18	0.42
1:A:62:MET:HE3	1:A:62:MET:HB3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:PHE:HE1	1:D:249:GLU:HB3	1.84	0.42
1:D:183:ARG:HA	1:D:183:ARG:HD3	1.82	0.42
1:D:176:LEU:HD12	1:D:194:VAL:HG11	2.01	0.41
1:A:190:PHE:CE1	1:A:207:GLN:HG3	2.54	0.41
1:C:167:PHE:HE1	1:C:249:GLU:HG2	1.84	0.41
1:A:40:LYS:HE2	1:A:234:SER:O	2.19	0.41
1:A:104:TYR:O	1:A:106:PRO:HD3	2.20	0.41
1:B:247:ARG:HD2	1:B:247:ARG:HA	1.87	0.41
1:D:184:TYR:CE2	1:D:226:PHE:HB2	2.56	0.41
1:A:176:LEU:HD22	1:A:203:ILE:HD11	2.02	0.40
1:A:266:PRO:HG3	1:D:97:LEU:HD11	2.02	0.40
1:B:43:VAL:O	1:B:55:CYS:HA	2.21	0.40
1:D:157:ASP:C	1:D:158:LEU:HD23	2.47	0.40
1:D:158:LEU:HD13	1:D:253:VAL:HG21	2.03	0.40
1:D:69:LEU:HD22	1:D:225:TYR:CE2	2.57	0.40
1:D:187:HIS:HB3	1:D:190:PHE:CD2	2.57	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	235/250 (94%)	225 (96%)	10 (4%)	0	100	100
1	B	236/250 (94%)	224 (95%)	12 (5%)	0	100	100
1	C	236/250 (94%)	228 (97%)	8 (3%)	0	100	100
1	D	235/250 (94%)	225 (96%)	10 (4%)	0	100	100
All	All	942/1000 (94%)	902 (96%)	40 (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	204/216 (94%)	201 (98%)	3 (2%)	57	83
1	B	205/216 (95%)	200 (98%)	5 (2%)	43	75
1	C	205/216 (95%)	203 (99%)	2 (1%)	68	88
1	D	204/216 (94%)	200 (98%)	4 (2%)	48	79
All	All	818/864 (95%)	804 (98%)	14 (2%)	53	81

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	THR
1	A	209	THR
1	A	255	ARG
1	B	33	ASN
1	B	34	CYS
1	B	140	ASP
1	B	168	ASN
1	B	247	ARG
1	C	34	CYS
1	C	257	LEU
1	D	37	PRO
1	D	120	GLN
1	D	130	SER
1	D	168	ASN

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

Mol	Chain	Res	Type
1	A	152	HIS
1	B	33	ASN
1	B	85	ASN
1	B	95	HIS
1	B	169	HIS

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Mol	Chain	Res	Type
1	C	237	GLN
1	D	54	GLN
1	D	85	ASN
1	D	120	GLN
1	D	169	HIS

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 ⓘ

6 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	E	1	2,1	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	1.21	3 (17%)
2	FUC	E	3	2	10,10,11	0.22	0	14,14,16	0.52	0
2	NAG	F	1	2,1	14,14,15	0.37	0	17,19,21	1.54	3 (17%)
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
2	FUC	F	3	2	10,10,11	0.20	0	14,14,16	0.51	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
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	4.84	129.39	122.90
2	E	2	NAG	C4-C3-C2	2.79	115.10	111.02
2	E	2	NAG	O5-C5-C4	-2.43	104.90	110.83
2	F	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	F	1	NAG	C1-C2-N2	2.15	113.82	110.43
2	E	2	NAG	C1-O5-C5	-2.12	109.35	112.19
2	F	1	NAG	O7-C7-N2	2.11	125.71	121.98
2	E	1	NAG	O5-C1-C2	-2.09	108.05	111.29
2	E	1	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

