



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 04:03 PM BST

PDB ID : 5ZSF
Title : Crystal structure of monkey TLR7 in complex with imiquimod
Authors : Zhang, Z.; Ohto, U.; Shimizu, T.
Deposited on : 2018-04-28
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

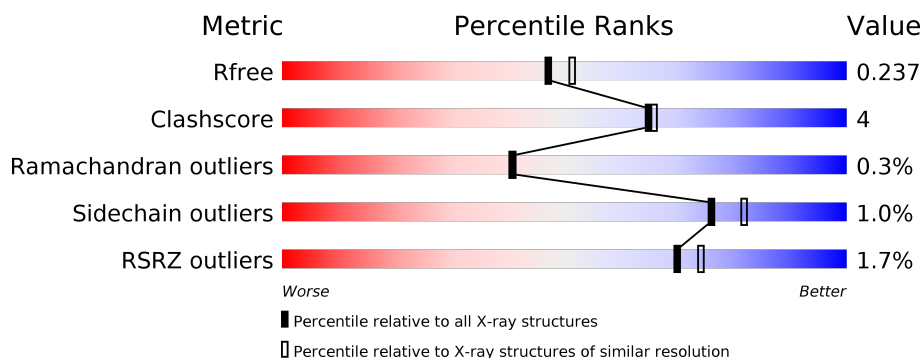
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	823	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	823	<div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13684 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 Toll-like receptor 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			
1	A	772	Total	C	N	O	S	0	1	0
			6258	4010	1066	1152	30			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	ARG	-	expression tag	UNP B3Y653
B	24	SER	-	expression tag	UNP B3Y653
B	25	PRO	-	expression tag	UNP B3Y653
B	26	TRP	-	expression tag	UNP B3Y653
B	167	GLN	ASN	engineered mutation	UNP B3Y653
B	389	GLN	ASN	engineered mutation	UNP B3Y653
B	440	LEU	SER	see sequence details	UNP B3Y653
B	441	VAL	GLU	see sequence details	UNP B3Y653
B	442	PRO	VAL	see sequence details	UNP B3Y653
B	443	ARG	GLY	see sequence details	UNP B3Y653
B	444	GLY	PHE	see sequence details	UNP B3Y653
B	445	SER	CYS	see sequence details	UNP B3Y653
B	488	GLN	ASN	engineered mutation	UNP B3Y653
B	799	GLN	ASN	engineered mutation	UNP B3Y653
B	840	GLU	-	expression tag	UNP B3Y653
B	841	PHE	-	expression tag	UNP B3Y653
B	842	LEU	-	expression tag	UNP B3Y653
B	843	VAL	-	expression tag	UNP B3Y653
B	844	PRO	-	expression tag	UNP B3Y653
B	845	ARG	-	expression tag	UNP B3Y653
A	23	ARG	-	expression tag	UNP B3Y653
A	24	SER	-	expression tag	UNP B3Y653
A	25	PRO	-	expression tag	UNP B3Y653
A	26	TRP	-	expression tag	UNP B3Y653
A	167	GLN	ASN	engineered mutation	UNP B3Y653

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Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLN	ASN	engineered mutation	UNP B3Y653
A	440	LEU	SER	see sequence details	UNP B3Y653
A	441	VAL	GLU	see sequence details	UNP B3Y653
A	442	PRO	VAL	see sequence details	UNP B3Y653
A	443	ARG	GLY	see sequence details	UNP B3Y653
A	444	GLY	PHE	see sequence details	UNP B3Y653
A	445	SER	CYS	see sequence details	UNP B3Y653
A	488	GLN	ASN	engineered mutation	UNP B3Y653
A	799	GLN	ASN	engineered mutation	UNP B3Y653
A	840	GLU	-	expression tag	UNP B3Y653
A	841	PHE	-	expression tag	UNP B3Y653
A	842	LEU	-	expression tag	UNP B3Y653
A	843	VAL	-	expression tag	UNP B3Y653
A	844	PRO	-	expression tag	UNP B3Y653
A	845	ARG	-	expression tag	UNP B3Y653

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



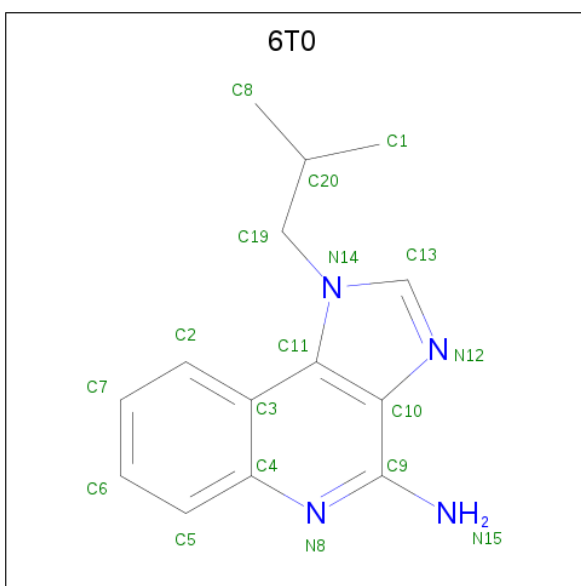
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is 1-(2-methylpropyl)imidazo[4,5-c]quinolin-4-amine (three-letter code: 6T0) (formula: C₁₄H₁₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			18	14	4		
5	A	1	Total	C	N	0	0
			18	14	4		

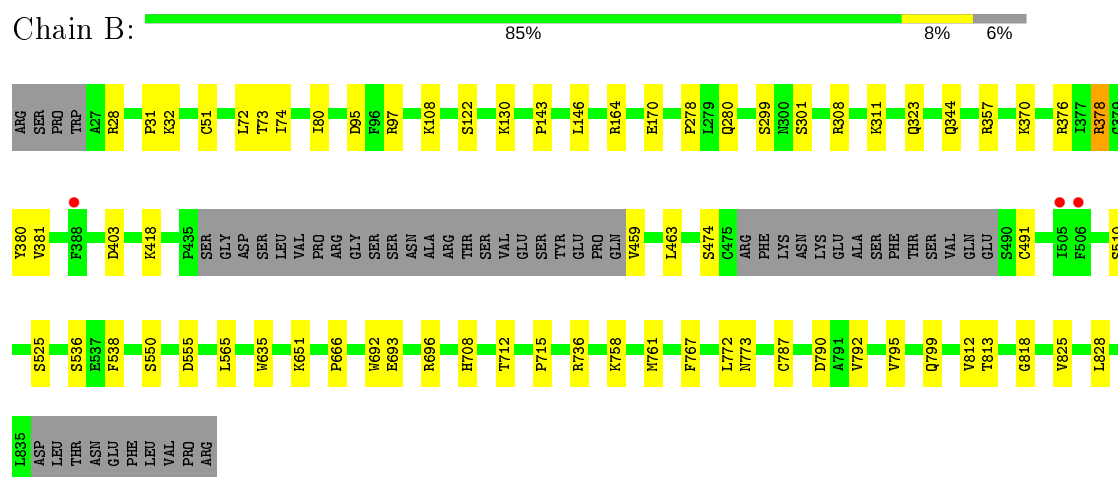
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	525	Total	O	0	0
			525	525		
6	A	340	Total	O	0	0
			340	340		

