



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:25 AM BST

PDB ID : 5YGS  
Title : Human TNFRSF25 death domain  
Authors : Yin, X.; Jin, T.  
Deposited on : 2017-09-26  
Resolution : 2.69 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](mailto: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.

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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

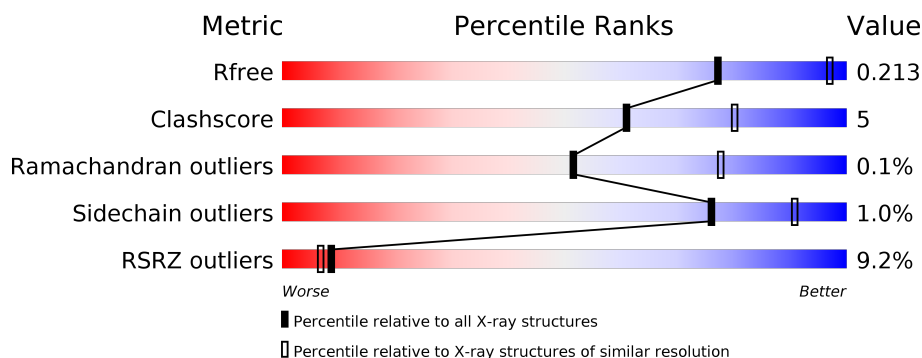
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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.




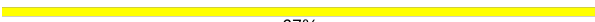

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	463	<div> <div>5%</div> <div>87%</div> <div>11%</div> </div>
1	B	463	<div> <div>8%</div> <div>89%</div> <div>10%</div> </div>
1	C	463	<div> <div>13%</div> <div>84%</div> <div>15%</div> </div>
1	D	463	<div> <div>10%</div> <div>89%</div> <div>10%</div> </div>
2	E	3	<div> <div>100%</div> </div>
2	F	3	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	3	 100%
2	H	3	 67%  33%

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
3	SO4	C	501	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 28638 atoms, of which 14212 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 Human TNRSF25 death domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	0	0
			7053	2268	3512	595	668	10			
1	B	456	Total	C	H	N	O	S	0	0	0
			7057	2268	3517	595	666	11			
1	C	457	Total	C	H	N	O	S	0	0	0
			7073	2273	3524	596	669	11			
1	D	458	Total	C	H	N	O	S	0	0	0
			7090	2279	3531	599	670	11			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	H	O	0	0	0
			66	18	32	16			
2	F	3	Total	C	H	O	0	0	0
			66	18	32	16			
2	G	3	Total	C	H	O	0	0	0
			66	18	32	16			
2	H	3	Total	C	H	O	0	0	0
			66	18	32	16			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

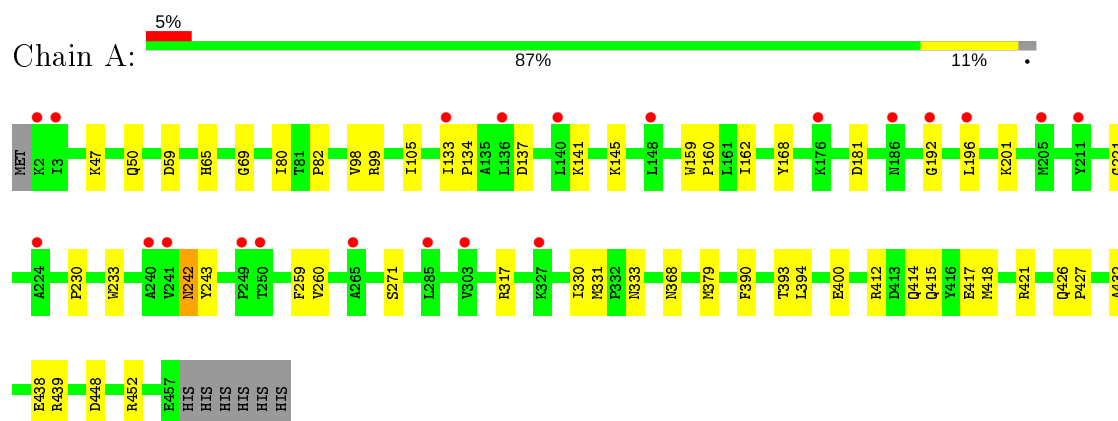
- Molecule 4 is water.

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

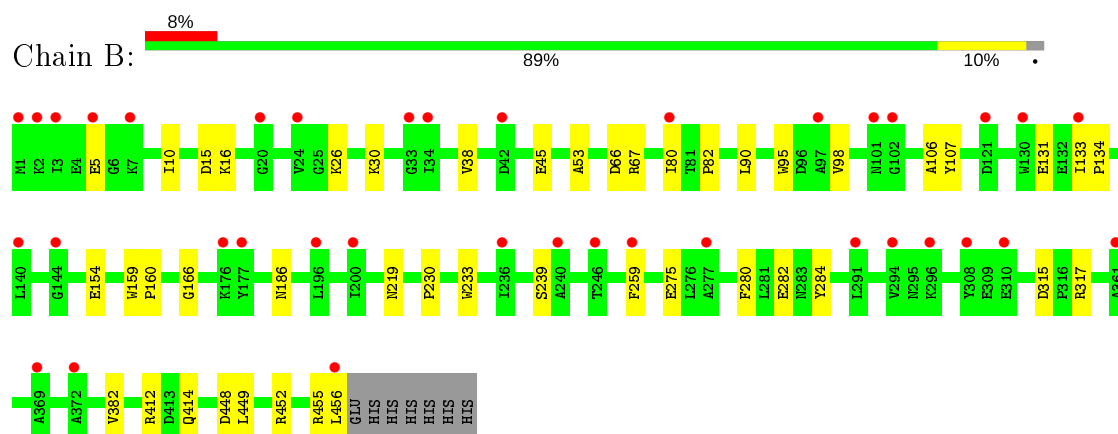
### 3 Residue-property plots

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.

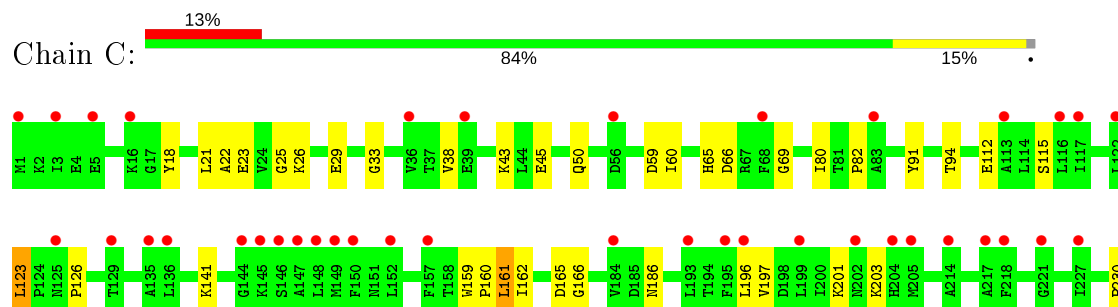
- Molecule 1: Human TNRSF25 death domain

