



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 AM UTC

PDB ID : 6VT2 / pdb_00006vt2
Title : Sialic acid binding region of Streptococcus sanguinis SK1 adhesin bound to sTa
Authors : Stubbs, H.E.; Iverson, T.M.
Deposited on : 2020-02-12
Resolution : 1.52 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

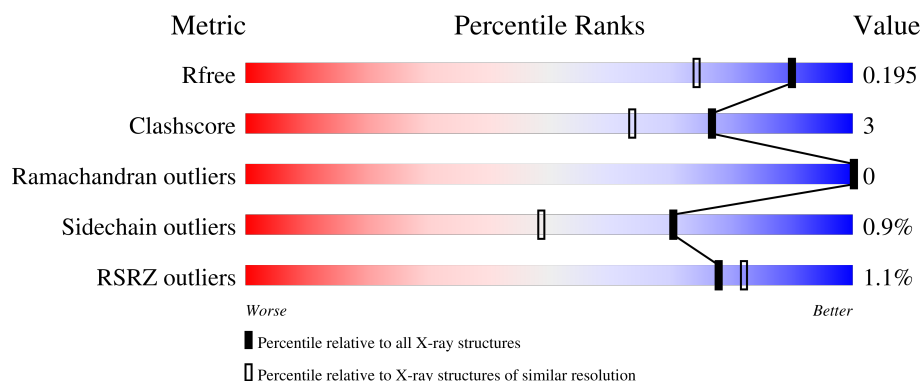
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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.



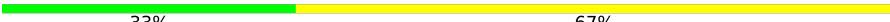
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	409	79% 19% .
1	E	409	81% 19%
2	C	3	33% 33% 33%
2	D	3	33% 33% 33%
2	F	3	33% 67%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	706	-	-	X	-

2 Entry composition [i](#)

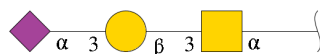
There are 6 unique types of molecules in this entry. The entry contains 14469 atoms, of which 6220 are hydrogens and 0 are deuteriums.

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 Adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	H	N	O	0	16	0
			6264	1976	3078	553	657			
1	E	409	Total	C	H	N	O	0	19	0
			6342	1990	3134	564	654			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.

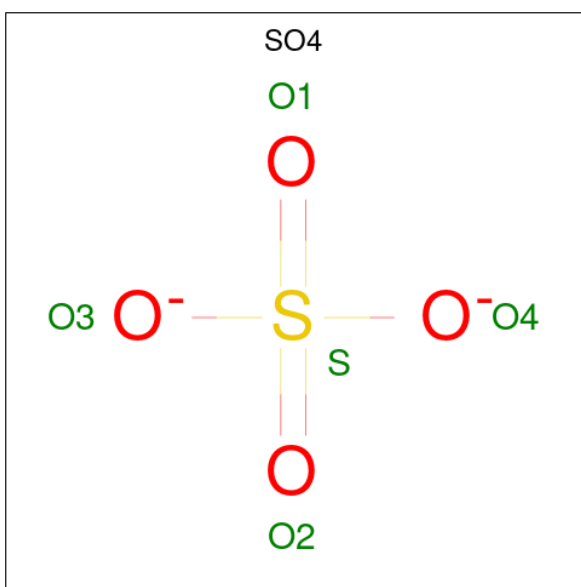


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	C	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	D	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	F	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

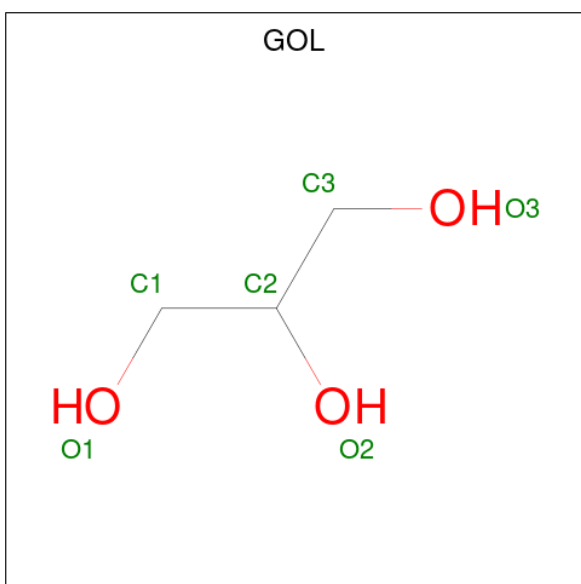
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	E	4	Total	Ca	0	0
			4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	H	O	0	0
			14	3	8	3		

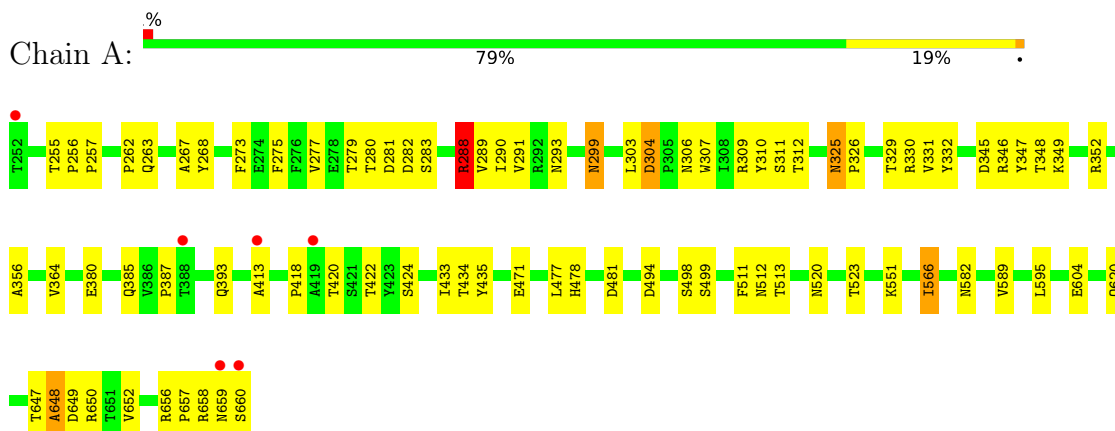
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	818	Total	O	0	0
			818	818		
6	E	814	Total	O	0	0
			814	814		

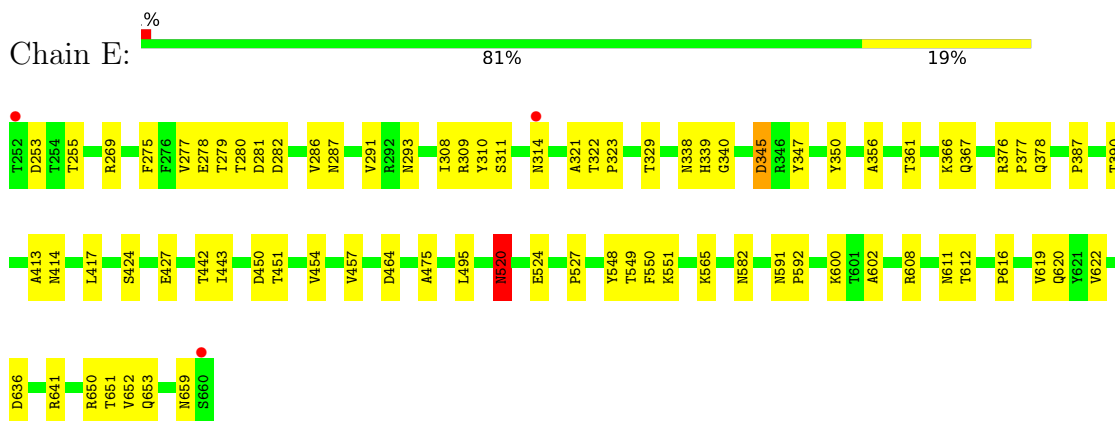
3 Residue-property plots

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: Adhesin



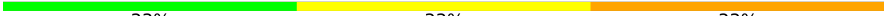
- Molecule 1: Adhesin



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

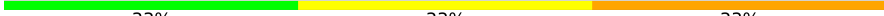


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain C:  33% 33% 33%

A2G1
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain D:  33% 33% 33%

A2G1
GAL2
SIA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain F:  33% 67%