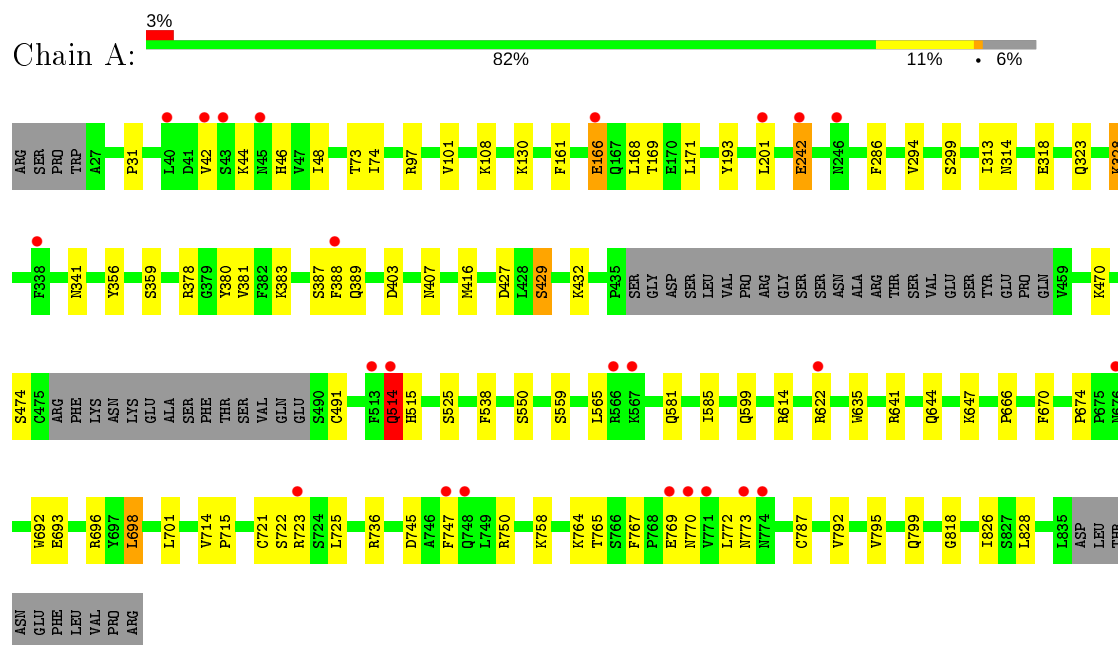
3 Residue-property plots

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: Toll-like receptor 7



- Molecule 1: Toll-like receptor 7



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

Chain C:  50% 50%

HA01
HA02

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

Chain D:  50% 50%

HA01
HA02

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

Chain E:  100%

HA01
HA02

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

Chain F:  50% 50%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.27Å 140.12Å 151.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.16 – 2.10 47.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.16-2.10) 100.0 (47.16-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.192 , 0.237 0.192 , 0.237	Depositor DCC
R_{free} test set	6049 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13684	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: 6T0, NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	5/6389 (0.1%)	0.65	5/8657 (0.1%)
1	B	0.45	1/6389 (0.0%)	0.64	4/8657 (0.0%)
All	All	0.46	6/12778 (0.0%)	0.65	9/17314 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLU	CB-CG	-8.24	1.36	1.52
1	A	328	LYS	CD-CE	6.85	1.68	1.51
1	A	514	GLN	CG-CD	5.86	1.64	1.51
1	A	242	GLU	CD-OE2	5.29	1.31	1.25
1	A	721	CYS	CB-SG	-5.09	1.73	1.81
1	B	280	GLN	CB-CG	-5.09	1.38	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	723	ARG	CG-CD-NE	9.21	131.15	111.80
1	A	42	VAL	CG1-CB-CG2	-8.00	98.10	110.90
1	B	280	GLN	CA-CB-CG	7.92	130.83	113.40
1	A	328	LYS	CG-CD-CE	6.39	131.09	111.90
1	A	328	LYS	CD-CE-NZ	5.51	124.37	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	GLU	CA-C-N	-5.44	105.22	117.20
1	B	378	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	378	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	280	GLN	CB-CA-C	5.14	120.69	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	514	GLN	Sidechain