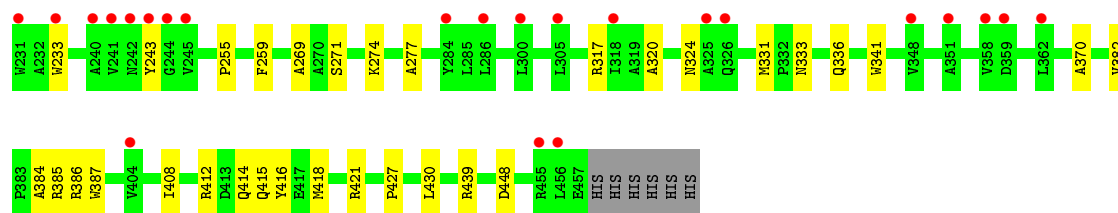


- Molecule 1: Human TNRSF25 death domain

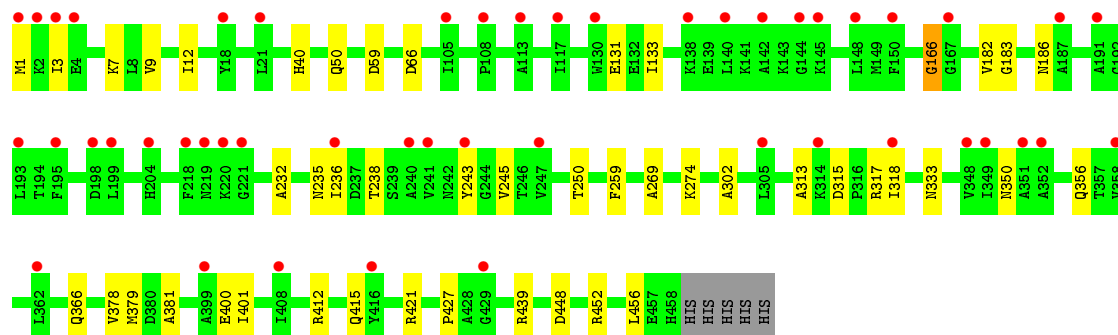
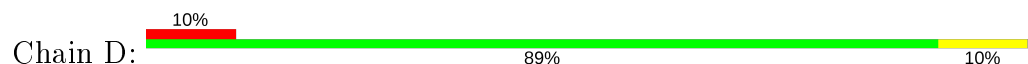


- Molecule 1: Human TNRSF25 death domain

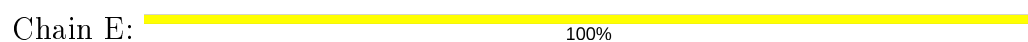




- Molecule 1: Human TNRSF25 death domain



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.69Å 153.55Å 98.24Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	98.25 – 2.69 46.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (98.25-2.69) 99.0 (46.80-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX v1.12-2829	Depositor
R, $R_{free}$	0.190 , 0.212 0.195 , 0.213	Depositor DCC
$R_{free}$ test set	3023 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	0 of 59934 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: GLC, 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	0.27	0/3621	0.42	0/4913
1	B	0.26	0/3620	0.42	0/4911
1	C	0.26	0/3629	0.41	0/4923
1	D	0.27	0/3640	0.41	0/4938
All	All	0.27	0/14510	0.42	0/19685