A2G1
GAL2
SIA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.21Å 269.86Å 47.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.66 – 1.52 35.66 – 1.52	Depositor EDS
% Data completeness (in resolution range)	91.2 (35.66-1.52) 91.2 (35.66-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.177 , 0.193 0.177 , 0.195	Depositor DCC
R_{free} test set	7382 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14469	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.61% 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: SIA, A2G, SO4, GAL, GOL, CA

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	1.50	77/3324 (2.3%)	1.11	16/4558 (0.4%)
1	E	1.51	70/3356 (2.1%)	1.09	10/4599 (0.2%)
All	All	1.51	147/6680 (2.2%)	1.10	26/9157 (0.3%)

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	THR	C-O	-19.14	1.02	1.24
1	E	454	VAL	C-O	-16.94	1.05	1.24
1	E	255[A]	THR	C-O	-16.04	1.05	1.24
1	E	255[B]	THR	C-O	-16.04	1.05	1.24
1	A	435	TYR	C-N	12.20	1.48	1.33
1	E	620[A]	GLN	C-O	-11.43	1.09	1.24
1	E	620[B]	GLN	C-O	-11.43	1.09	1.24
1	E	622	VAL	C-O	-10.76	1.12	1.24
1	A	279	THR	C-O	-10.37	1.12	1.24
1	E	347	TYR	C-O	-9.96	1.12	1.23
1	A	277	VAL	C-O	-9.95	1.12	1.24
1	A	513	THR	C-N	9.93	1.46	1.34
1	E	377	PRO	C-O	-9.22	1.13	1.23
1	A	275	PHE	C-O	-9.01	1.12	1.23
1	E	280[A]	THR	C-O	-8.85	1.12	1.23
1	E	280[B]	THR	C-O	-8.85	1.12	1.23
1	E	279	THR	C-O	-8.58	1.12	1.24
1	A	304	ASP	C-O	-8.49	1.15	1.24
1	E	293	ASN	C-O	-8.36	1.13	1.23
1	A	262	PRO	C-O	-8.21	1.14	1.23
1	E	652	VAL	C-O	-8.10	1.15	1.24
1	A	331	VAL	C-O	-8.02	1.15	1.24
1	E	322	THR	C-O	-7.92	1.15	1.23
1	E	367	GLN	C-O	-7.91	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	TYR	C-O	-7.91	1.15	1.23
1	E	527	PRO	C-O	-7.71	1.14	1.23
1	A	280[A]	THR	C-O	-7.70	1.14	1.23
1	A	280[B]	THR	C-O	-7.70	1.14	1.23
1	E	277	VAL	C-O	-7.64	1.15	1.24
1	A	289[A]	VAL	C-O	-7.59	1.16	1.24
1	A	289[B]	VAL	C-O	-7.59	1.16	1.24
1	A	566	ILE	C-O	-7.56	1.14	1.24
1	A	332	TYR	C-O	-7.46	1.15	1.23
1	A	422	THR	C-O	-7.42	1.14	1.23
1	E	275	PHE	C-O	-7.35	1.14	1.23
1	A	346	ARG	C-O	-7.33	1.14	1.23
1	A	256	PRO	C-O	-7.25	1.16	1.24
1	E	278[A]	GLU	N-CA	7.06	1.54	1.46
1	E	278[B]	GLU	N-CA	7.06	1.54	1.46
1	E	387	PRO	C-O	-6.94	1.15	1.24
1	A	293	ASN	C-O	-6.88	1.15	1.23
1	A	280[A]	THR	N-CA	6.88	1.55	1.45
1	A	280[B]	THR	N-CA	6.88	1.55	1.45
1	E	592	PRO	C-O	-6.82	1.15	1.24
1	A	471	GLU	C-N	-6.82	1.24	1.33
1	E	323	PRO	C-O	-6.81	1.15	1.24
1	A	290	ILE	C-O	-6.74	1.17	1.24
1	E	314	ASN	C-O	-6.73	1.15	1.23
1	E	350	TYR	C-O	-6.73	1.15	1.24
1	A	523	THR	C-O	-6.67	1.15	1.23
1	A	352	ARG	C-O	-6.67	1.15	1.23
1	A	289[A]	VAL	N-CA	6.65	1.54	1.46
1	A	289[B]	VAL	N-CA	6.65	1.54	1.46
1	E	443[A]	ILE	N-CA	6.64	1.54	1.46
1	E	443[B]	ILE	N-CA	6.64	1.54	1.46
1	A	511	PHE	C-O	-6.57	1.16	1.24
1	E	339	HIS	CE1-NE2	-6.57	1.25	1.32
1	E	376	ARG	C-O	-6.55	1.17	1.24
1	E	457	VAL	C-O	-6.50	1.17	1.24
1	E	651[A]	THR	C-O	-6.42	1.15	1.24
1	E	651[B]	THR	C-O	-6.42	1.15	1.24
1	A	433	ILE	C-O	-6.34	1.17	1.24
1	A	326	PRO	C-O	-6.33	1.16	1.23
1	A	309	ARG	C-O	-6.33	1.15	1.23
1	A	364	VAL	C-O	-6.30	1.17	1.24
1	A	424	SER	C-O	-6.27	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	329	THR	C-O	-6.23	1.16	1.24
1	A	267[A]	ALA	N-CA	6.22	1.53	1.46
1	A	267[B]	ALA	N-CA	6.22	1.53	1.46
1	E	600	LYS	C-O	-6.20	1.16	1.24
1	A	291	VAL	C-O	-6.19	1.17	1.24
1	E	591	ASN	C-O	-6.19	1.18	1.24
1	E	549	THR	C-O	-6.18	1.16	1.24
1	A	282	ASP	C-O	-6.16	1.16	1.24
1	E	551	LYS	C-O	-6.15	1.17	1.24
1	E	345	ASP	C-O	-6.10	1.17	1.23
1	A	349	LYS	C-O	-6.09	1.16	1.23