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	6258	0	6303	53	0
1	B	6258	0	6301	52	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	56	0	52	1	0
3	B	84	0	78	3	0
4	A	5	0	0	1	0
4	B	10	0	0	1	0
5	A	18	0	0	1	0
5	B	18	0	0	1	0
6	A	340	0	0	8	0
6	B	525	0	0	10	0
All	All	13684	0	12834	105	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 4.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD23	1:B:170:GLU:CD	2.01	0.79
1:B:146:LEU:HD23	1:B:170:GLU:OE2	1.84	0.77
1:B:510:SER:OG	1:B:536:SER:O	2.04	0.76
1:B:73:THR:HG22	1:B:74:ILE:HG13	1.67	0.75
1:A:767:PHE:HB3	1:A:772:LEU:HD11	1.70	0.72
1:A:599:GLN:OE1	1:A:622:ARG:NH2	2.23	0.71
1:A:514:GLN:OE1	1:A:515:HIS:CE1	2.44	0.70
1:A:432:LYS:NZ	6:A:1006:HOH:O	2.22	0.69
1:B:459:VAL:N	6:B:1006:HOH:O	2.23	0.69
1:B:95:ASP:OD2	6:B:1001:HOH:O	2.11	0.68
1:A:97:ARG:NH1	6:A:1009:HOH:O	2.27	0.67
1:B:696:ARG:HD3	3:B:908:NAG:H82	1.76	0.67
1:B:773:ASN:OD1	6:B:1002:HOH:O	2.13	0.66
1:A:765:THR:OG1	6:A:1001:HOH:O	2.14	0.65
1:A:773:ASN:ND2	6:A:1004:HOH:O	2.21	0.64
1:A:581:GLN:OE1	6:A:1002:HOH:O	2.16	0.63
1:B:146:LEU:N	1:B:146:LEU:HD22	2.14	0.62
1:A:670:PHE:CD2	1:A:698:LEU:HD21	2.35	0.62
1:B:143:PRO:O	1:B:146:LEU:HD21	1.99	0.62
1:B:130:LYS:HD3	2:D:2:NAG:H83	1.82	0.60
1:A:769:GLU:HG3	1:A:769:GLU:O	2.01	0.60
1:B:378:ARG:HD2	1:B:403:ASP:OD2	2.01	0.60
1:A:286:PHE:HB3	1:A:313:ILE:HD11	1.84	0.59
1:A:314:ASN:O	1:A:341:ASN:ND2	2.36	0.59
1:A:201:LEU:O	6:A:1003:HOH:O	2.17	0.58
1:B:32:LYS:NZ	6:B:1019:HOH:O	2.36	0.57
1:A:73:THR:HG22	1:A:74:ILE:HG13	1.87	0.57
1:B:146:LEU:CD2	1:B:170:GLU:OE2	2.52	0.57
1:B:767:PHE:HB3	1:B:772:LEU:HD11	1.88	0.55
1:A:559:SER:N	4:A:909:SO4:O4	2.31	0.55
1:A:693:GLU:O	1:A:696:ARG:HG3	2.07	0.54
1:B:164:ARG:NE	6:B:1004:HOH:O	2.18	0.54
1:A:387:SER:HB3	1:A:416:MET:HB2	1.90	0.53
1:B:635:TRP:HB3	1:B:666:PRO:HG2	1.90	0.53
1:B:787:CYS:HB3	1:B:828:LEU:HD21	1.90	0.53
1:B:146:LEU:HD23	1:B:170:GLU:OE1	2.07	0.53
1:B:712:THR:O	6:B:1003:HOH:O	2.18	0.52
1:A:378:ARG:HD2	1:A:403:ASP:OD2	2.10	0.51
1:B:692:TRP:CE2	1:B:715:PRO:HD3	2.45	0.51
1:A:764:LYS:NZ	6:A:1026:HOH:O	2.43	0.51
1:B:692:TRP:CD2	1:B:715:PRO:HD3	2.47	0.50
1:B:357:ARG:NH1	1:B:380:TYR:OH	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:HIS:HD2	6:B:1489:HOH:O	1.94	0.49
1:A:380:TYR:N	1:A:407:ASN:OD1	2.43	0.49
1:A:97:ARG:NH2	1:A:474:SER:O	2.45	0.49
1:A:714:VAL:HB	1:A:715:PRO:HD2	1.93	0.49
1:B:299:SER:HA	1:B:323:GLN:O	2.14	0.48
1:A:747:PHE:O	1:A:750:ARG:NH2	2.47	0.48
1:B:491:CYS:HB3	3:B:901:NAG:H81	1.95	0.48
1:A:294:VAL:HG22	1:A:318:GLU:HB3	1.96	0.47
1:A:356:TYR:CZ	1:A:383:LYS:HG2	2.49	0.47
1:B:376:ARG:NH1	4:B:911:SO4:O1	2.39	0.47
1:A:736:ARG:HG2	1:A:758:LYS:HB2	1.95	0.47
1:A:168:LEU:HD22	1:A:171:LEU:HD12	1.97	0.47
1:B:795:VAL:HG21	1:B:828:LEU:HD23	1.97	0.47
1:A:166:GLU:O	1:A:169:THR:HG22	2.15	0.47
1:B:31:PRO:HB3	1:B:799:GLN:O	2.15	0.47
1:A:674:PRO:HB2	6:A:1115:HOH:O	2.14	0.47
1:B:311:LYS:NZ	1:B:311:LYS:HB2	2.30	0.46
1:A:299:SER:HA	1:A:323:GLN:O	2.15	0.46
1:B:370:LYS:HD2	6:B:1216:HOH:O	2.16	0.46
1:A:644:GLN:HG2	1:A:647:LYS:HD2	1.98	0.46
1:B:97:ARG:NH2	1:B:474:SER:O	2.49	0.46
1:B:308:ARG:HD2	1:B:311:LYS:HE2	1.98	0.45
1:A:31:PRO:HB3	1:A:799:GLN:O	2.16	0.45
1:B:51:CYS:HB2	1:B:72:LEU:HD23	1.98	0.45
1:A:525:SER:HA	1:A:550:SER:O	2.17	0.45
1:A:538:PHE:HB3	1:A:565:LEU:HD21	1.99	0.45
1:A:692:TRP:CD2	1:A:715:PRO:HD3	2.52	0.45
1:A:722:SER:OG	1:A:725:LEU:HB2	2.17	0.45
1:B:555:ASP:OD1	5:B:913:6T0:N15	2.50	0.44
1:A:635:TRP:HB3	1:A:666:PRO:HG2	1.99	0.44
1:A:787:CYS:HB3	1:A:828:LEU:HD21	1.98	0.44
1:A:491:CYS:HB3	3:A:901:NAG:H81	1.98	0.44
1:B:308:ARG:CD	1:B:311:LYS:HE2	2.48	0.43
1:B:693:GLU:O	1:B:696:ARG:HG3	2.17	0.43
1:A:692:TRP:CE2	1:A:715:PRO:HD3	2.54	0.43
1:B:736:ARG:HG2	1:B:758:LYS:HB2	2.01	0.43
1:B:525:SER:HA	1:B:550:SER:O	2.19	0.43
1:A:359:SER:HB2	1:A:389:GLN:NE2	2.34	0.42
1:A:585:ILE:HG23	5:A:910:6T0:N15	2.33	0.42
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.72	0.42
1:B:418:LYS:NZ	3:B:904:NAG:O6	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:THR:HA	1:B:97:ARG:O	2.19	0.42
1:B:80:ILE:HG22	1:B:122:SER:HB3	2.01	0.42
1:A:403:ASP:HA	1:A:427:ASP:HB3	2.00	0.42
1:A:795:VAL:HG21	1:A:828:LEU:HD23	2.02	0.42
1:B:812:VAL:HG12	1:B:825:VAL:HG13	2.02	0.42
1:A:427:ASP:OD2	1:A:429:SER:HB2	2.19	0.42
1:A:614:ARG:HD3	1:A:641:ARG:HB3	2.02	0.41
1:B:97:ARG:HH11	1:B:97:ARG:HD3	1.75	0.41
1:B:146:LEU:N	1:B:146:LEU:CD2	2.82	0.41
1:A:46:HIS:HB3	1:A:48:ILE:HD11	2.03	0.41
1:B:278:PRO:HB3	1:B:301:SER:O	2.20	0.41
1:B:761:MET:HE1	1:B:790:ASP:HB3	2.02	0.41
1:A:387:SER:HB3	1:A:416:MET:CB	2.50	0.41
1:A:698:LEU:HB3	1:A:701:LEU:HB2	2.02	0.41
1:B:28:ARG:NH2	6:B:1061:HOH:O	2.54	0.41
1:A:745:ASP:HA	1:A:747:PHE:CZ	2.56	0.41
1:B:463:LEU:HD12	1:B:463:LEU:HA	1.91	0.40
1:B:344:GLN:HG3	6:B:1145:HOH:O	2.21	0.40
1:B:651:LYS:HB3	1:B:651:LYS:HE2	1.75	0.40
1:A:826:ILE:HA	1:A:826:ILE:HD13	1.79	0.40
1:A:161:PHE:HA	1:A:193:TYR:CE1	2.57	0.40
1:B:538:PHE:HB3	1:B:565:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	767/823 (93%)	724 (94%)	40 (5%)	3 (0%)	34	32
1	B	767/823 (93%)	728 (95%)	37 (5%)	2 (0%)	41	41
All	All	1534/1646 (93%)	1452 (95%)	77 (5%)	5 (0%)	41	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	818	GLY
1	A	242	GLU
1	A	818	GLY
1	B	381	VAL
1	A	381	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	726/774 (94%)	715 (98%)	11 (2%)	65	71
1	B	726/774 (94%)	723 (100%)	3 (0%)	91	94
All	All	1452/1548 (94%)	1438 (99%)	14 (1%)	76	82

