



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:04 AM UTC

PDB ID : 5YGS / pdb_00005ygs
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

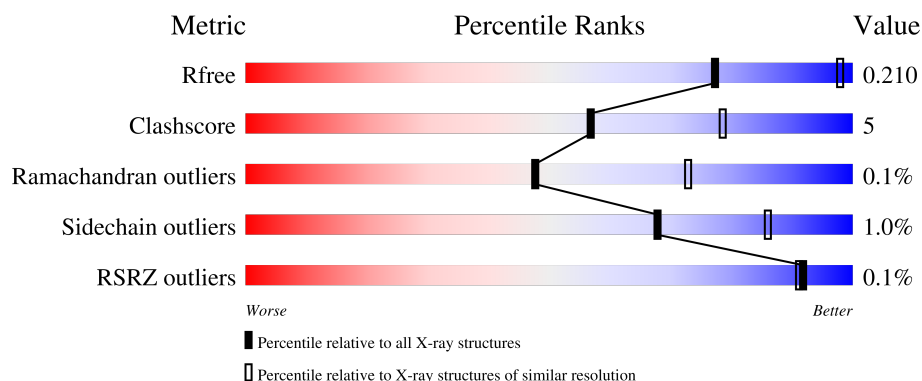
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

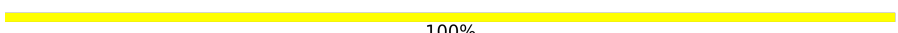
The reported resolution of this entry is 2.69 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	463	 87% 11% .
1	B	463	 89% 10% .
1	C	463	 83% 15% .
1	D	463	 89% 10% .
2	E	3	 100%

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Mol	Chain	Length	Quality of chain
2	F	3	 100%
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 (CCD ID: SO4) (formula: O₄S).



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	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		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

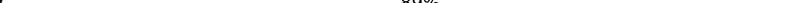
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		

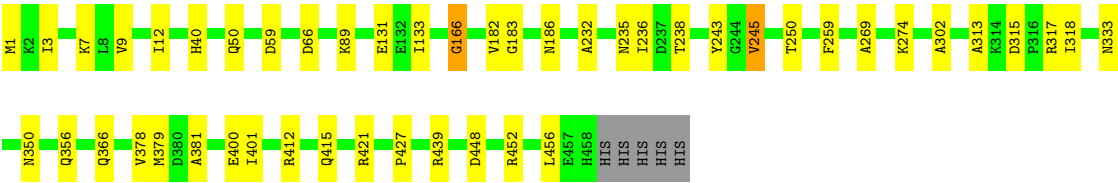
● Molecule 1: Human TNRSF25 death domain

I330	I331	P332	N333	N368	M379	F390	T393	L394	E400	R412	D413	Q414	Q415	Y416	E417	M418	R421	Q426	P427	A432	E438	A439	D448	R452	E457	HIS	HIS	HIS	HIS	HIS	HIS	F259	V260	S271	F377
K47	Q50	D59	H65	G69	T80	T81	P82	V88	I105	I133	P134	D137	K141	K145	Y159	P160	L161	I162	Y168	D181	G192	L196	K201	G221	P230	W233	M242	Y243	F259	V260	S271	F377			

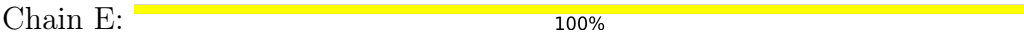
H1	L281 E282 Y284	D316 F316 R317	K26 V382	K30 R412	V39 Q414	E45 Q425	A53 D448 L449	D66 R67 R452	I80 L455 R456	T81 G82	L90	W95	V98	A106 Y107	E131 G132 I133 P134	E134	W159 P160	G166	M166	N219	P230	W233	S239	E275	F280
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R421	V197	W1
P427	K201	Y18
L430	N202	L21
R439	K203	A22
D448	M225	E23
E457	P230	V24
HIS	P233	K26
HIS	Y243	E29
HIS	P255	G33
HIS	A269	V38
HIS	A270	K43
HIS	S271	L44
	K274	E46
	A277	Q50
	R317	D59
	A320	I60
	E323	H65
	N324	D66
	K327	G69
	M331	I80
	P332	T81
	N333	P82
	Q336	Y91
	W341	T94
	A370	E112
	V382	A113
	P383	L114
	A384	S115
	R385	L123
	R386	P126
	W387	K141
	I408	W159
	R412	P160
	D413	L161
	Q414	I162
	Q415	D165
	E417	G166
	M418	W186