1	E	602	ALA	C-O	-6.08	1.17	1.24
1	E	280[A]	THR	N-CA	6.08	1.53	1.45
1	E	280[B]	THR	N-CA	6.08	1.53	1.45
1	A	393	GLN	N-CA	6.06	1.53	1.46
1	E	653	GLN	C-O	-6.05	1.17	1.24
1	E	424	SER	C-O	-6.02	1.16	1.23
1	A	595	LEU	C-O	-6.00	1.16	1.23
1	A	325	ASN	C-O	-5.99	1.17	1.24
1	A	288	ARG	C-O	-5.97	1.17	1.23
1	E	340	GLY	C-O	-5.94	1.15	1.23
1	A	303	LEU	C-O	-5.90	1.17	1.23
1	A	413	ALA	C-O	-5.90	1.16	1.24
1	A	311	SER	C-O	-5.89	1.16	1.23
1	A	348	THR	C-O	-5.87	1.16	1.24
1	A	283	SER	C-O	-5.86	1.16	1.24
1	E	550	PHE	C-O	-5.84	1.16	1.23
1	E	378	GLN	C-O	-5.83	1.16	1.24
1	A	312	THR	C-O	-5.82	1.17	1.24
1	E	611	ASN	C-O	-5.79	1.16	1.24
1	A	330	ARG	C-O	-5.77	1.17	1.24
1	A	307	TRP	C-O	-5.76	1.16	1.24
1	E	310	TYR	C-O	-5.72	1.16	1.23
1	A	657	PRO	C-O	-5.70	1.16	1.23
1	E	548	TYR	C-O	-5.67	1.17	1.24
1	A	306	ASN	C-O	-5.67	1.16	1.24
1	E	269	ARG	C-O	-5.66	1.17	1.23
1	A	434	THR	C-O	-5.64	1.17	1.24
1	E	286	VAL	C-O	-5.63	1.18	1.24
1	E	291	VAL	C-O	-5.59	1.18	1.24
1	A	648	ALA	C-O	-5.57	1.17	1.24
1	E	524	GLU	C-O	-5.56	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	450	ASP	C-O	-5.55	1.17	1.23
1	E	309	ARG	C-O	-5.54	1.16	1.23
1	E	464	ASP	C-O	-5.52	1.17	1.24
1	A	268	TYR	C-O	-5.51	1.17	1.23
1	A	512[A]	ASN	C-O	5.51	1.30	1.24
1	A	512[B]	ASN	C-O	5.51	1.30	1.24
1	E	475	ALA	C-O	-5.50	1.17	1.24
1	E	311	SER	C-O	-5.49	1.17	1.23
1	A	513	THR	C-O	-5.46	1.18	1.24
1	A	498	SER	C-O	-5.45	1.17	1.24
1	A	281	ASP	C-O	-5.38	1.17	1.23
1	E	321	ALA	C-O	-5.38	1.15	1.23
1	E	287[A]	ASN	N-CA	5.33	1.53	1.46
1	E	287[B]	ASN	N-CA	5.33	1.53	1.46
1	E	390	THR	C-O	-5.33	1.17	1.24
1	A	656	ARG	C-O	-5.32	1.17	1.24
1	A	310	TYR	C-O	-5.31	1.17	1.23
1	E	282	ASP	C-O	-5.30	1.17	1.24
1	A	435	TYR	C-O	-5.26	1.17	1.23
1	A	649	ASP	C-O	-5.26	1.17	1.24
1	A	647	THR	C-O	-5.24	1.16	1.23
1	E	338	ASN	C-O	-5.22	1.17	1.24
1	A	329	THR	C-O	-5.21	1.17	1.24
1	A	418	PRO	C-O	-5.20	1.17	1.23
1	A	267[A]	ALA	C-O	-5.14	1.18	1.24
1	A	267[B]	ALA	C-O	-5.14	1.18	1.24
1	A	273	PHE	C-O	-5.13	1.17	1.23
1	E	308	ILE	C-O	-5.13	1.18	1.24
1	E	281	ASP	C-O	-5.12	1.17	1.23
1	A	620	GLN	C-O	-5.11	1.17	1.24
1	A	478[A]	HIS	N-CA	5.11	1.52	1.46
1	A	478[B]	HIS	N-CA	5.11	1.52	1.46
1	E	361	THR	C-O	-5.07	1.17	1.23
1	E	253	ASP	C-O	-5.06	1.18	1.24
1	A	299	ASN	C-O	-5.04	1.17	1.24
1	E	255[A]	THR	N-CA	5.03	1.54	1.45
1	E	255[B]	THR	N-CA	5.03	1.54	1.45
1	A	481	ASP	CG-OD1	-5.03	1.15	1.25
1	A	257	PRO	C-O	-5.01	1.17	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	THR	O-C-N	-8.62	113.61	121.37
1	A	435	TYR	O-C-N	-8.09	112.47	121.53
1	E	520	ASN	CA-CB-CG	-6.91	105.69	112.60
1	E	443[A]	ILE	N-CA-C	-6.73	97.93	107.75
1	E	443[B]	ILE	N-CA-C	-6.73	97.93	107.75
1	A	435	TYR	CA-C-O	6.32	127.96	120.88
1	A	658	ARG	CB-CA-C	6.05	119.86	109.51
1	E	451	THR	CA-C-N	-5.85	114.41	122.30
1	E	451	THR	C-N-CA	-5.85	114.41	122.30
1	A	288	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	477	LEU	CA-C-N	-5.79	113.34	122.73
1	A	477	LEU	C-N-CA	-5.79	113.34	122.73
1	E	277	VAL	CA-C-N	-5.75	114.89	122.99
1	E	277	VAL	C-N-CA	-5.75	114.89	122.99
1	E	442	THR	CA-C-N	-5.36	115.98	123.10
1	E	442	THR	C-N-CA	-5.36	115.98	123.10
1	A	512[A]	ASN	CA-C-O	5.30	125.86	120.24
1	A	512[B]	ASN	CA-C-O	5.30	125.86	120.24
1	A	288	ARG	CG-CD-NE	5.21	123.45	112.00
1	A	304	ASP	CB-CA-C	5.20	117.13	109.22
1	A	435	TYR	CA-C-N	5.16	124.82	119.56
1	A	435	TYR	C-N-CA	5.16	124.82	119.56
1	A	494	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	512[A]	ASN	O-C-N	-5.11	117.29	123.27
1	A	512[B]	ASN	O-C-N	-5.11	117.29	123.27
1	E	524	GLU	N-CA-C	-5.07	105.75	111.28