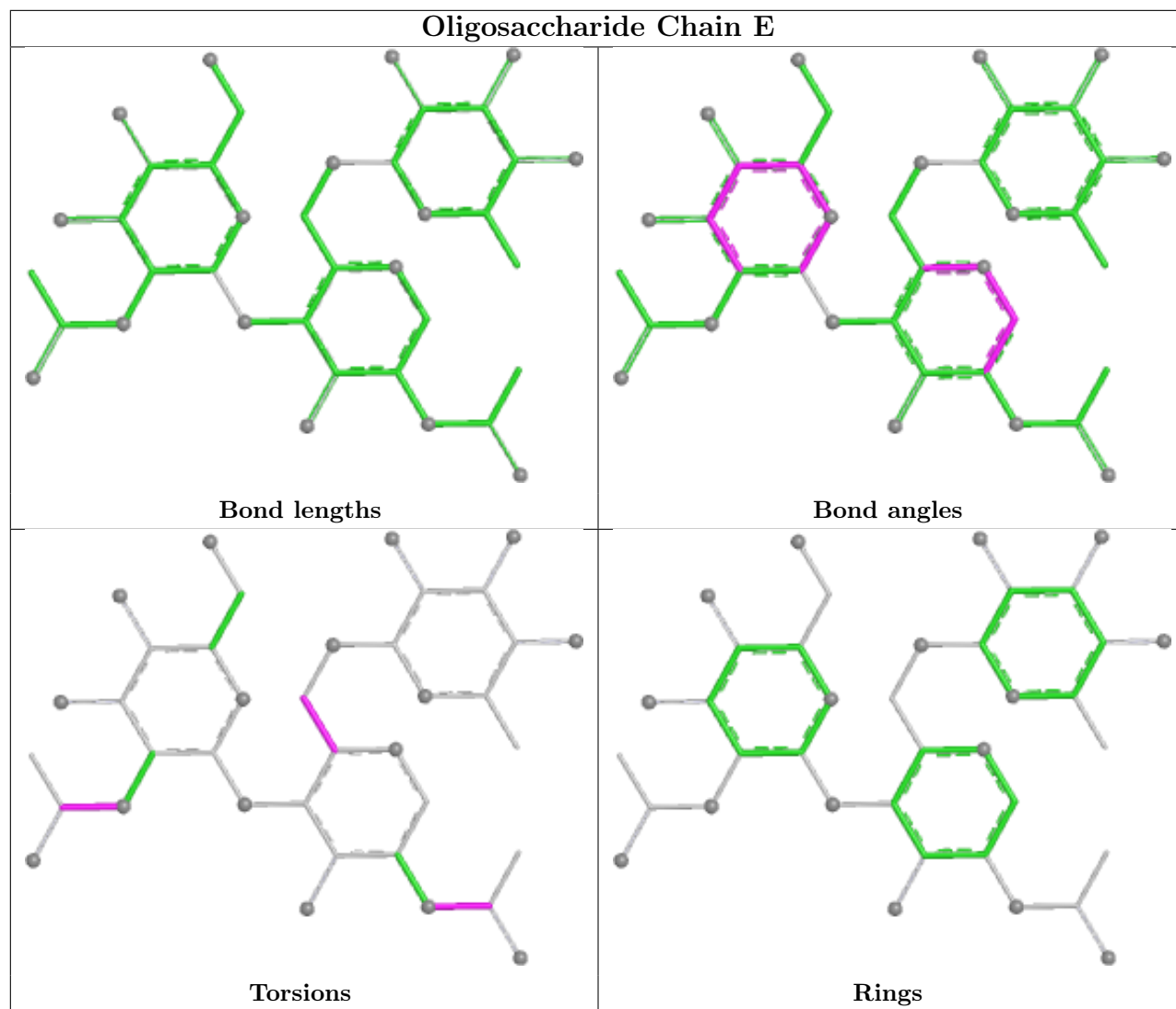
All (10) torsion outliers are listed below:

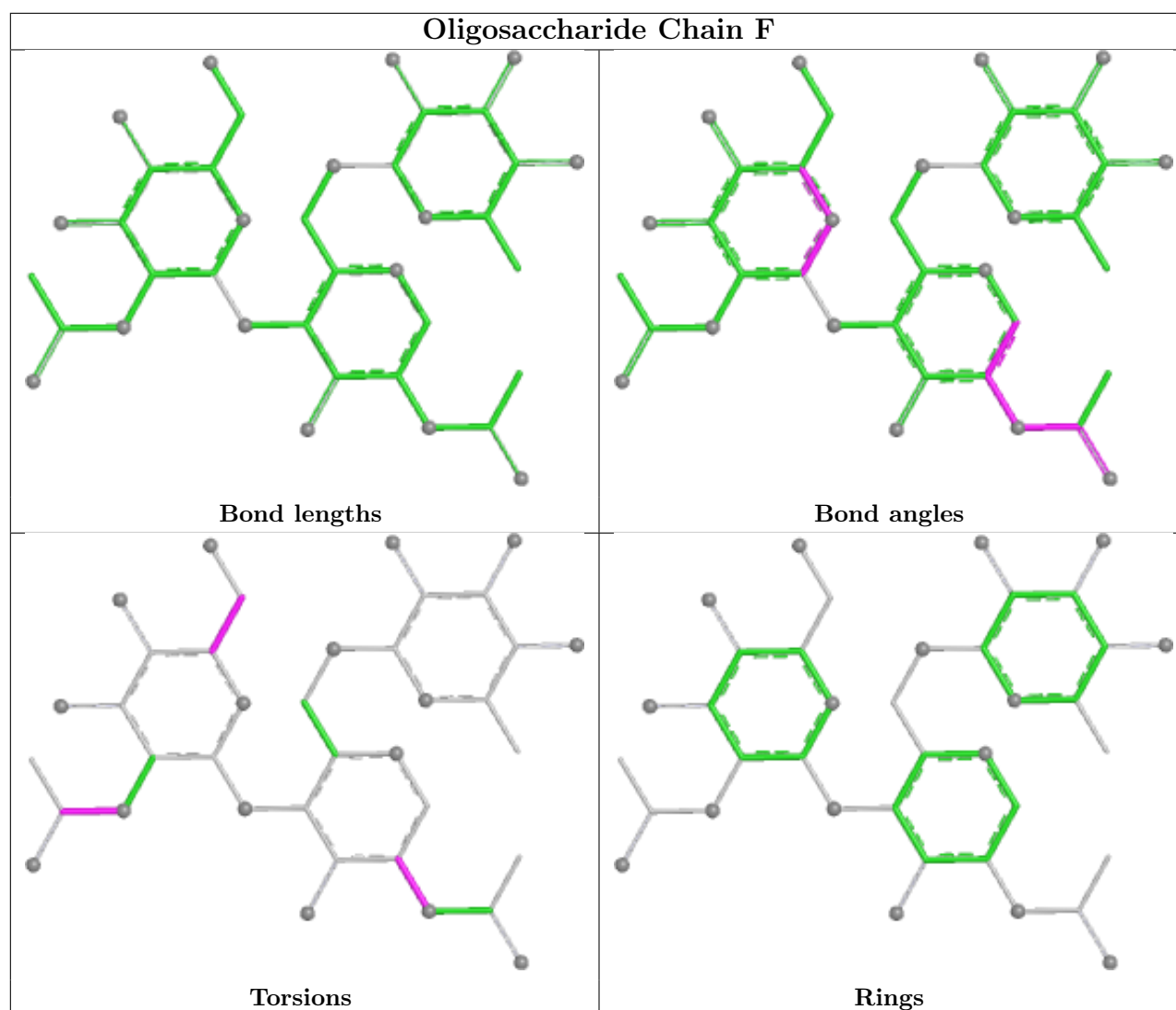
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C1-C2-N2-C7
2	F	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

4 ligands 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	SO4	A	301	-	4,4,4	0.44	0	6,6,6	0.11	0
4	NAG	D	301	1	14,14,15	0.49	0	17,19,21	0.61	0
3	SO4	B	301	-	4,4,4	0.42	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	301	1	14,14,15	0.41	0	17,19,21	0.92	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
4	NAG	D	301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	301	1	-	1/6/23/26	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(°)
4	C	301	NAG	C1-O5-C5	-2.18	109.27	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	NAG	O5-C5-C6-O6
4	D	301	NAG	O5-C5-C6-O6