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

Mol	Chain	Res	Type
1	B	108	LYS
1	B	792	VAL
1	B	813	THR
1	A	44	LYS
1	A	101	VAL
1	A	108	LYS
1	A	166	GLU
1	A	328	LYS
1	A	388	PHE
1	A	429	SER
1	A	470	LYS
1	A	698	LEU
1	A	770	ASN
1	A	792	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	GLN
1	A	515	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 ⓘ

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$
2	NAG	C	1	1,2	14,14,15	0.47	0	17,19,21	0.55	0
2	NAG	C	2	2	14,14,15	0.46	0	17,19,21	0.73	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.49	0	17,19,21	0.46	0
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.57	0
2	NAG	E	1	1,2	14,14,15	0.38	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	0.63	0
2	NAG	F	1	1,2	14,14,15	0.47	0	17,19,21	0.51	0
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.88	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	3.21	116.53	112.19
2	C	2	NAG	C1-O5-C5	2.51	115.59	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

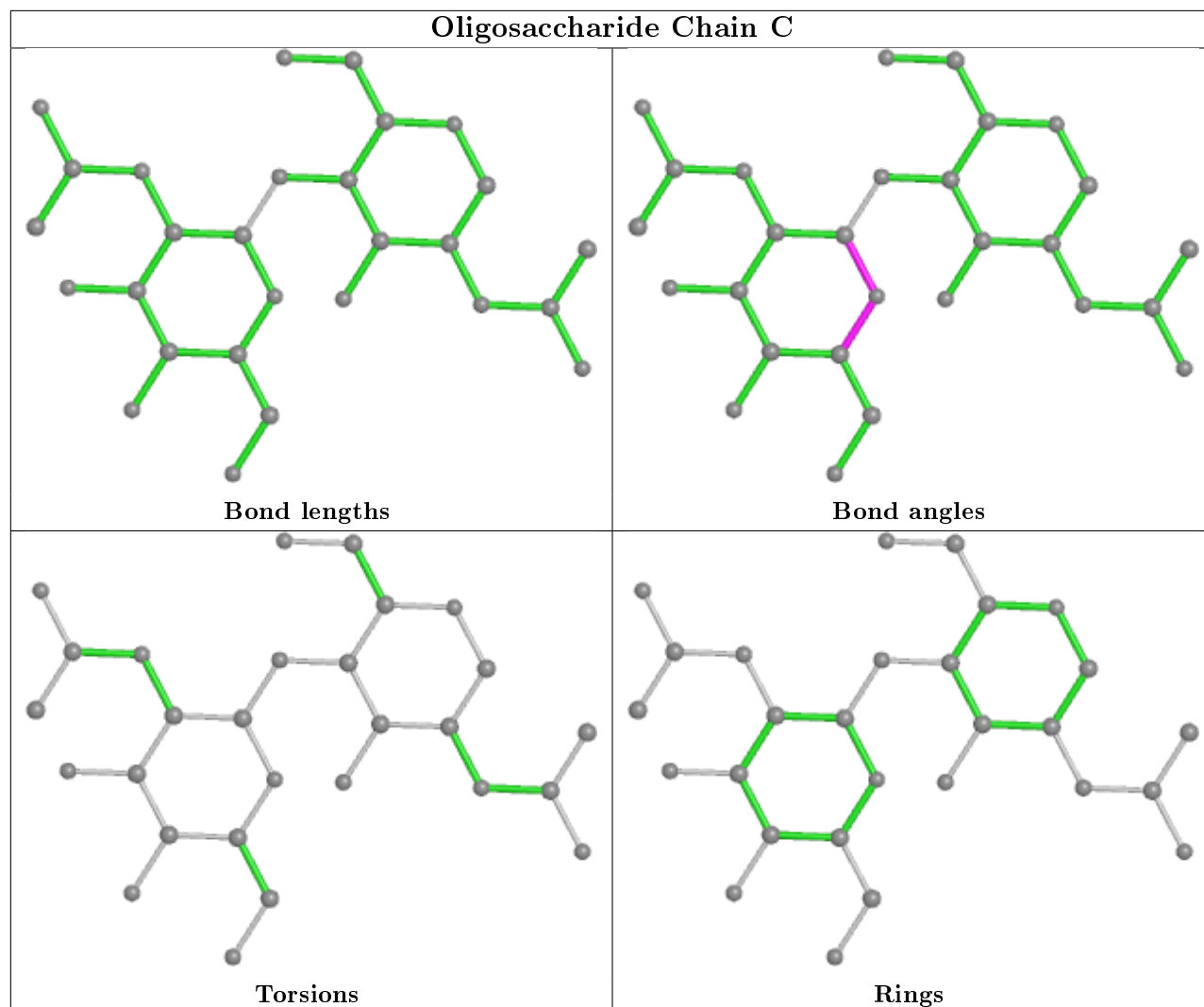
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C3-C2-N2-C7