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	3186	3078	3018	19	4
1	E	3208	3134	3043	15	4
2	C	46	0	37	1	0
2	D	46	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	46	0	37	0	0
2	K	46	0	37	0	0
3	A	4	0	0	0	0
3	E	4	0	0	0	0
4	A	10	0	0	6	1
4	E	15	0	0	0	0
5	E	6	8	8	0	0
6	A	818	0	0	14	6
6	E	814	0	0	9	6
All	All	8249	6220	6217	38	13

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 3.

All (38) 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:604:GLU:HG2	6:A:845:HOH:O	1.53	1.07
1:E:650[A]:ARG:NH1	6:E:1501:HOH:O	1.93	1.00
4:A:706:SO4:S	6:A:801:HOH:O	2.21	0.98
4:A:706:SO4:O3	6:A:801:HOH:O	1.86	0.93
1:A:604:GLU:CG	6:A:845:HOH:O	2.12	0.89
1:E:366:LYS:NZ	6:E:1502:HOH:O	2.17	0.70
1:A:387:PRO:O	6:A:802:HOH:O	2.12	0.66
1:E:636:ASP:OD1	1:E:641[B]:ARG:HD3	1.97	0.65
1:A:604:GLU:CD	6:A:845:HOH:O	2.41	0.59
4:A:706:SO4:O4	6:A:801:HOH:O	2.14	0.58
1:E:413:ALA:O	6:E:1503:HOH:O	2.17	0.58
1:A:288:ARG:HH21	1:A:288:ARG:HG2	1.68	0.58
1:A:288:ARG:NH2	4:A:706:SO4:O3	2.39	0.56
1:E:366:LYS:NZ	6:E:1504:HOH:O	2.20	0.54
1:E:565[A]:LYS:HG2	6:E:1509:HOH:O	2.08	0.53
1:A:288:ARG:NH2	4:A:706:SO4:S	2.67	0.53
1:A:551:LYS:HG2	1:A:566:ILE:HD13	1.92	0.51
1:A:380:GLU:OE2	6:A:803:HOH:O	2.18	0.51
1:A:520:ASN:ND2	6:A:820:HOH:O	2.45	0.50
1:E:427:GLU:HG3	6:E:1611:HOH:O	2.13	0.49
1:E:356:ALA:HB3	6:E:1589:HOH:O	2.12	0.48
1:A:345:ASP:HA	2:C:3:SIA:H113	1.96	0.47
1:A:648:ALA:O	1:A:652[B]:VAL:HG22	2.15	0.47
1:A:356:ALA:HB3	6:A:869:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASN:CG	1:A:650:ARG:HD2	2.40	0.47
1:E:520:ASN:CG	6:E:1505:HOH:O	2.59	0.46
1:E:345:ASP:HA	2:D:3:SIA:H113	1.98	0.45
1:A:325:ASN:ND2	6:A:830:HOH:O	2.49	0.45
1:E:616:PRO:HD2	1:E:619[B]:VAL:CG2	2.48	0.44
1:A:589:VAL:CG2	1:A:652[A]:VAL:HG13	2.48	0.43
1:E:414:ASN:HB3	1:E:417:LEU:HG	2.02	0.42
1:E:608[A]:ARG:O	1:E:612:THR:HG23	2.19	0.42
1:A:499:SER:OG	6:A:805:HOH:O	2.21	0.42
1:A:385:GLN:NE2	6:A:811:HOH:O	2.38	0.42
4:A:706:SO4:O4	6:A:804:HOH:O	2.20	0.41
1:E:582:ASN:OD1	1:E:650[A]:ARG:HD3	2.20	0.41
1:E:650[B]:ARG:NH2	6:E:1536:HOH:O	2.53	0.41
1:A:288:ARG:HH21	1:A:288:ARG:CG	2.34	0.40

All (13) 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)
6:A:1434:HOH:O	6:A:1581:HOH:O[1_554]	1.52	0.68
1:A:660:SER:CA	6:E:2081:HOH:O[1_556]	1.84	0.36
1:A:659:ASN:OD1	1:E:659:ASN:OD1[1_556]	1.93	0.27
6:A:1357:HOH:O	6:A:1579:HOH:O[2_765]	1.97	0.23
6:A:1491:HOH:O	6:E:2296:HOH:O[4_556]	1.98	0.22
6:E:1536:HOH:O	6:E:1962:HOH:O[2_765]	1.98	0.22
1:A:299:ASN:O	1:E:608[B]:ARG:NH2[4_555]	2.04	0.16
6:A:1466:HOH:O	6:A:1510:HOH:O[2_765]	2.04	0.16
6:E:1536:HOH:O	6:E:2081:HOH:O[2_765]	2.13	0.07
6:A:1431:HOH:O	6:E:2010:HOH:O[2_765]	2.14	0.06
6:A:830:HOH:O	6:E:1978:HOH:O[4_556]	2.16	0.04
1:A:299:ASN:O	1:E:608[B]:ARG:HH22[4_555]	1.59	0.01
1:E:612:THR:CG2	4:A:706:SO4:O1[4_455]	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	A	423/409 (103%)	416 (98%)	7 (2%)	0	100	100
1	E	426/409 (104%)	420 (99%)	6 (1%)	0	100	100
All	All	849/818 (104%)	836 (98%)	13 (2%)	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	362/349 (104%)	358 (99%)	4 (1%)	65	40
1	E	368/349 (105%)	366 (100%)	2 (0%)	81	66
All	All	730/698 (105%)	724 (99%)	6 (1%)	70	53

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	288	ARG
1	A	304	ASP
1	A	420	THR
1	E	495	LEU
1	E	520	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
1	A	400	GLN
1	A	502	ASN
1	A	520	ASN

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Mol	Chain	Res	Type
1	E	263	GLN
1	E	385	GLN
1	E	624	ASN

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 ⓘ

12 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	A2G	C	1	2	15,15,15	0.42	0	21,21,21	1.14	2 (9%)
2	GAL	C	2	2	11,11,12	0.58	0	15,15,17	0.84	0
2	SIA	C	3	2	20,20,21	1.63	2 (10%)	21,28,31	1.25	3 (14%)
2	A2G	D	1	2	15,15,15	0.38	0	21,21,21	1.25	2 (9%)
2	GAL	D	2	2	11,11,12	0.67	0	15,15,17	0.82	0
2	SIA	D	3	2	20,20,21	1.73	2 (10%)	21,28,31	1.49	3 (14%)
2	A2G	F	1	2	15,15,15	0.46	0	21,21,21	1.24	3 (14%)
2	GAL	F	2	2	11,11,12	0.58	0	15,15,17	0.84	0
2	SIA	F	3	2	20,20,21	1.60	1 (5%)	21,28,31	1.36	3 (14%)
2	A2G	K	1	2	15,15,15	0.42	0	21,21,21	1.35	2 (9%)
2	GAL	K	2	2	11,11,12	0.59	0	15,15,17	0.89	0
2	SIA	K	3	2	20,20,21	1.67	1 (5%)	21,28,31	1.47	2 (9%)

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	A2G	C	1	2	-	0/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	SIA	C	3	2	-	0/18/34/38	0/1/1/1
2	A2G	D	1	2	-	0/6/26/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	A2G	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	SIA	F	3	2	-	0/18/34/38	0/1/1/1
2	A2G	K	1	2	-	0/6/26/26	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	SIA	K	3	2	-	0/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	C2-C1	6.28	1.59	1.52
2	K	3	SIA	C2-C1	6.01	1.59	1.52
2	F	3	SIA	C2-C1	5.94	1.59	1.52
2	C	3	SIA	C2-C1	5.88	1.59	1.52
2	D	3	SIA	C7-C6	2.35	1.55	1.52
2	C	3	SIA	C7-C6	2.11	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	A2G	C1-C2-N2	-4.85	105.11	110.73
2	D	3	SIA	O1A-C1-C2	-4.28	113.61	122.85
2	K	3	SIA	O1A-C1-C2	-4.11	113.96	122.85
2	D	1	A2G	C1-C2-N2	-3.94	106.17	110.73
2	F	1	A2G	C1-C2-N2	-3.53	106.64	110.73
2	C	1	A2G	C1-C2-N2	-3.41	106.78	110.73
2	D	1	A2G	C3-C2-N2	-3.18	104.76	110.62
2	F	3	SIA	O6-C2-C3	-3.13	106.35	110.56
2	C	1	A2G	C3-C2-N2	-2.97	105.14	110.62
2	K	3	SIA	O6-C2-C3	-2.93	106.62	110.56
2	F	3	SIA	O1A-C1-C2	-2.89	116.61	122.85
2	C	3	SIA	O6-C2-C3	-2.75	106.86	110.56
2	D	3	SIA	O6-C2-C3	-2.74	106.87	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	A2G	C3-C2-N2	-2.67	105.70	110.62
2	C	3	SIA	O1A-C1-C2	-2.64	117.15	122.85
2	F	3	SIA	O1B-C1-O1A	2.35	129.41	124.08
2	C	3	SIA	O1B-C1-O1A	2.34	129.40	124.08
2	D	3	SIA	O1B-C1-O1A	2.09	128.83	124.08
2	K	1	A2G	C2-N2-C7	-2.07	118.25	123.11
2	F	1	A2G	C6-C5-C4	-2.04	108.00	113.02

There are no chirality outliers.