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

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	237/250 (94%)	0.59	32 (13%) 7 5	38, 57, 127, 151	0
1	B	238/250 (95%)	0.83	29 (12%) 8 6	40, 62, 105, 137	0
1	C	238/250 (95%)	0.49	19 (7%) 18 13	34, 56, 102, 128	0
1	D	237/250 (94%)	2.05	109 (45%) 0 0	48, 104, 143, 160	0
All	All	950/1000 (95%)	0.99	189 (19%) 3 2	34, 68, 130, 160	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PRO	6.8
1	D	167	PHE	6.3
1	B	162	PRO	6.3
1	D	157	ASP	6.1
1	D	163	THR	5.9
1	D	251	LEU	5.6
1	D	188	PRO	5.5
1	D	202	GLN	5.0
1	D	162	PRO	5.0
1	B	86	ALA	4.8
1	D	165	GLY	4.8
1	B	163	THR	4.8
1	A	83	PRO	4.8
1	D	193	ALA	4.8
1	D	166	ALA	4.7
1	B	84	LYS	4.7
1	D	161	ARG	4.7
1	D	237	GLN	4.5
1	D	183	ARG	4.5
1	B	85	ASN	4.4
1	D	173	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	200	THR	4.3
1	D	170	SER	4.3
1	D	164	ALA	4.3
1	B	164	ALA	4.2
1	C	181	ARG	4.1
1	D	192	ALA	4.1
1	D	196	TYR	4.1
1	B	269	SER	4.1
1	C	32	ASP	4.0
1	A	86	ALA	3.9
1	D	226	PHE	3.9
1	D	194	VAL	3.9
1	D	199	PRO	3.9
1	B	102	GLY	3.8
1	A	90	VAL	3.8
1	D	172	LEU	3.8
1	D	169	HIS	3.7
1	C	164	ALA	3.7
1	D	204	GLU	3.7
1	D	179	LEU	3.6
1	D	208	GLN	3.6
1	D	252	GLN	3.6
1	D	268	PHE	3.6
1	D	259	TYR	3.6
1	D	242	LEU	3.6
1	D	189	LYS	3.5
1	A	84	LYS	3.5
1	D	250	PRO	3.5
1	D	195	HIS	3.5
1	D	187	HIS	3.5
1	D	203	ILE	3.4
1	C	122	THR	3.4
1	D	241	GLY	3.4
1	D	136	THR	3.4
1	C	162	PRO	3.3
1	D	263	GLU	3.3
1	D	230	ILE	3.3
1	D	206	ARG	3.3
1	A	88	THR	3.3
1	D	126	TRP	3.2
1	A	32	ASP	3.2
1	D	147	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	162	PRO	3.1
1	D	214	ALA	3.1
1	D	177	ARG	3.1
1	B	165	GLY	3.1
1	A	95	HIS	3.0
1	B	101	ASP	3.0
1	C	161	ARG	3.0
1	D	159	ARG	3.0
1	A	99	ASP	3.0
1	D	213	ALA	3.0
1	C	167	PHE	3.0
1	D	261	LEU	2.9
1	D	249	GLU	2.9
1	A	97	LEU	2.9
1	B	53	CYS	2.9
1	D	185	ARG	2.9
1	B	121	GLN	2.9
1	D	205	LEU	2.9
1	B	67	SER	2.8
1	D	266	PRO	2.8
1	D	262	ASP	2.8
1	C	211	GLN	2.8
1	D	53	CYS	2.8
1	D	124	VAL	2.8
1	D	260	TYR	2.8
1	D	135	ARG	2.7
1	D	254	GLU	2.7
1	D	148	LEU	2.7
1	D	176	LEU	2.7
1	D	184	TYR	2.7
1	B	96	ALA	2.7
1	D	240	GLY	2.7
1	A	268	PHE	2.7
1	A	125	CYS	2.7
1	C	84	LYS	2.7
1	A	33	ASN	2.7
1	D	239	ARG	2.7
1	B	146	ASP	2.7
1	D	267	LYS	2.7
1	A	94	GLU	2.7
1	D	247	ARG	2.6
1	B	240	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	246	VAL	2.6
1	D	174	ALA	2.6
1	D	160	HIS	2.6
1	D	215	GLY	2.6
1	B	100	ASN	2.6
1	A	87	ARG	2.6
1	B	135	ARG	2.6
1	D	178	ARG	2.6
1	C	240	GLY	2.6
1	C	209	THR	2.6
1	C	33	ASN	2.6
1	B	167	PHE	2.6
1	A	252	GLN	2.5
1	A	82	ALA	2.5
1	D	134	ARG	2.5
1	D	257	LEU	2.5
1	D	131	VAL	2.5
1	D	258	ILE	2.5
1	D	121	GLN	2.5
1	A	139	GLY	2.5
1	A	164	ALA	2.5
1	D	191	VAL	2.5
1	D	207	GLN	2.4
1	A	89	LEU	2.4
1	B	103	LEU	2.4
1	D	155	LEU	2.4
1	D	229	ASP	2.4
1	D	245	ARG	2.4
1	B	166	ALA	2.4
1	C	243	ASP	2.4
1	C	206	ARG	2.3
1	D	181	ARG	2.3
1	B	122	THR	2.3
1	C	248	GLY	2.3
1	A	96	ALA	2.3
1	D	127	CYS	2.3
1	A	120	GLN	2.3
1	B	95	HIS	2.3
1	D	190	PHE	2.3
1	D	182	GLU	2.3
1	C	138	LYS	2.3
1	D	138	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	219	ILE	2.3
1	A	85	ASN	2.3
1	D	180	PHE	2.3
1	B	82	ALA	2.3
1	D	175	GLU	2.3
1	D	137	ASP	2.3
1	D	115	LYS	2.3
1	A	93	SER	2.3
1	D	209	THR	2.3
1	D	120	GLN	2.2
1	B	161	ARG	2.2
1	C	159	ARG	2.2
1	A	240	GLY	2.2
1	D	116	ALA	2.2
1	A	100	ASN	2.2
1	D	158	LEU	2.2
1	D	156	ILE	2.2
1	D	256	THR	2.2
1	A	102	GLY	2.2
1	A	117	ARG	2.2
1	C	163	THR	2.2
1	D	243	ASP	2.2
1	D	264	ILE	2.1
1	A	198	GLN	2.1
1	D	84	LYS	2.1
1	B	249	GLU	2.1
1	D	171	ASP	2.1
1	B	123	SER	2.1
1	D	119	CYS	2.1
1	A	98	VAL	2.1
1	D	41	MET	2.1
1	D	212	LYS	2.1
1	A	101	ASP	2.1
1	D	111	GLU	2.1
1	C	160	HIS	2.1
1	A	92	PRO	2.1
1	B	143	LEU	2.1
1	D	150	ARG	2.1
1	D	44	CYS	2.0
1	D	218	ASP	2.0
1	D	255	ARG	2.0
1	D	32	ASP	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](#)