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3541	3512	3512	29	0
1	B	3540	3517	3517	29	0
1	C	3549	3524	3524	46	0
1	D	3559	3531	3531	29	0
2	E	34	32	29	0	0
2	F	34	32	29	4	0
2	G	34	32	29	3	0
2	H	34	32	29	1	0
3	A	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	1	0
3	C	20	0	0	3	0
3	D	25	0	0	1	0
4	A	1	0	0	0	0
All	All	14426	14212	14200	129	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 (129) 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:421:ARG:NH1	1:D:427:PRO:O	2.00	0.95
1:C:421:ARG:NH1	1:C:427:PRO:O	2.06	0.89
1:C:66:ASP:OD2	2:G:2:GLC:O3	1.92	0.85
1:C:269:ALA:O	1:C:274:LYS:NZ	2.09	0.85
1:D:448:ASP:OD1	1:D:452:ARG:NH1	2.11	0.83
1:C:382:VAL:O	1:C:412:ARG:NH2	2.11	0.83
1:D:379:MET:O	1:D:412:ARG:NH1	2.14	0.80
1:D:66:ASP:OD2	2:H:2:GLC:O3	1.99	0.80
1:A:368:ASN:ND2	1:A:400:GLU:OE1	2.16	0.79
1:D:243:TYR:OH	1:D:317:ARG:NH1	2.19	0.76
1:B:5:GLU:OE1	1:B:5:GLU:N	2.20	0.74
1:B:382:VAL:O	1:B:412:ARG:NH2	2.20	0.74
1:C:415:GLN:OE1	1:C:439:ARG:NH2	2.23	0.71
1:A:421:ARG:NH1	1:A:427:PRO:O	2.23	0.71
1:D:131:GLU:OE1	1:D:131:GLU:N	2.23	0.70
1:D:50:GLN:NE2	3:D:503:SO4:O3	2.25	0.69
1:B:131:GLU:N	1:B:131:GLU:OE1	2.26	0.68
1:D:415:GLN:OE1	1:D:439:ARG:NH2	2.23	0.68
1:A:243:TYR:OH	1:A:317:ARG:NH1	2.26	0.67
1:C:385:ARG:N	3:C:501:SO4:O1	2.27	0.67
1:B:154:GLU:OE1	2:F:2:GLC:O6	2.14	0.65
1:B:67:ARG:NH1	2:F:3:GLC:O3	2.32	0.63
1:C:165:ASP:OD1	1:C:165:ASP:N	2.32	0.63
1:D:400:GLU:OE2	1:D:401:ILE:N	2.39	0.56
1:B:45:GLU:OE1	1:B:45:GLU:N	2.39	0.56
1:C:243:TYR:OH	1:C:317:ARG:NH1	2.39	0.56
1:D:269:ALA:O	1:D:274:LYS:NZ	2.39	0.55
1:C:18:TYR:O	1:C:22:ALA:N	2.38	0.54
1:C:29:GLU:O	1:C:33:GLY:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:O	1:B:239:SER:OG	2.15	0.53
1:A:168:TYR:OH	1:A:181:ASP:OD1	2.26	0.53
1:A:379:MET:O	1:A:412:ARG:NH1	2.42	0.53
1:C:123:LEU:O	1:C:123:LEU:HD23	2.09	0.52
1:A:201:LYS:N	1:A:201:LYS:HD2	2.25	0.52
1:D:3:ILE:HD13	1:D:59:ASP:OD2	2.11	0.51
1:A:47:LYS:NZ	3:A:503:SO4:O3	2.44	0.51
1:A:69:GLY:HA3	1:A:333:ASN:O	2.11	0.51
1:A:133:ILE:HG12	1:A:134:PRO:HD3	1.92	0.51
1:A:59:ASP:OD2	1:A:271:SER:OG	2.29	0.51
1:C:50:GLN:NE2	3:C:504:SO4:O2	2.42	0.51
1:C:112:GLU:OE1	2:G:1:GLC:O2	2.24	0.51
1:C:60:ILE:HD11	1:C:277:ALA:HB1	1.94	0.49
1:A:415:GLN:OE1	1:A:439:ARG:NH2	2.41	0.49
1:C:43:LYS:HE2	1:C:45:GLU:OE2	2.13	0.49
1:A:448:ASP:OD1	1:A:452:ARG:NH1	2.41	0.48
1:C:320:ALA:O	1:C:324:ASN:ND2	2.44	0.48
1:A:159:TRP:N	1:A:160:PRO:CD	2.77	0.48
1:B:107:TYR:OH	1:B:282:GLU:OE2	2.27	0.48
1:C:69:GLY:HA3	1:C:333:ASN:O	2.14	0.48
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.49	0.47
1:C:414:GLN:O	1:C:418:MET:N	2.42	0.47
1:C:197:VAL:O	1:C:201:LYS:HG2	2.14	0.47
1:C:341:TRP:HB3	2:G:3:GLC:O5	2.15	0.47
1:A:50:GLN:O	1:A:414:GLN:NE2	2.48	0.47
1:B:26:LYS:O	1:B:30:LYS:N	2.49	0.46
1:C:80:ILE:HG22	1:C:82:PRO:HD3	1.98	0.46
1:B:448:ASP:OD1	1:B:452:ARG:HD2	2.16	0.46
1:C:370:ALA:HB1	1:D:456:LEU:CD2	2.46	0.46
1:C:387:TRP:HB2	1:C:412:ARG:NH1	2.31	0.46
1:C:416:TYR:CZ	1:C:439:ARG:NH1	2.84	0.46
1:D:183:GLY:O	1:D:186:ASN:ND2	2.49	0.46
1:C:166:GLY:O	1:C:186:ASN:ND2	2.49	0.45
1:B:275:GLU:N	1:B:275:GLU:OE1	2.44	0.45
1:C:115:SER:OG	1:C:324:ASN:ND2	2.48	0.45
1:B:98:VAL:HG21	1:B:106:ALA:HB3	1.99	0.45
1:C:159:TRP:N	1:C:160:PRO:CD	2.80	0.45
1:C:25:GLY:O	1:C:29:GLU:N	2.36	0.45
1:D:235:ASN:O	1:D:238:THR:OG1	2.31	0.45
1:C:141:LYS:NZ	1:C:203:LYS:O	2.48	0.45
1:C:65:HIS:NE2	1:C:331:MET:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HG23	1:B:38:VAL:HA	1.99	0.44
1:C:21:LEU:HD23	1:C:38:VAL:HG11	2.00	0.44
1:C:59:ASP:OD2	1:C:271:SER:OG	2.29	0.44
1:D:66:ASP:HA	1:D:333:ASN:HA	1.98	0.44
1:D:378:VAL:O	1:D:381:ALA:N	2.47	0.44
1:C:161:LEU:HD12	1:C:162:ILE:N	2.33	0.44
1:C:23:GLU:HA	1:C:26:LYS:HE3	1.99	0.44
1:D:1:MET:HB3	1:D:7:LYS:NZ	2.32	0.44
1:B:315:ASP:OD1	1:B:317:ARG:N	2.49	0.44
1:D:245:VAL:CG2	1:D:317:ARG:HA	2.47	0.44
1:B:15:ASP:OD1	1:B:16:LYS:NZ	2.40	0.44
1:D:12:ILE:O	1:D:40:HIS:HA	2.17	0.44
1:A:65:HIS:NE2	1:A:331:MET:O	2.47	0.43
1:D:232:ALA:O	1:D:236:ILE:HD12	2.18	0.43
1:A:438:GLU:OE2	1:A:452:ARG:NH1	2.50	0.43
1:D:9:VAL:N	1:D:59:ASP:OD2	2.37	0.43
1:B:166:GLY:O	1:B:186:ASN:ND2	2.45	0.43
1:D:350:ASN:HB3	1:D:356:GLN:HG2	2.01	0.43
1:B:455:ARG:HD3	3:B:504:SO4:O2	2.18	0.43
1:A:137:ASP:O	1:A:141:LYS:N	2.45	0.43
1:B:133:ILE:N	1:B:134:PRO:CD	2.81	0.43
1:C:161:LEU:HD12	1:C:162:ILE:HG13	2.00	0.43
1:D:315:ASP:O	1:D:318:ILE:HG22	2.18	0.43
1:C:448:ASP:OD1	1:C:448:ASP:C	2.56	0.43
1:D:166:GLY:O	1:D:186:ASN:ND2	2.52	0.42
1:D:313:ALA:HA	1:D:318:ILE:HG21	2.02	0.42
1:B:159:TRP:N	1:B:160:PRO:CD	2.82	0.42
1:D:302:ALA:HA	1:D:318:ILE:HD11	2.01	0.42
1:B:90:LEU:HD12	1:B:95:TRP:CZ2	2.55	0.42
1:C:123:LEU:HD21	1:C:126:PRO:CA	2.50	0.42
1:C:384:ALA:O	1:C:386:ARG:HG3	2.20	0.42
1:A:242:ASN:OD1	1:A:242:ASN:N	2.52	0.42
1:B:80:ILE:HG22	1:B:82:PRO:HD3	2.02	0.42
1:A:418:MET:HG2	1:A:432:ALA:HB3	2.01	0.42
1:C:336:GLN:N	1:C:336:GLN:OE1	2.52	0.42
1:D:182:VAL:O	1:D:366:GLN:NE2	2.52	0.41
1:A:145:LYS:NZ	1:A:221:GLY:O	2.40	0.41
1:A:394:LEU:HD11	1:B:449:LEU:HD23	2.02	0.41
1:C:387:TRP:CH2	1:C:408:ILE:HG21	2.55	0.41
1:A:80:ILE:HG22	1:A:82:PRO:HD3	2.02	0.41
1:D:133:ILE:HD12	1:D:133:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.55	0.41
1:B:66:ASP:OD2	2:F:2:GLC:O3	2.25	0.41
1:A:390:PHE:O	1:A:393:THR:N	2.54	0.41
1:B:53:ALA:N	1:B:414:GLN:OE1	2.47	0.41
1:C:412:ARG:NH1	3:C:501:SO4:O4	2.53	0.41
1:A:133:ILE:N	1:A:134:PRO:CD	2.84	0.41
1:A:137:ASP:OD2	1:A:141:LYS:HE2	2.20	0.41
1:C:91:TYR:O	1:C:94:THR:OG1	2.34	0.41
1:B:280:PHE:O	1:B:284:TYR:HB2	2.21	0.41
1:C:430:LEU:H	1:C:430:LEU:HD12	1.86	0.40
1:A:162:ILE:HA	1:A:192:GLY:HA3	2.04	0.40
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.56	0.40
1:B:16:LYS:NZ	2:F:1:GLC:O1	2.54	0.40
1:B:133:ILE:CG1	1:B:134:PRO:HD3	2.51	0.40
1:A:98:VAL:O	1:A:105:ILE:HG12	2.22	0.40
1:A:260:VAL:HB	1:A:330:ILE:HA	2.04	0.40
1:B:275:GLU:OE2	1:C:255:PRO:HG2	2.21	0.40
1:C:370:ALA:HB1	1:D:456:LEU:HD23	2.04	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	454/463 (98%)	434 (96%)	20 (4%)	0	100	100
1	B	454/463 (98%)	435 (96%)	19 (4%)	0	100	100
1	C	455/463 (98%)	434 (95%)	21 (5%)	0	100	100
1	D	456/463 (98%)	437 (96%)	18 (4%)	1 (0%)	47	73
All	All	1819/1852 (98%)	1740 (96%)	78 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	166	GLY

### 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	356/363 (98%)	350 (98%)	6 (2%)	60	84
1	B	356/363 (98%)	354 (99%)	2 (1%)	86	95
1	C	357/363 (98%)	353 (99%)	4 (1%)	73	90
1	D	358/363 (99%)	356 (99%)	2 (1%)	86	95
All	All	1427/1452 (98%)	1413 (99%)	14 (1%)	76	91