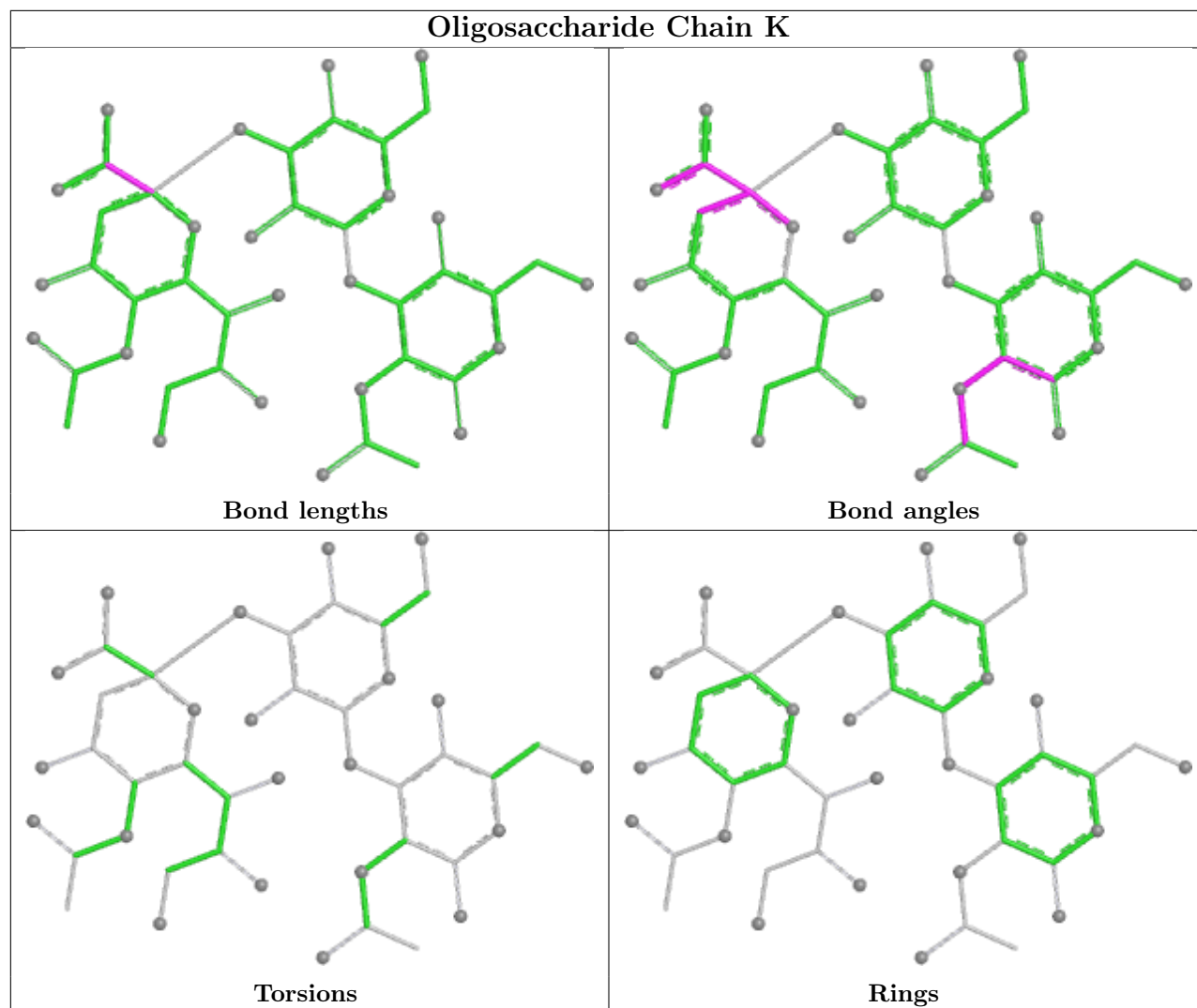
There are no torsion outliers.

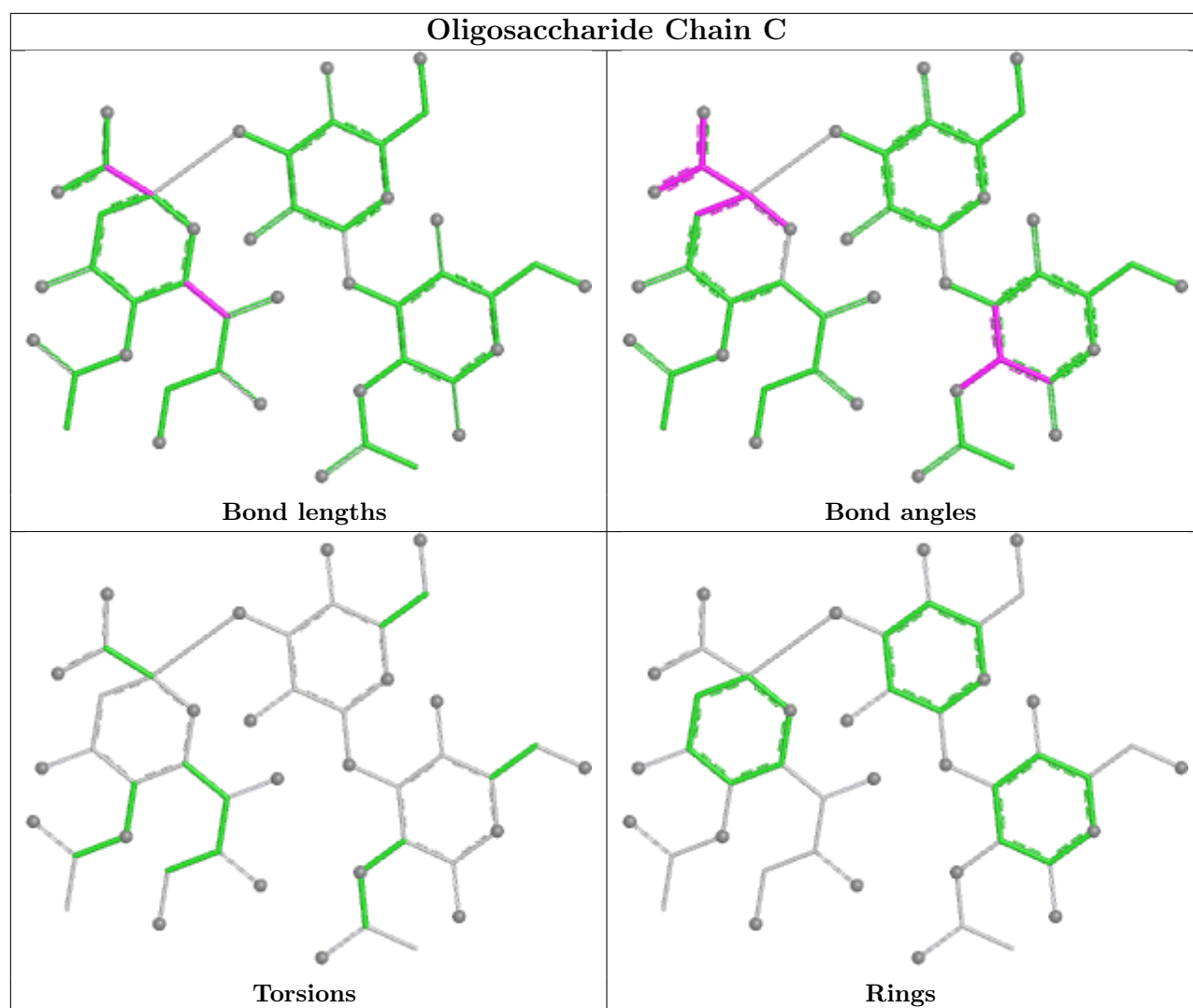
There are no ring outliers.