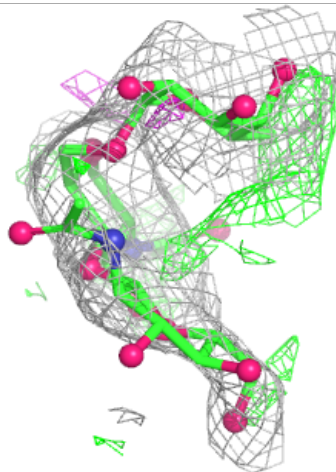
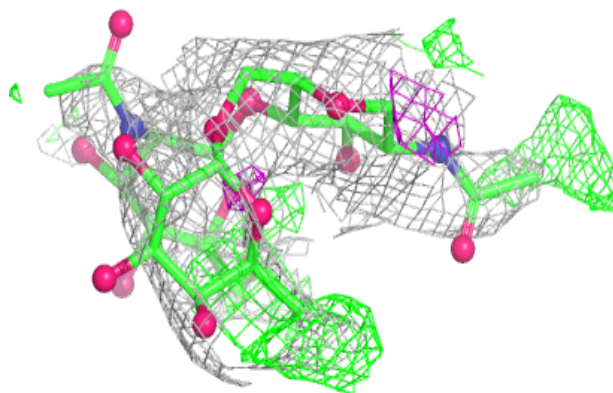
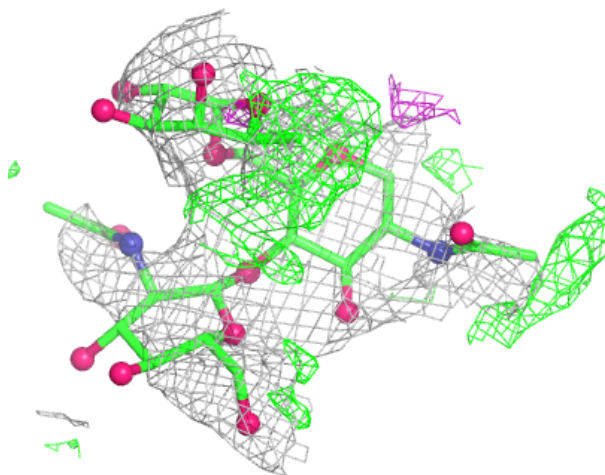
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