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

Mol	Chain	Res	Type
1	A	99	ARG
1	A	196	LEU
1	A	242	ASN
1	A	259	PHE
1	A	417	GLU
1	A	426	GLN
1	B	259	PHE
1	B	456	LEU
1	C	123	LEU
1	C	161	LEU
1	C	196	LEU
1	C	259	PHE
1	D	250	THR
1	D	259	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 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	GLC	E	1	2	12,12,12	1.26	1 (8%)	17,17,17	1.57	3 (17%)
2	GLC	E	2	2	11,11,12	1.53	3 (27%)	15,15,17	1.01	1 (6%)
2	GLC	E	3	2	11,11,12	1.72	2 (18%)	15,15,17	1.46	2 (13%)
2	GLC	F	1	2	12,12,12	1.24	1 (8%)	17,17,17	0.73	0
2	GLC	F	2	2	11,11,12	1.67	3 (27%)	15,15,17	1.09	1 (6%)
2	GLC	F	3	2	11,11,12	1.93	3 (27%)	15,15,17	1.39	2 (13%)
2	GLC	G	1	2	12,12,12	1.26	1 (8%)	17,17,17	0.79	0
2	GLC	G	2	2	11,11,12	1.54	2 (18%)	15,15,17	1.00	0
2	GLC	G	3	2	11,11,12	1.75	2 (18%)	15,15,17	1.13	1 (6%)
2	GLC	H	1	2	12,12,12	1.29	1 (8%)	17,17,17	1.10	0
2	GLC	H	2	2	11,11,12	1.63	2 (18%)	15,15,17	0.99	1 (6%)
2	GLC	H	3	2	11,11,12	1.82	2 (18%)	15,15,17	0.90	1 (6%)

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	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	2	-	2/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	2/2/19/22	0/1/1/1
2	GLC	G	3	2	-	2/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	GLC	O5-C1	5.13	1.51	1.43
2	H	3	GLC	O5-C1	4.90	1.51	1.43
2	E	3	GLC	O5-C1	4.67	1.51	1.43
2	G	3	GLC	O5-C1	4.66	1.51	1.43
2	H	2	GLC	O5-C1	3.83	1.49	1.43
2	F	2	GLC	O5-C1	3.72	1.49	1.43
2	G	2	GLC	O5-C1	3.46	1.49	1.43
2	E	2	GLC	O5-C1	3.33	1.49	1.43
2	E	1	GLC	O5-C1	2.87	1.50	1.42
2	H	2	GLC	O5-C5	2.78	1.49	1.43
2	F	2	GLC	O5-C5	2.76	1.49	1.43
2	G	1	GLC	O5-C1	2.76	1.49	1.42
2	H	1	GLC	O5-C1	2.73	1.49	1.42
2	E	2	GLC	O5-C5	2.68	1.48	1.43
2	F	1	GLC	O5-C1	2.68	1.49	1.42
2	F	3	GLC	O5-C5	2.58	1.48	1.43
2	G	2	GLC	O5-C5	2.50	1.48	1.43
2	H	3	GLC	O5-C5	2.46	1.48	1.43
2	G	3	GLC	O5-C5	2.34	1.48	1.43
2	F	2	GLC	C2-C3	-2.26	1.49	1.52
2	F	3	GLC	C2-C3	-2.18	1.49	1.52
2	E	3	GLC	O5-C5	2.14	1.47	1.43
2	E	2	GLC	C2-C3	-2.02	1.49	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	GLC	C1-C2-C3	3.93	114.50	109.67
2	E	1	GLC	O5-C1-C2	3.75	116.98	110.28
2	E	1	GLC	C1-C2-C3	3.53	117.64	110.31
2	G	3	GLC	C1-C2-C3	2.97	113.32	109.67
2	E	2	GLC	C1-O5-C5	-2.93	108.22	112.19
2	F	3	GLC	C1-O5-C5	2.85	116.06	112.19
2	F	3	GLC	C1-C2-C3	2.60	112.87	109.67
2	E	3	GLC	C1-O5-C5	-2.40	108.94	112.19
2	H	3	GLC	C1-C2-C3	2.28	112.47	109.67
2	H	2	GLC	C3-C4-C5	2.18	114.13	110.24
2	F	2	GLC	C3-C4-C5	2.09	113.96	110.24
2	E	1	GLC	C4-C3-C2	2.01	114.32	110.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	GLC	O5-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
2	F	3	GLC	C4-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	G	3	GLC	O5-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	G	2	GLC	O5-C5-C6-O6
2	G	2	GLC	C4-C5-C6-O6
2	G	3	GLC	C4-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 8 short contacts:

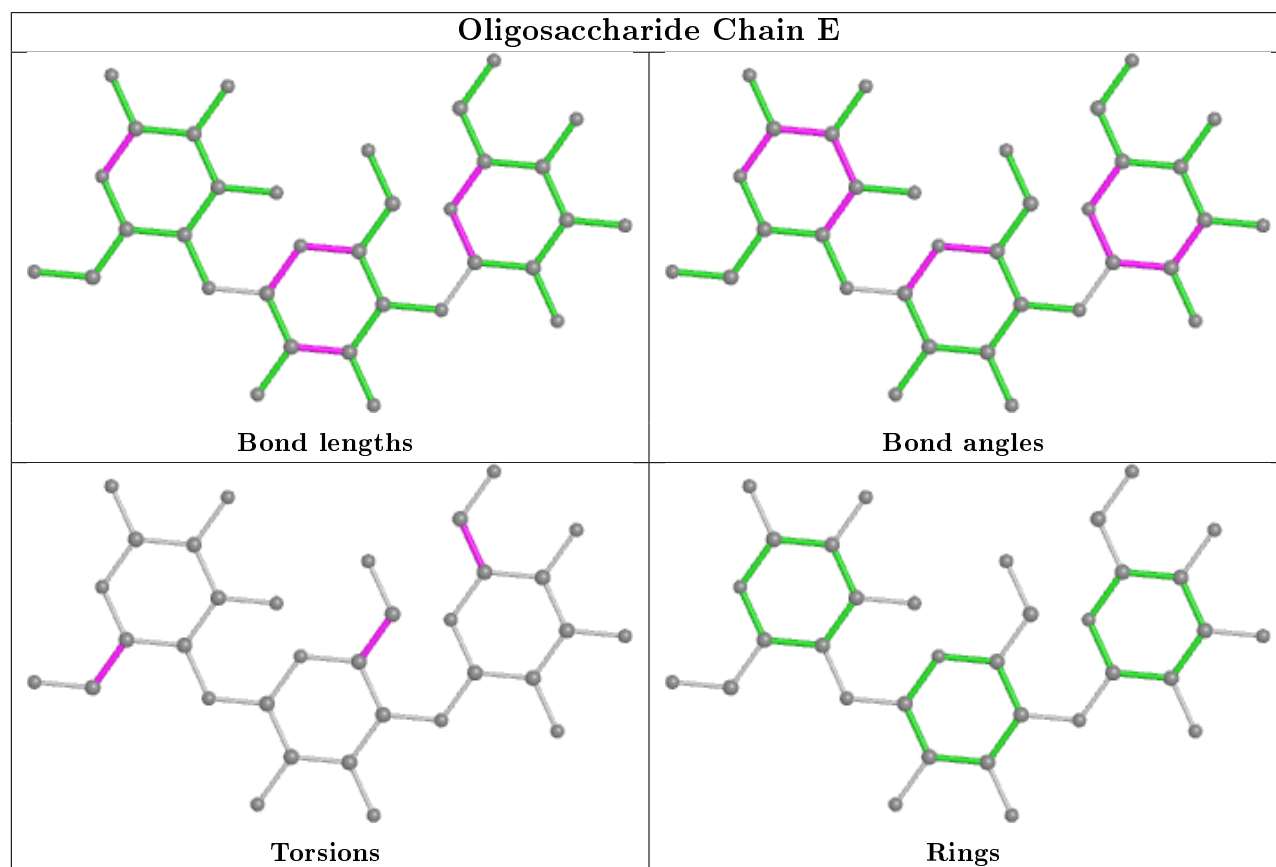
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	GLC	1	0
2	H	2	GLC	1	0
2	F	2	GLC	2	0
2	G	2	GLC	1	0