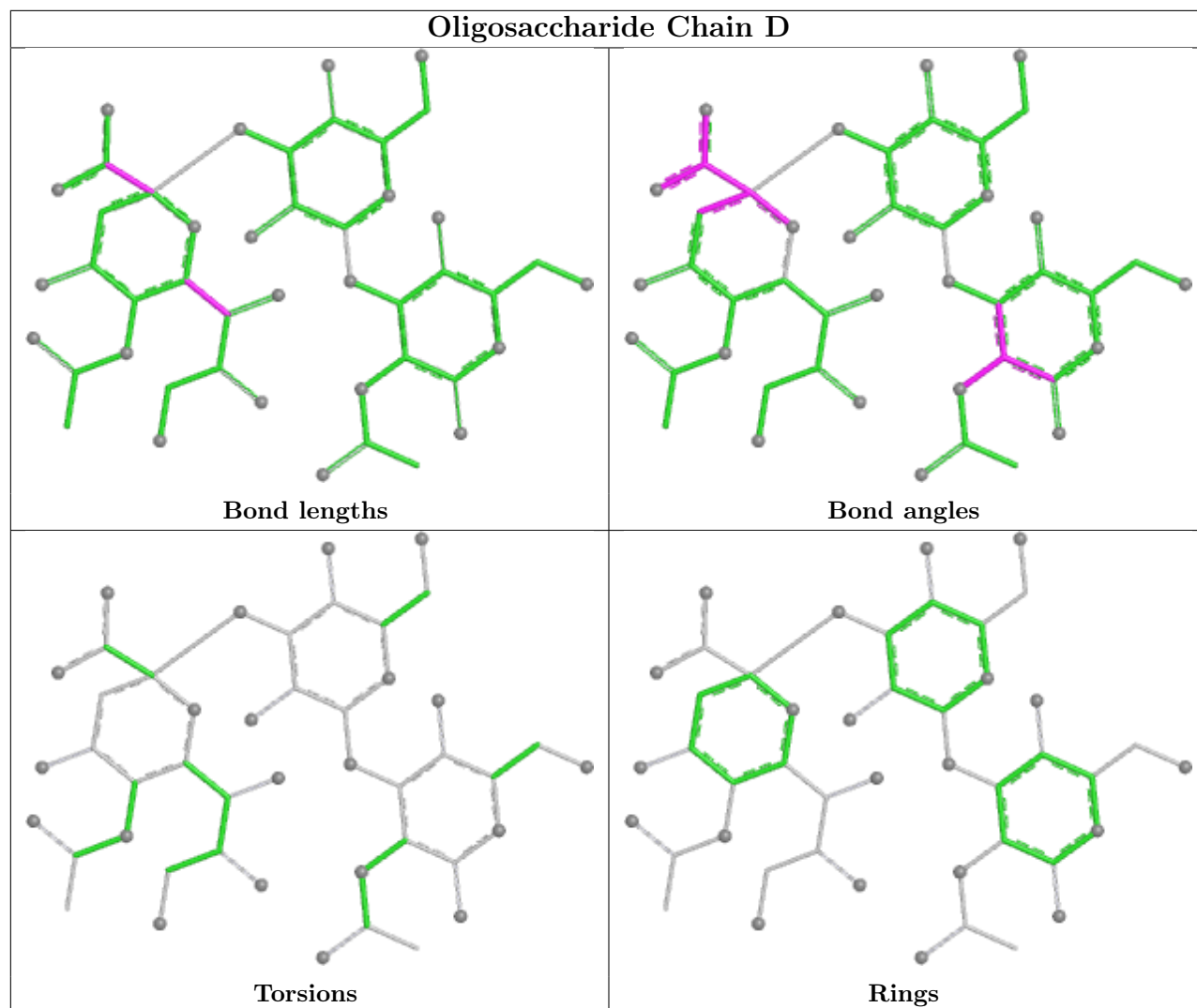
2 monomers are involved in 2 short contacts:

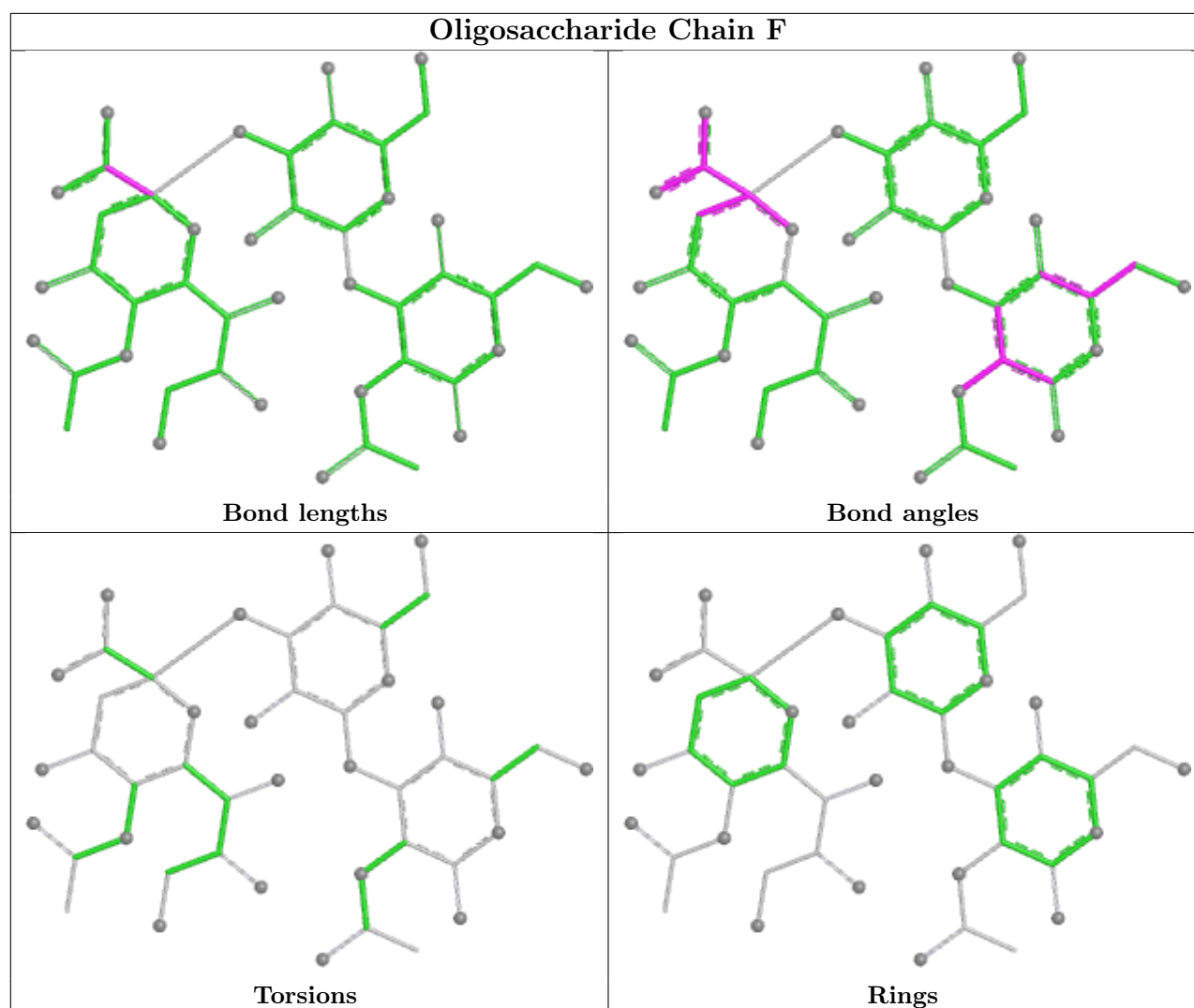
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	SIA	1	0
2	C	3	SIA	1	0