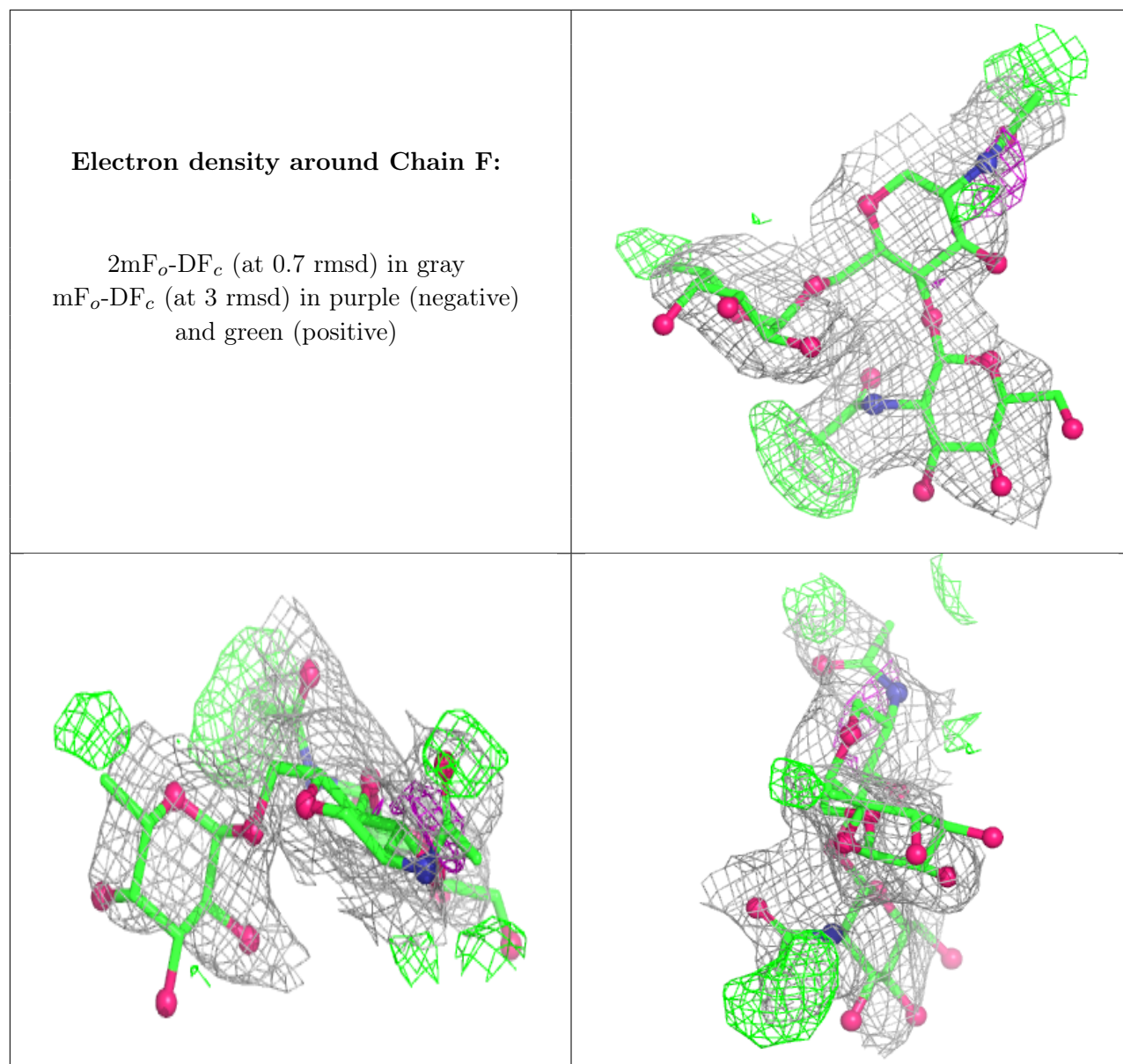
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	E	3	10/11	-0.06	0.28	136,144,148,152	0
2	FUC	F	3	10/11	0.16	0.24	124,136,145,145	0
2	NAG	F	2	14/15	0.18	0.26	121,126,130,130	0
2	NAG	E	2	14/15	0.41	0.31	124,134,140,140	0
2	NAG	E	1	14/15	0.61	0.22	102,122,127,138	0
2	NAG	F	1	14/15	0.74	0.20	83,98,123,131	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.

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
4	NAG	D	301	14/15	0.14	0.23	139,153,157,158	0
4	NAG	C	301	14/15	0.44	0.22	113,125,128,128	0
3	SO4	A	301	5/5	0.90	0.19	70,72,76,87	0
3	SO4	B	301	5/5	0.90	0.15	72,72,78,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.