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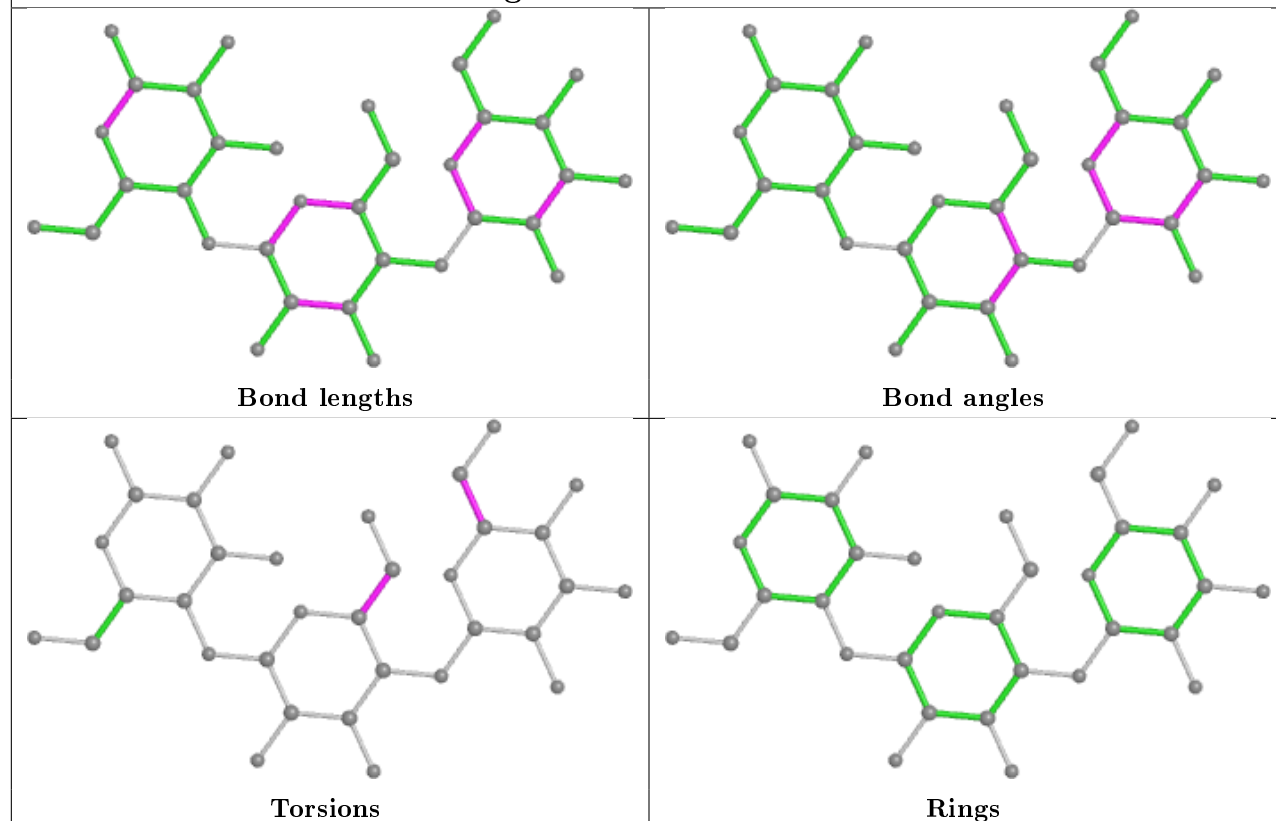
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	1	0
2	G	3	GLC	1	0
2	G	1	GLC	1	0

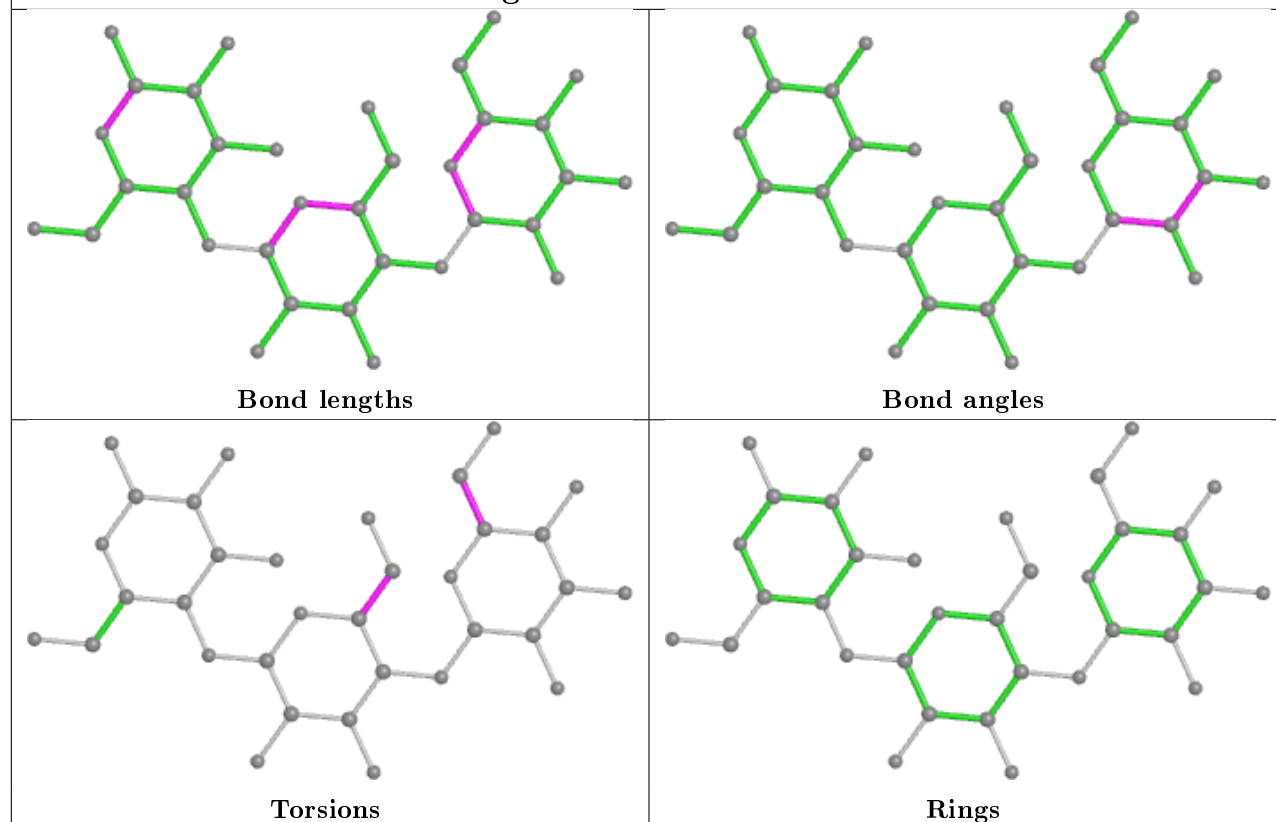
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