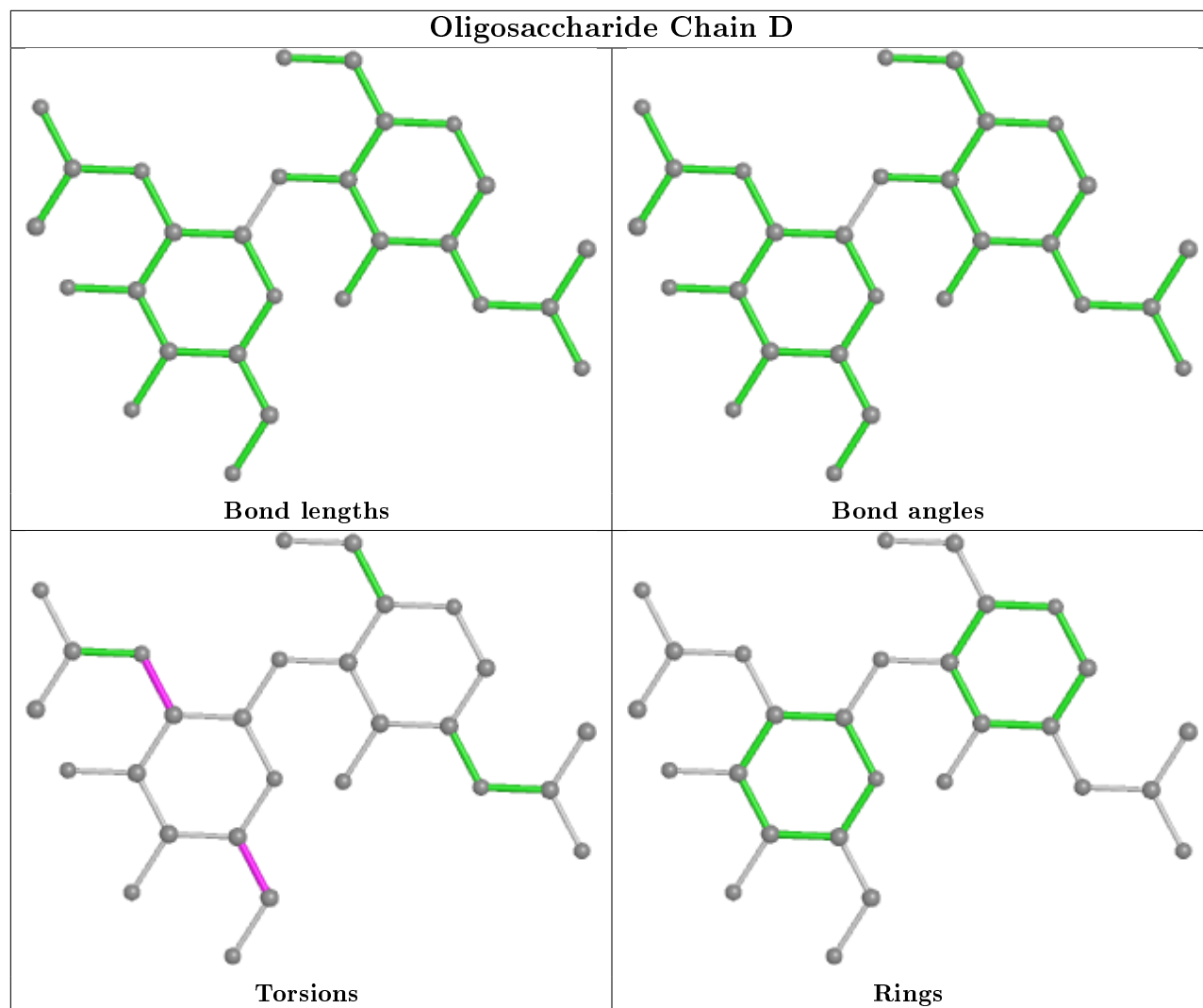
There are no ring outliers.

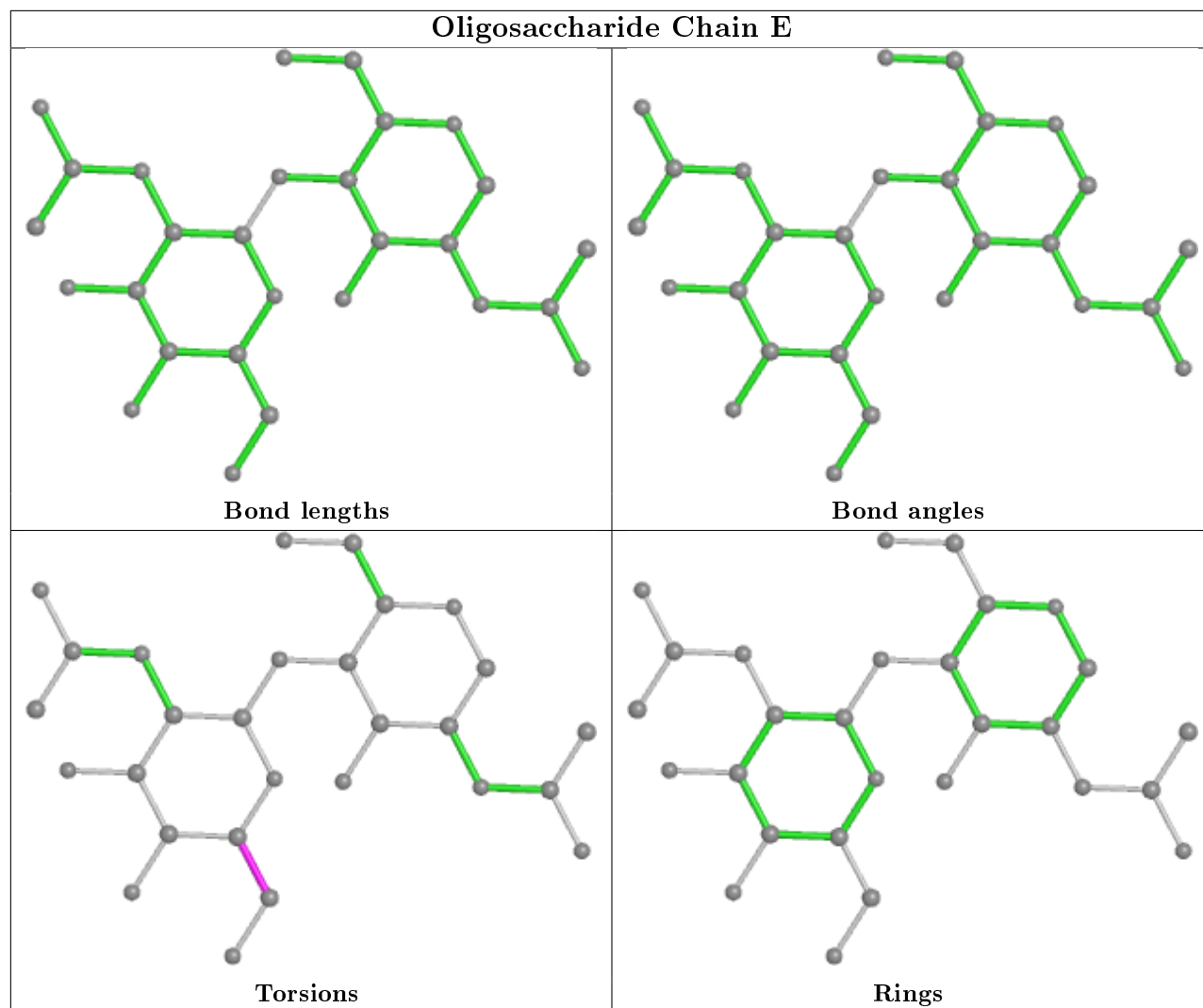
1 monomer is involved in 1 short contact:

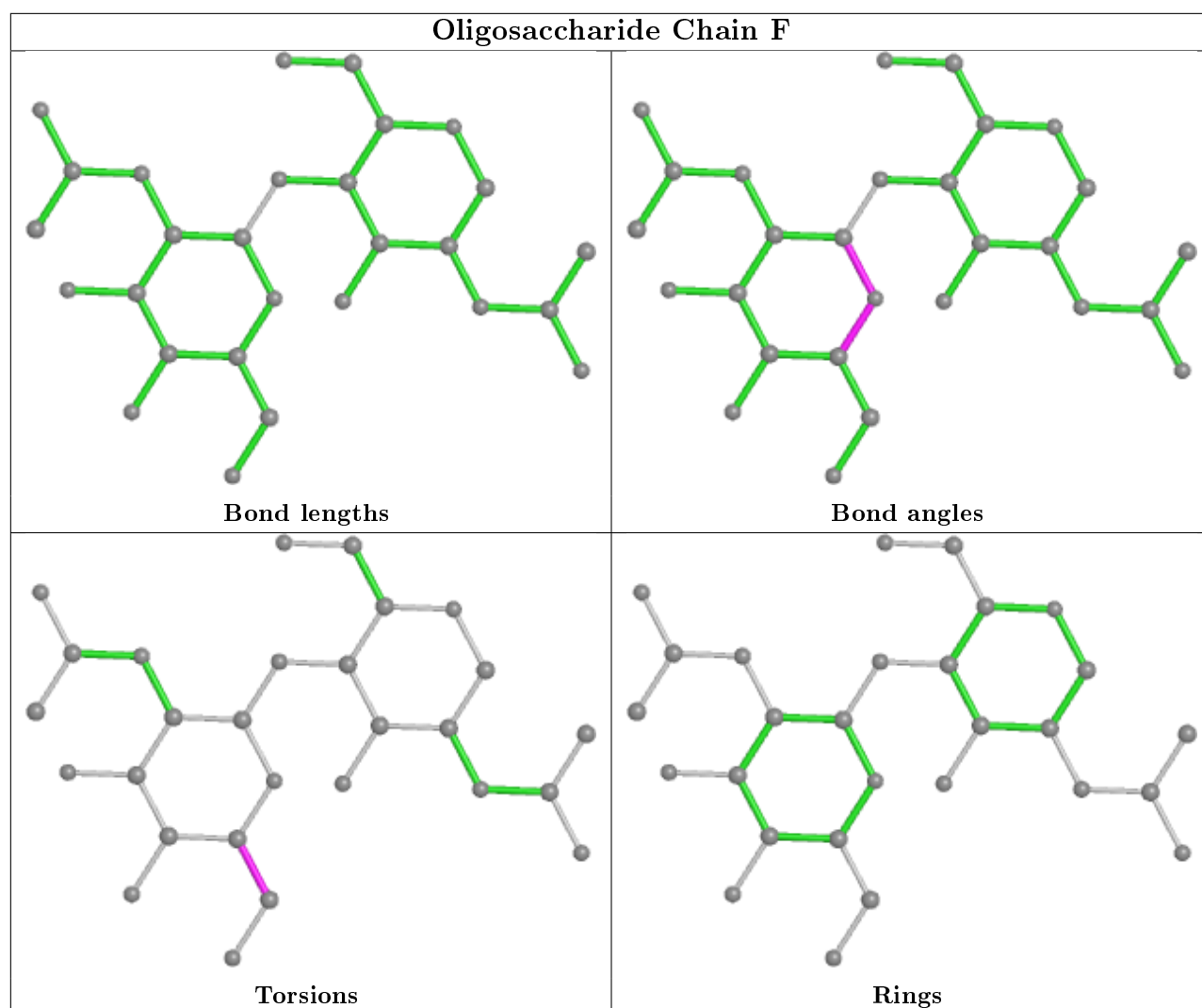
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0

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 ⓘ

15 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	NAG	B	908	1	14,14,15	0.97	1 (7%)	17,19,21	0.87	1 (5%)
3	NAG	A	908	1	14,14,15	0.20	0	17,19,21	0.53	0
4	SO4	B	911	-	4,4,4	0.16	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	909	1	14,14,15	0.57	0	17,19,21	0.46	0
3	NAG	A	907	1	14,14,15	0.46	0	17,19,21	0.38	0
4	SO4	A	909	-	4,4,4	0.21	0	6,6,6	0.31	0
3	NAG	A	906	1	14,14,15	0.24	0	17,19,21	0.73	0
5	6T0	A	910	-	16,20,20	1.42	1 (6%)	20,29,29	1.33	3 (15%)
3	NAG	B	901	1	14,14,15	0.55	0	17,19,21	0.56	0
3	NAG	A	901	1	14,14,15	0.68	0	17,19,21	0.72	0
5	6T0	B	913	-	16,20,20	1.50	1 (6%)	20,29,29	1.22	2 (10%)
3	NAG	B	907	1	14,14,15	0.65	0	17,19,21	0.70	1 (5%)
4	SO4	B	912	-	4,4,4	0.17	0	6,6,6	0.12	0
3	NAG	B	904	1	14,14,15	0.27	0	17,19,21	0.73	0
3	NAG	B	910	1	14,14,15	0.41	0	17,19,21	0.43	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
3	NAG	B	908	1	-	0/6/23/26	0/1/1/1
3	NAG	A	908	1	-	2/6/23/26	0/1/1/1
3	NAG	B	909	1	-	2/6/23/26	0/1/1/1
3	NAG	A	907	1	-	2/6/23/26	0/1/1/1
3	NAG	A	906	1	-	2/6/23/26	0/1/1/1
5	6T0	A	910	-	-	0/3/4/4	0/3/3/3
3	NAG	B	901	1	-	0/6/23/26	0/1/1/1
3	NAG	A	901	1	-	2/6/23/26	0/1/1/1
5	6T0	B	913	-	-	1/3/4/4	0/3/3/3
3	NAG	B	907	1	-	2/6/23/26	0/1/1/1
3	NAG	B	904	1	-	2/6/23/26	0/1/1/1
3	NAG	B	910	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	913	6T0	C3-C4	4.57	1.50	1.41
5	A	910	6T0	C3-C4	4.32	1.49	1.41
3	B	908	NAG	O5-C1	3.20	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	NAG	C1-O5-C5	3.19	116.51	112.19
5	A	910	6T0	C10-C9-N8	-3.10	118.97	121.01
5	B	913	6T0	C11-C3-C4	-2.92	117.43	119.65
5	B	913	6T0	C10-C9-N8	-2.84	119.14	121.01
5	A	910	6T0	C11-C3-C4	-2.73	117.58	119.65
3	B	907	NAG	C1-O5-C5	2.08	115.01	112.19
5	A	910	6T0	N15-C9-N8	2.05	122.54	117.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	907	NAG	O5-C5-C6-O6
3	B	909	NAG	C4-C5-C6-O6
3	A	906	NAG	C4-C5-C6-O6
3	B	907	NAG	C4-C5-C6-O6
3	B	910	NAG	O5-C5-C6-O6
3	A	906	NAG	O5-C5-C6-O6
3	A	908	NAG	C4-C5-C6-O6
3	B	910	NAG	C4-C5-C6-O6
3	A	908	NAG	O5-C5-C6-O6
3	B	909	NAG	O5-C5-C6-O6
3	B	904	NAG	C4-C5-C6-O6
3	A	901	NAG	C4-C5-C6-O6
3	A	901	NAG	O5-C5-C6-O6
5	B	913	6T0	N14-C19-C20-C1
3	B	904	NAG	O5-C5-C6-O6
3	A	907	NAG	C4-C5-C6-O6
3	A	907	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	908	NAG	1	0
4	B	911	SO4	1	0
4	A	909	SO4	1	0
5	A	910	6T0	1	0
3	B	901	NAG	1	0
3	A	901	NAG	1	0
5	B	913	6T0	1	0
3	B	904	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	772/823 (93%)	0.36	24 (3%) 49 55	32, 47, 65, 84	0
1	B	772/823 (93%)	0.20	3 (0%) 92 93	24, 39, 55, 79	0
All	All	1544/1646 (93%)	0.28	27 (1%) 70 74	24, 42, 61, 84	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	GLN	5.0
1	A	566	ARG	4.4
1	A	773	ASN	4.0
1	A	388	PHE	3.8
1	A	338	PHE	3.3
1	A	769	GLU	3.0
1	A	747	PHE	2.9
1	A	43	SER	2.9
1	A	774	ASN	2.8
1	A	42	VAL	2.8
1	A	676	ASN	2.7
1	A	40	LEU	2.7
1	A	771	VAL	2.6
1	A	45	ASN	2.5
1	A	723	ARG	2.5
1	A	567	LYS	2.4
1	A	622	ARG	2.4
1	A	770	ASN	2.3
1	A	246	ASN	2.3
1	B	388	PHE	2.3
1	B	506	PHE	2.3
1	A	166	GLU	2.3
1	A	242	GLU	2.2
1	A	201	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	513	PHE	2.1
1	B	505	ILE	2.0
1	A	514	GLN	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](#)