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









5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	705	-	4,4,4	0.19	0	6,6,6	0.56	0
4	SO4	E	1407	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	E	1406	-	4,4,4	0.49	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	1408	-	4,4,4	0.53	0	6,6,6	0.59	0
5	GOL	E	1401	-	5,5,5	1.50	0	5,5,5	0.81	0
4	SO4	A	706	-	4,4,4	0.79	0	6,6,6	0.49	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	GOL	E	1401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1401	GOL	C1-C2-C3-O3
5	E	1401	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	SO4	6	1

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	409/409 (100%)	-0.18	6 (1%) 72 77	7, 15, 30, 54	7 (1%)
1	E	409/409 (100%)	-0.27	3 (0%) 84 88	6, 15, 28, 55	8 (1%)
All	All	818/818 (100%)	-0.22	9 (1%) 78 82	6, 15, 29, 55	15 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	660	SER	5.3
1	A	660	SER	4.8
1	A	659	ASN	3.4
1	A	252	THR	3.2
1	E	252	THR	2.4
1	A	413	ALA	2.1
1	E	314	ASN	2.0
1	A	388	THR	2.0
1	A	419	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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

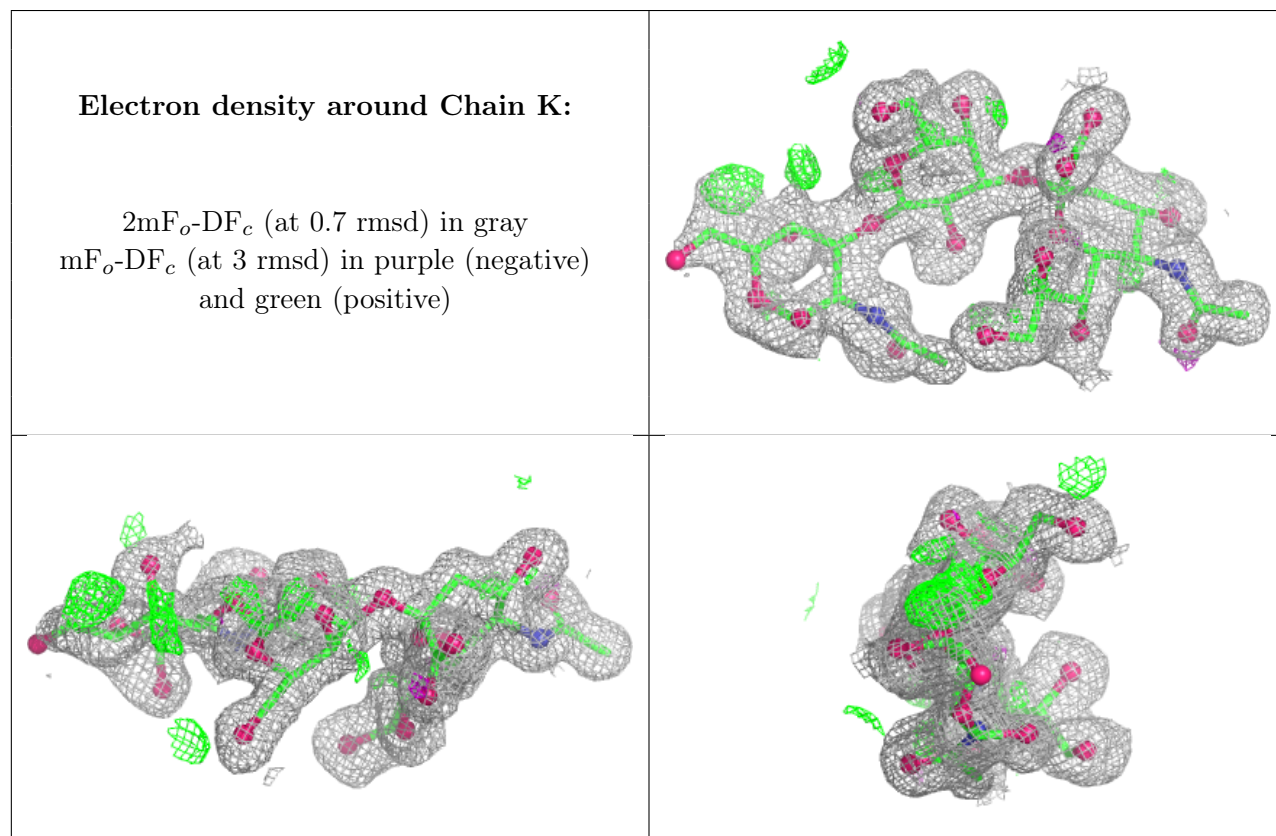
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A2G	K	1	15/15	-	-	29,38,44,52	0

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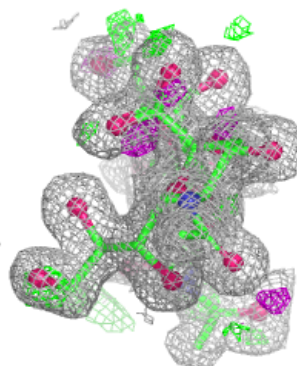
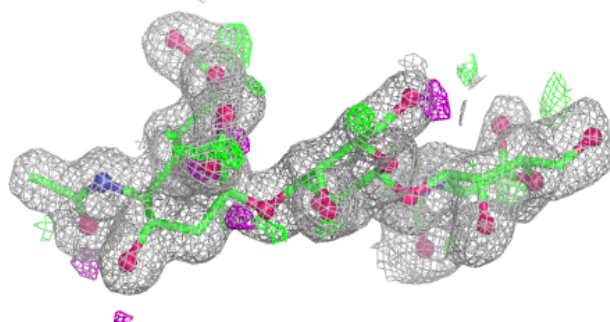
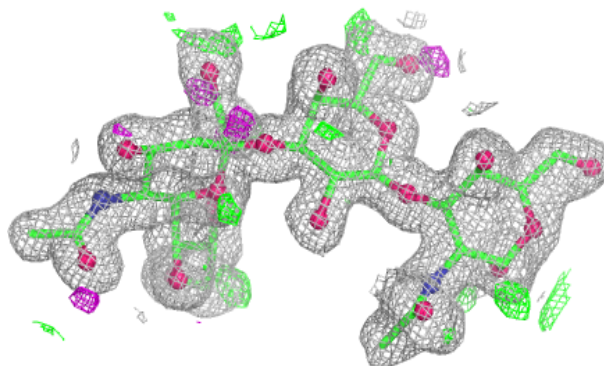
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	K	2	11/12	-	-	18,22,25,26	0
2	SIA	K	3	20/21	-	-	11,15,19,20	0
2	A2G	F	1	15/15	0.76	0.17	33,42,51,55	0
2	A2G	C	1	15/15	0.78	0.15	15,19,32,33	0
2	GAL	F	2	11/12	0.91	0.09	17,21,25,27	0
2	GAL	C	2	11/12	0.92	0.09	11,13,16,16	0
2	SIA	C	3	20/21	0.93	0.08	8,11,13,14	0
2	A2G	D	1	15/15	0.93	0.10	13,20,32,35	0
2	GAL	D	2	11/12	0.94	0.07	10,12,13,16	0
2	SIA	F	3	20/21	0.94	0.07	11,15,19,21	0
2	SIA	D	3	20/21	0.95	0.07	8,11,14,14	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.