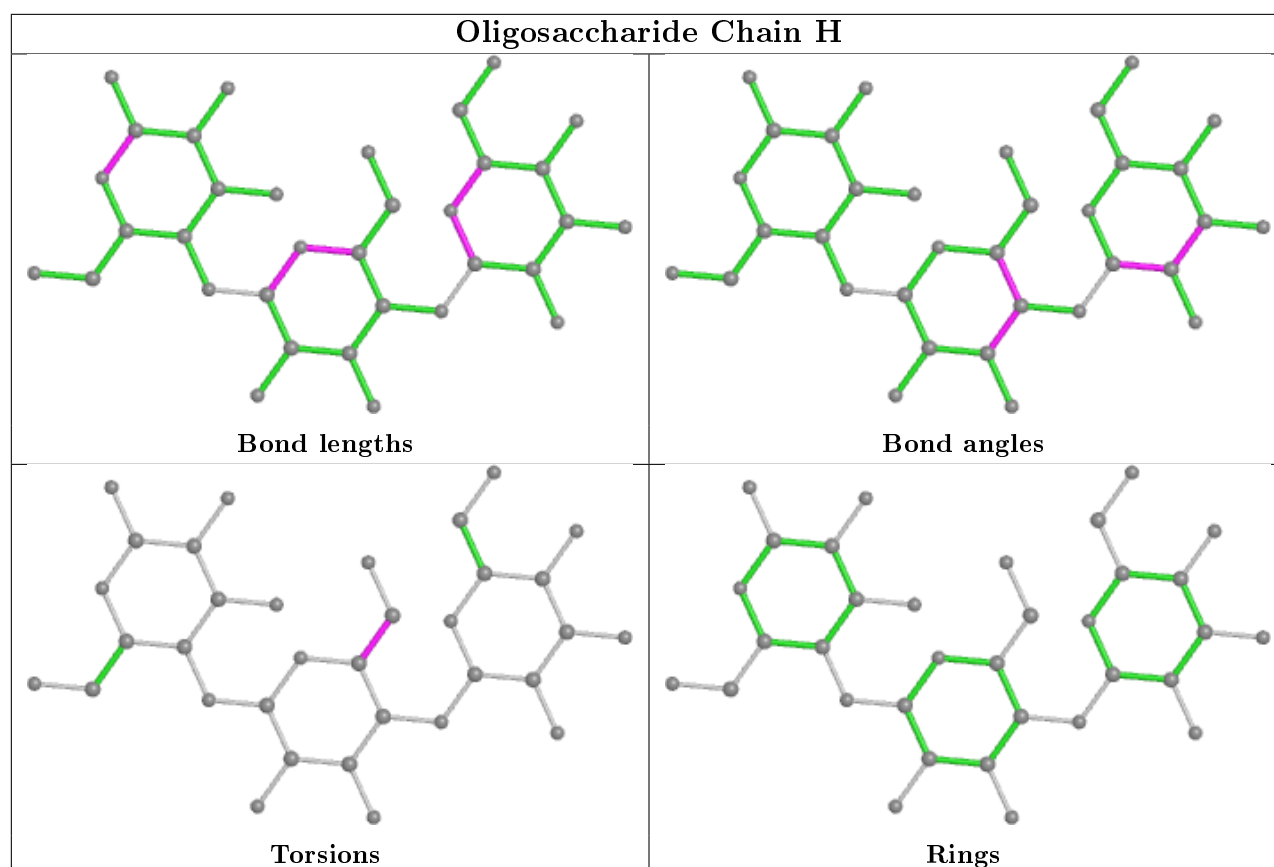


## Oligosaccharide Chain F



## Oligosaccharide Chain G





## 5.6 Ligand geometry [i](#)

20 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	D	504	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	C	501	-	4,4,4	0.18	0	6,6,6	0.10	0
3	SO4	D	501	-	4,4,4	0.16	0	6,6,6	0.05	0
3	SO4	A	501	-	4,4,4	0.17	0	6,6,6	0.08	0
3	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	D	502	-	4,4,4	0.13	0	6,6,6	0.11	0
3	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	C	504	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	SO4	1	0
3	C	501	SO4	2	0
3	C	504	SO4	1	0
3	A	503	SO4	1	0
3	D	503	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	456/463 (98%)	0.60	21 (4%)	32 31	38, 64, 100, 172	0
1	B	456/463 (98%)	0.75	37 (8%)	12 10	40, 66, 109, 211	0
1	C	457/463 (98%)	0.93	62 (13%)	3 2	44, 78, 128, 219	0
1	D	458/463 (98%)	0.87	48 (10%)	6 4	48, 75, 118, 186	0
All	All	1827/1852 (98%)	0.79	168 (9%)	9 7	38, 71, 115, 219	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	LYS	12.5
1	B	3	ILE	10.9
1	D	1	MET	10.6
1	D	3	ILE	9.4
1	C	145	LYS	8.3
1	C	148	LEU	7.7
1	C	129	THR	7.5
1	B	121	ASP	7.1
1	C	243	TYR	6.6
1	C	358	VAL	6.6
1	A	2	LYS	6.2
1	D	352	ALA	6.1
1	D	240	ALA	5.8
1	C	199	LEU	5.6
1	C	146	SER	5.5
1	B	196	LEU	5.3
1	B	5	GLU	5.1
1	D	117	ILE	5.0
1	B	240	ALA	4.9
1	C	221	GLY	4.9
1	A	3	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	142	ALA	4.8
1	C	135	ALA	4.7
1	C	147	ALA	4.7
1	A	250	THR	4.6
1	C	245	VAL	4.5
1	D	105	ILE	4.5
1	C	150	PHE	4.4
1	D	221	GLY	4.4
1	B	33	GLY	4.3
1	C	240	ALA	4.2
1	B	24	VAL	4.1
1	C	36	VAL	4.0
1	C	214	ALA	4.0
1	D	243	TYR	3.9
1	D	220	LYS	3.9
1	C	300	LEU	3.9
1	D	4	GLU	3.9
1	D	305	LEU	3.8
1	B	140	LEU	3.7
1	B	259	PHE	3.6
1	B	310	GLU	3.6
1	C	157	PHE	3.6
1	A	211	TYR	3.6
1	C	83	ALA	3.6
1	D	247	VAL	3.5
1	C	326	GLN	3.5
1	D	148	LEU	3.4
1	C	362	LEU	3.3
1	D	150	PHE	3.3
1	C	204	HIS	3.2
1	D	399	ALA	3.2
1	A	186	ASN	3.1
1	A	240	ALA	3.1
1	C	136	LEU	3.1
1	A	133	ILE	3.1
1	A	148	LEU	3.1
1	C	218	PHE	3.1
1	D	351	ALA	3.1
1	A	196	LEU	3.1
1	C	116	LEU	3.1
1	D	204	HIS	3.0
1	D	113	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	3.0
1	C	227	ILE	2.9
1	C	144	GLY	2.9
1	C	68	PHE	2.9
1	C	233	TRP	2.8
1	D	241	VAL	2.8
1	D	138	LYS	2.8
1	B	200	ILE	2.8
1	B	2	LYS	2.8
1	B	296	LYS	2.8
1	C	113	ALA	2.8
1	B	34	ILE	2.8
1	D	187	ALA	2.7
1	C	359	ASP	2.7
1	B	133	ILE	2.7
1	C	202	ASN	2.7
1	C	149	MET	2.7
1	D	140	LEU	2.7
1	A	327	LYS	2.7
1	D	314	LYS	2.7
1	B	456	LEU	2.7
1	D	167	GLY	2.7
1	D	199	LEU	2.7
1	C	325	ALA	2.7
1	A	192	GLY	2.7
1	B	291	LEU	2.6
1	D	348	VAL	2.6
1	D	145	LYS	2.6
1	B	294	VAL	2.6
1	C	196	LEU	2.6
1	B	97	ALA	2.6
1	B	7	LYS	2.6
1	C	39	GLU	2.6
1	D	218	PHE	2.6
1	B	372	ALA	2.6
1	B	236	ILE	2.5
1	D	236	ILE	2.5
1	A	140	LEU	2.5
1	C	241	VAL	2.5
1	A	224	ALA	2.5
1	D	416	TYR	2.5
1	D	358	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	102	GLY	2.5
1	B	144	GLY	2.5
1	C	318	ILE	2.4
1	C	242	ASN	2.4
1	B	176	LYS	2.4
1	C	305	LEU	2.4
1	C	286	LEU	2.4
1	B	130	TRP	2.4
1	B	361	ALA	2.4
1	D	362	LEU	2.4
1	D	21	LEU	2.4
1	B	80	ILE	2.4
1	B	20	GLY	2.4
1	D	191	ALA	2.4
1	A	241	VAL	2.4
1	B	101	ASN	2.3
1	D	219	ASN	2.3
1	D	429	GLY	2.3
1	C	3	ILE	2.3
1	C	217	ALA	2.3
1	C	455	ARG	2.3
1	D	18	TYR	2.3
1	D	193	LEU	2.3
1	C	351	ALA	2.3
1	C	1	MET	2.3
1	A	265	ALA	2.3
1	C	5	GLU	2.3
1	D	408	ILE	2.3
1	B	177	TYR	2.3
1	C	16	LYS	2.2
1	C	195	PHE	2.2
1	D	108	PRO	2.2
1	B	1	MET	2.2
1	D	198	ASP	2.2
1	C	184	VAL	2.2
1	C	125	ASN	2.2
1	A	205	MET	2.2
1	D	195	PHE	2.2
1	C	348	VAL	2.2
1	C	56	ASP	2.2
1	C	231	TRP	2.2
1	D	318	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	122	LEU	2.1
1	C	117	ILE	2.1
1	C	284	TYR	2.1
1	A	249	PRO	2.1
1	C	456	LEU	2.1
1	C	152	LEU	2.1
1	B	369	ALA	2.1
1	A	176	LYS	2.1
1	A	303	VAL	2.1
1	D	349	ILE	2.1
1	C	244	GLY	2.1
1	B	277	ALA	2.1
1	B	246	THR	2.1
1	D	144	GLY	2.1
1	A	285	LEU	2.0
1	B	42	ASP	2.0
1	C	205	MET	2.0
1	D	130	TRP	2.0
1	C	404	VAL	2.0
1	B	308	TYR	2.0
1	C	193	LEU	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, 95<sup>th</sup> 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.