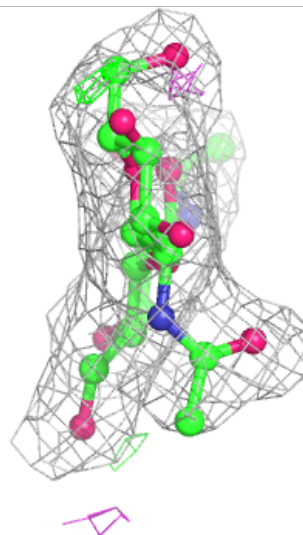
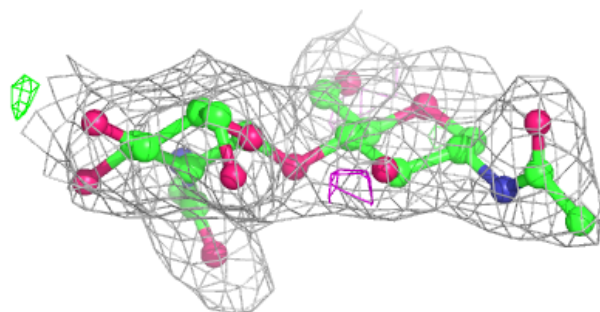
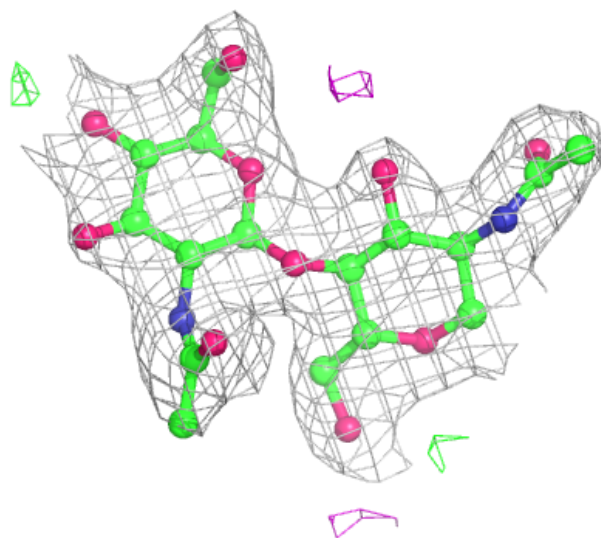
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	D	2	14/15	0.86	0.25	63,67,74,83	0
2	NAG	F	2	14/15	0.89	0.27	64,67,78,82	0
2	NAG	E	2	14/15	0.91	0.10	56,63,69,70	0
2	NAG	C	2	14/15	0.92	0.10	54,58,64,66	0
2	NAG	F	1	14/15	0.94	0.12	48,54,57,60	0
2	NAG	D	1	14/15	0.95	0.12	42,51,56,59	0
2	NAG	E	1	14/15	0.96	0.11	40,45,50,57	0
2	NAG	C	1	14/15	0.97	0.09	40,46,53,56	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.

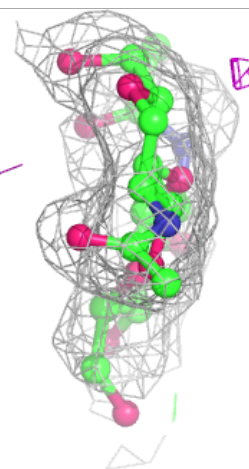
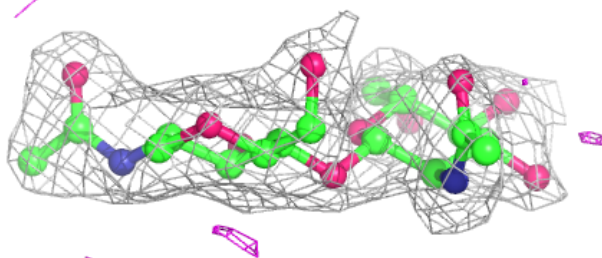
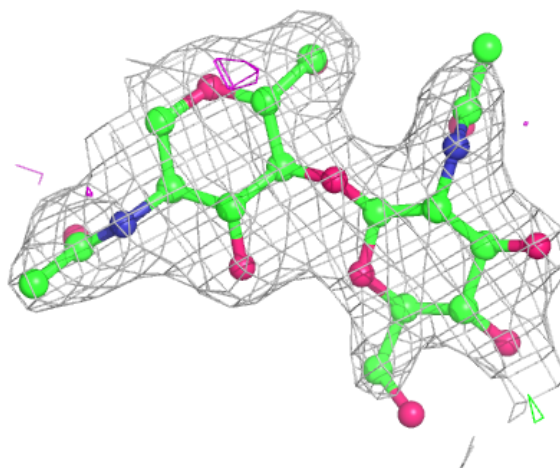
Electron density around Chain C:

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



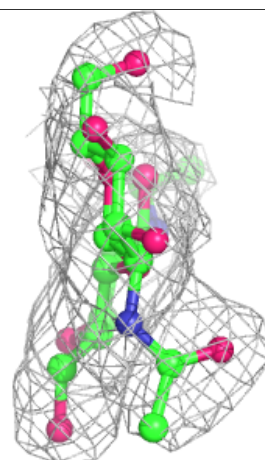
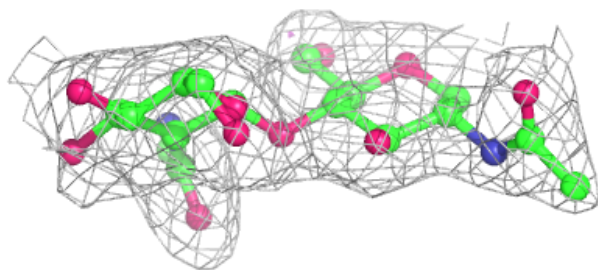
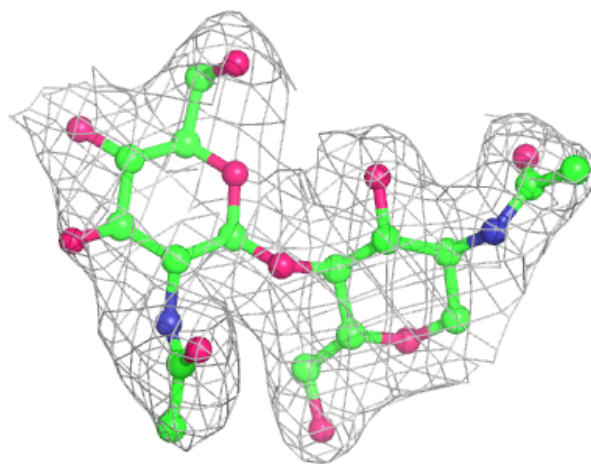
Electron density around Chain D:

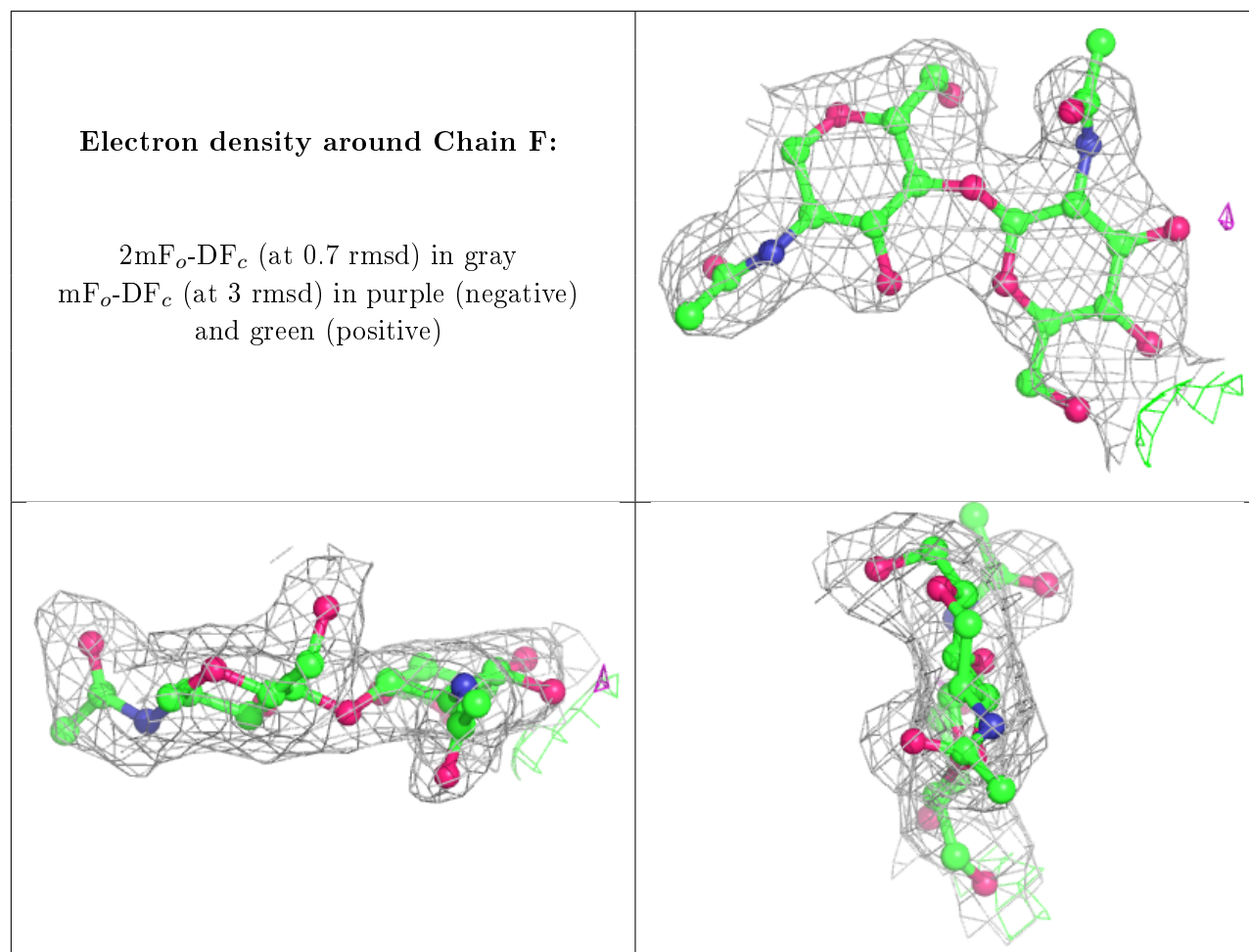
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\AA^2)	Q<0.9
4	SO4	A	909	5/5	0.86	0.16	72,78,80,92	0
3	NAG	B	910	14/15	0.86	0.11	59,66,73,73	0
4	SO4	B	911	5/5	0.87	0.34	53,64,73,81	0
3	NAG	A	906	14/15	0.88	0.14	65,73,74,77	0
3	NAG	B	909	14/15	0.88	0.16	54,61,73,77	0
3	NAG	A	908	14/15	0.89	0.18	65,68,72,73	0
3	NAG	B	907	14/15	0.90	0.15	48,57,60,71	0
4	SO4	B	912	5/5	0.91	0.17	73,74,81,92	0
3	NAG	A	907	14/15	0.91	0.26	68,72,80,85	0
3	NAG	A	901	14/15	0.92	0.13	40,45,48,48	0
3	NAG	B	904	14/15	0.93	0.11	50,54,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	6T0	A	910	18/18	0.94	0.20	44,47,60,60	0
3	NAG	B	901	14/15	0.95	0.13	28,35,39,43	0
3	NAG	B	908	14/15	0.95	0.11	43,46,51,52	0
5	6T0	B	913	18/18	0.97	0.17	39,43,49,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.