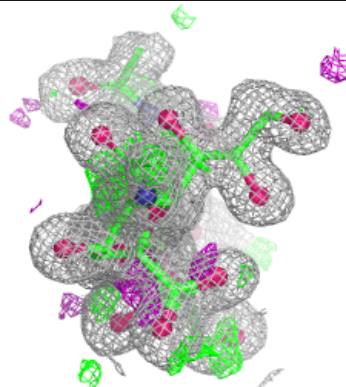
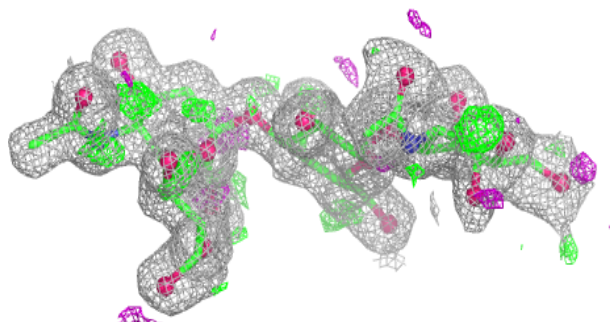
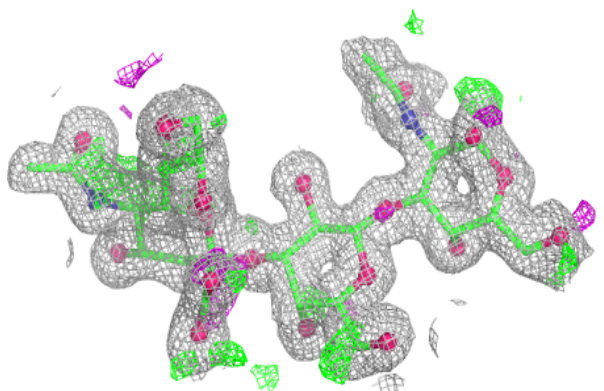


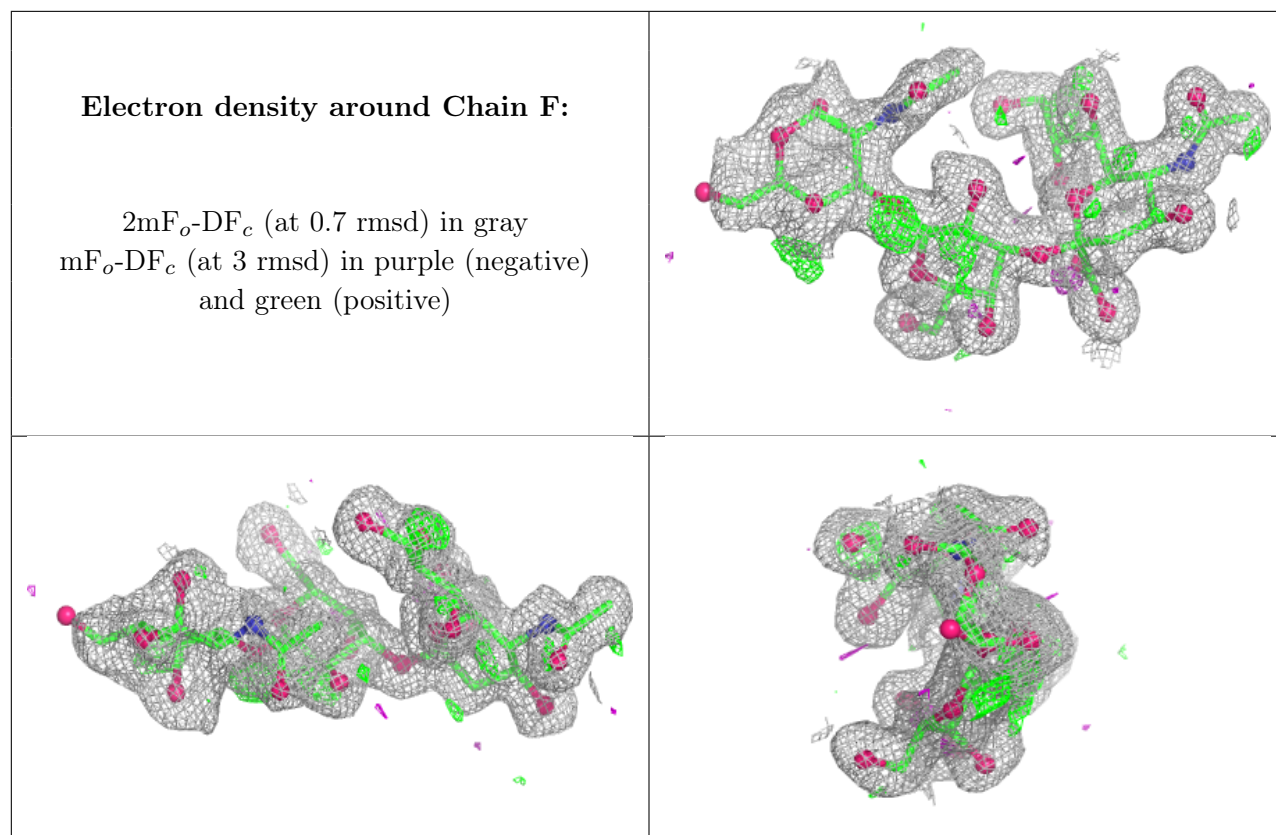
Electron density around Chain C:

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

**Electron density around Chain D:**

$2mF_o-DF_c$ (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
5	GOL	E	1401	6/6	0.66	0.21	24,38,53,57	0
4	SO4	E	1408	5/5	0.69	0.24	72,75,104,105	0
4	SO4	A	706	5/5	0.81	0.23	149,149,160,162	0
4	SO4	E	1407	5/5	0.83	0.13	46,48,62,77	0
4	SO4	E	1406	5/5	0.94	0.16	10,12,17,17	5
3	CA	E	1405	1/1	0.96	0.06	16,16,16,16	0
4	SO4	A	705	5/5	0.97	0.09	16,21,26,26	5
3	CA	E	1404	1/1	0.97	0.04	13,13,13,13	0
3	CA	A	704	1/1	0.97	0.04	12,12,12,12	0
3	CA	A	703	1/1	0.98	0.06	17,17,17,17	0
3	CA	E	1403	1/1	0.98	0.04	13,13,13,13	0
3	CA	A	701	1/1	0.99	0.03	11,11,11,11	0
3	CA	A	702	1/1	0.99	0.04	13,13,13,13	0
3	CA	E	1402	1/1	0.99	0.03	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.