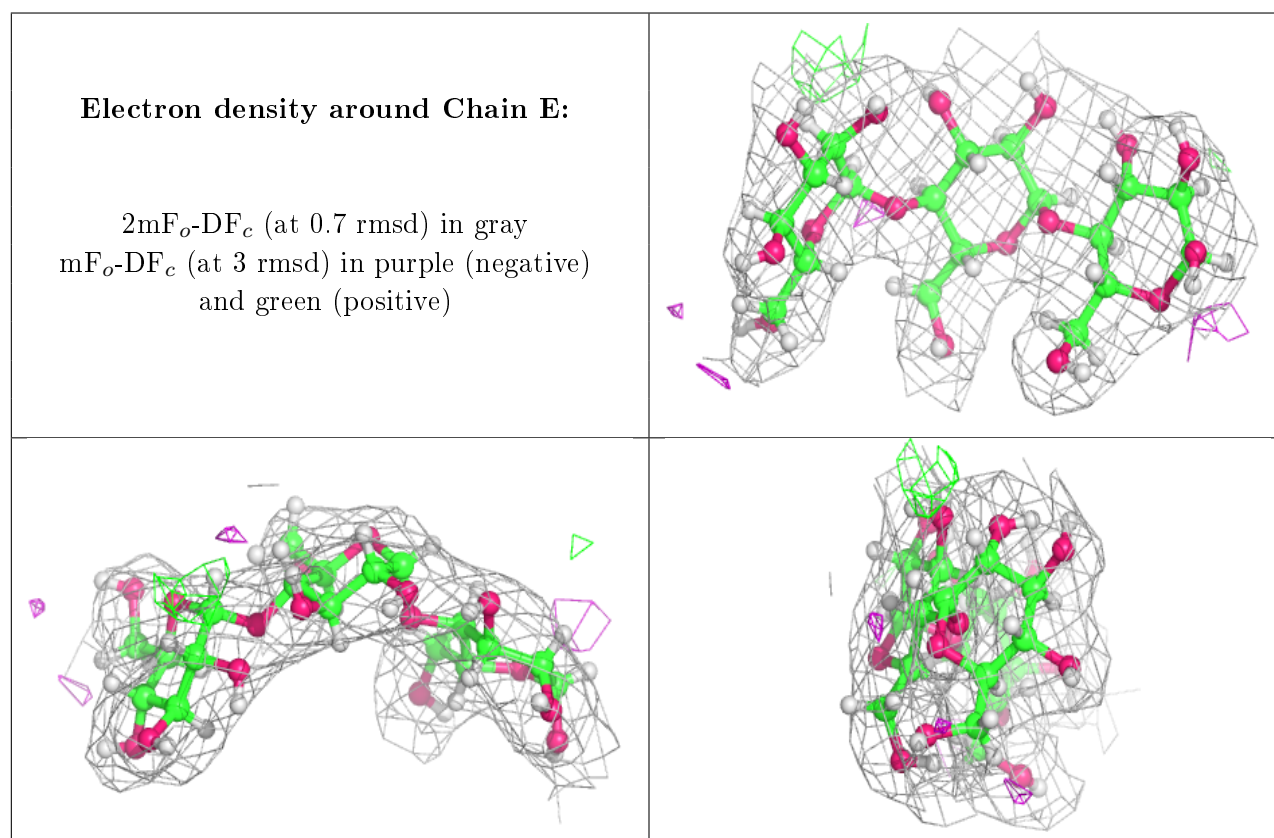
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	G	3	11/12	0.86	0.50	80,94,107,113	0
2	GLC	H	3	11/12	0.92	0.16	58,64,75,77	0
2	GLC	G	1	12/12	0.92	0.21	56,58,69,71	0
2	GLC	H	2	11/12	0.93	0.16	46,51,60,61	0
2	GLC	E	1	12/12	0.93	0.18	44,46,55,56	0
2	GLC	E	3	11/12	0.94	0.13	51,55,65,66	0
2	GLC	G	2	11/12	0.95	0.19	47,59,71,74	0

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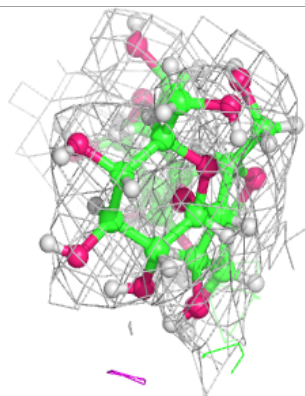
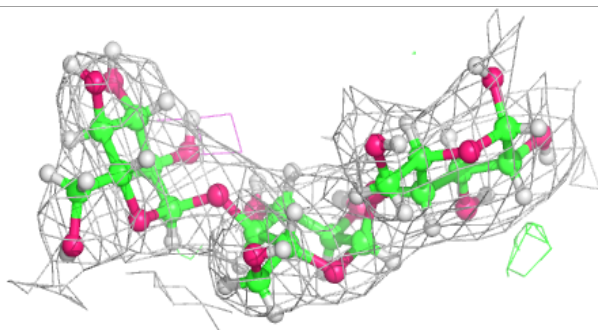
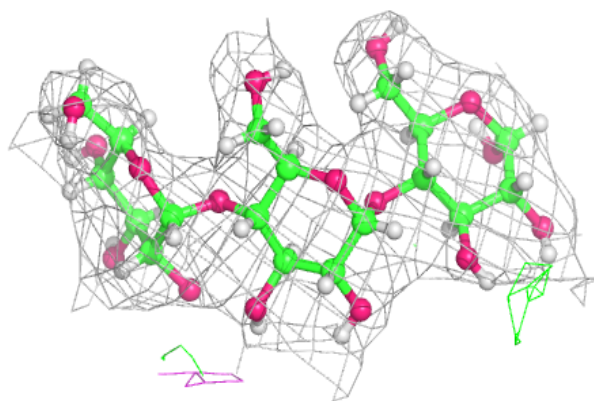
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	F	3	11/12	0.95	0.20	57,62,74,74	0
2	GLC	E	2	11/12	0.96	0.15	43,44,53,54	0
2	GLC	F	2	11/12	0.97	0.18	32,49,59,59	0
2	GLC	H	1	12/12	0.97	0.17	49,50,59,60	0
2	GLC	F	1	12/12	0.97	0.18	51,54,65,65	0

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.

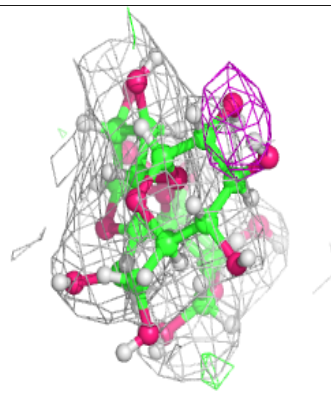
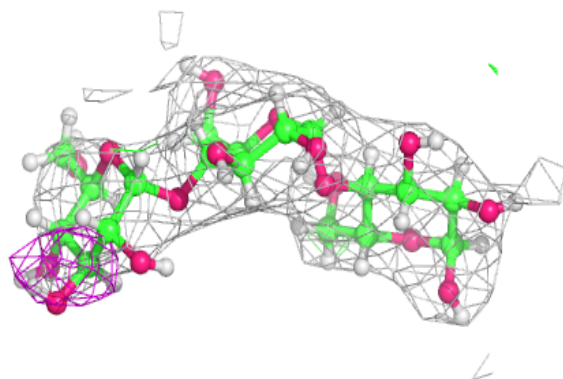
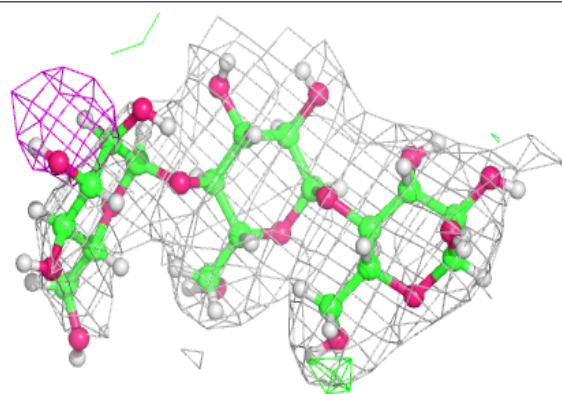


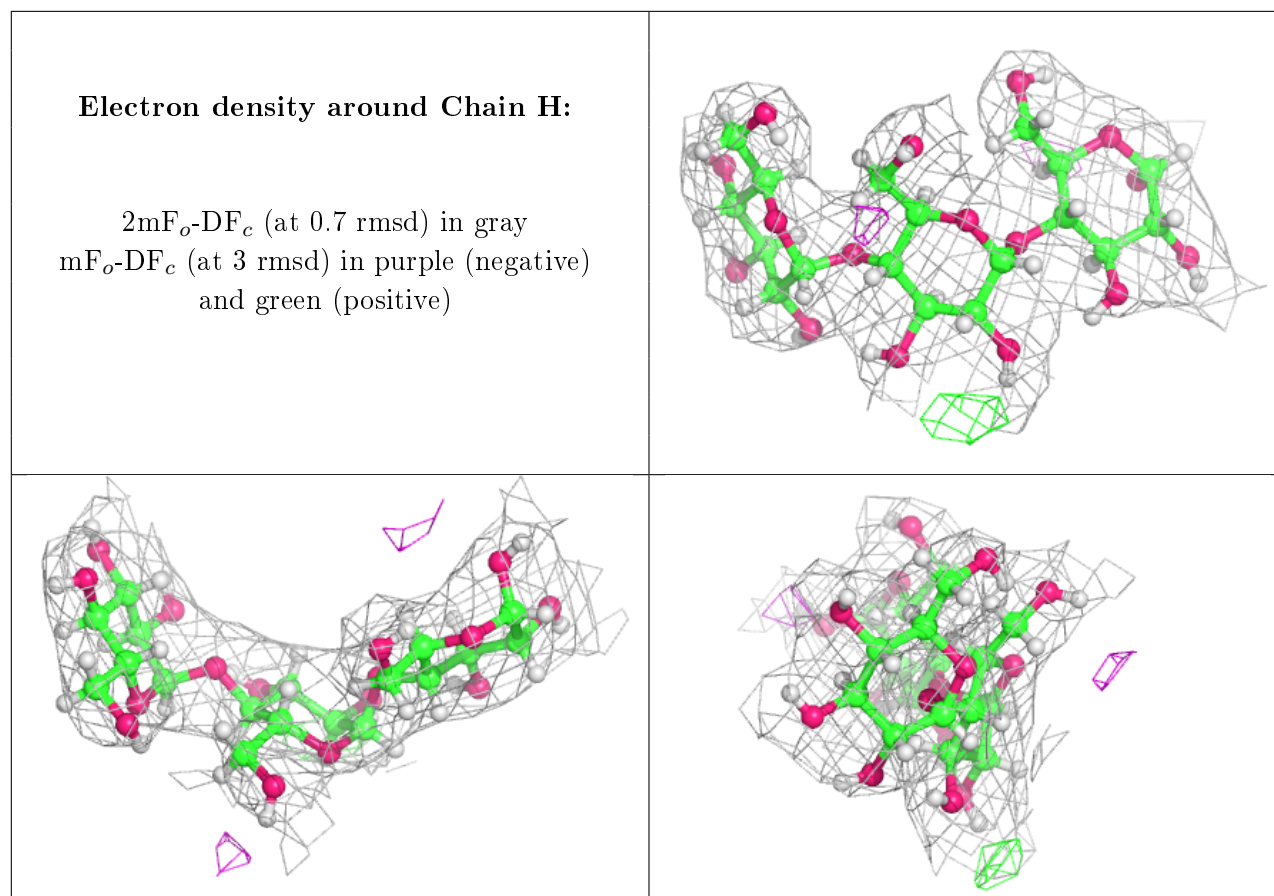
**Electron density around Chain F:**

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

**Electron density around Chain G:**

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





## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	C	502	5/5	0.82	0.22	104,104,104,104	0
3	SO4	B	504	5/5	0.84	0.24	128,128,128,128	0
3	SO4	B	505	5/5	0.87	0.21	86,87,87,87	0
3	SO4	B	503	5/5	0.89	0.17	75,75,75,75	0
3	SO4	C	504	5/5	0.89	0.19	108,109,109,109	0
3	SO4	A	504	5/5	0.90	0.20	106,106,106,106	0
3	SO4	D	503	5/5	0.90	0.29	119,119,119,120	0
3	SO4	A	505	5/5	0.93	0.16	80,81,81,81	0
3	SO4	B	506	5/5	0.93	0.17	89,89,89,89	0
3	SO4	C	501	5/5	0.95	0.25	88,88,89,90	0
3	SO4	B	502	5/5	0.95	0.14	78,79,79,79	0
3	SO4	A	503	5/5	0.95	0.14	69,69,69,70	0
3	SO4	C	503	5/5	0.95	0.11	79,79,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	502	5/5	0.95	0.16	73,73,73,74	0
3	SO4	D	505	5/5	0.96	0.18	94,95,95,95	0
3	SO4	A	502	5/5	0.96	0.13	80,80,80,80	0
3	SO4	A	501	5/5	0.96	0.28	89,89,90,91	0
3	SO4	D	501	5/5	0.97	0.21	63,64,64,64	0
3	SO4	D	504	5/5	0.97	0.14	83,83,83,83	0
3	SO4	B	501	5/5	0.97	0.18	46,55,59,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.