Chain D:  89% 10%



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



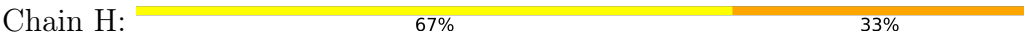
● Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



● 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, α , β , γ	73.69Å 153.55Å 98.24Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	98.25 – 2.69 98.24 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.6 (98.25-2.69) 99.0 (98.24-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX v1.12-2829	Depositor
R, R_{free}	0.190 , 0.212 0.193 , 0.210	Depositor DCC
R_{free} test set	3023 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	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	0.96	EDS
Total number of atoms	28638	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: SO4, GLC

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	0.15	0/3621	0.30	0/4913
1	B	0.14	0/3620	0.29	0/4911
1	C	0.14	0/3629	0.29	0/4923
1	D	0.13	0/3640	0.29	0/4938
All	All	0.14	0/14510	0.29	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	47	0
1	D	3559	3531	3531	30	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	131	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 (131) 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:N	1:B:5:GLU:OE1	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:N	1:D:131:GLU:OE1	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:N	1:C:165:ASP:OD1	2.32	0.63
1:D:400:GLU:OE2	1:D:401:ILE:N	2.39	0.56
1:B:45:GLU:N	1:B:45:GLU:OE1	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:HD23	1:C:123:LEU:O	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:59:ASP:OD2	1:A:271:SER:OG	2.29	0.51
1:A:133:ILE:HG12	1:A:134:PRO:HD3	1.92	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:B:66:ASP:OD2	2:F:2:GLC:O3	2.25	0.49
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:448:ASP:OD1	1:C:448:ASP:C	2.56	0.47
1:C:59:ASP:OD2	1:C:271:SER:OG	2.29	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:OE1	1:B:275:GLU:N	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:25:GLY:O	1:C:29:GLU:N	2.36	0.45
1:C:159:TRP:N	1:C:160:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:OE1	1:C:336:GLN:N	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:C:323:GLU:OE2	1:C:327:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.55	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:HD12	1:C:430:LEU:H	1.86	0.40
1:A:162:ILE:HA	1:A:192:GLY:HA3	2.04	0.40
1:B:16:LYS:NZ	2:F:1:GLC:O1	2.54	0.40
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.56	0.40
1:D:378:VAL:O	1:D:379:MET:C	2.65	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 ⓘ

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	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%)	43	68
All	All	1819/1852 (98%)	1740 (96%)	78 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	166	GLY

5.3.2 Protein sidechains [i](#)

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%)	351 (99%)	5 (1%)	59	82
1	B	356/363 (98%)	354 (99%)	2 (1%)	78	91
1	C	357/363 (98%)	354 (99%)	3 (1%)	73	88
1	D	358/363 (99%)	354 (99%)	4 (1%)	65	85
All	All	1427/1452 (98%)	1413 (99%)	14 (1%)	68	86

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

Mol	Chain	Res	Type
1	A	196	LEU
1	A	242	ASN
1	A	259	PHE
1	A	417	GLU
1	A	426	GLN
1	B	425	GLN
1	B	456	LEU
1	C	123	LEU
1	C	165	ASP
1	C	225	MET
1	D	89	LYS
1	D	245	VAL
1	D	250	THR
1	D	259	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	366	GLN
1	B	40	HIS
1	B	426	GLN
1	C	235	ASN
1	C	326	GLN
1	D	40	HIS
1	D	458	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 ⓘ

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	1.27	1 (8%)	17,17,17	1.58	2 (11%)
2	GLC	E	2	2	11,11,12	1.50	2 (18%)	15,15,17	1.01	1 (6%)
2	GLC	E	3	2	11,11,12	1.67	2 (18%)	15,15,17	1.30	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	1.63	3 (27%)	15,15,17	1.03	1 (6%)
2	GLC	F	3	2	11,11,12	1.88	3 (27%)	15,15,17	1.29	2 (13%)
2	GLC	G	1	2	12,12,12	1.26	1 (8%)	17,17,17	0.78	0
2	GLC	G	2	2	11,11,12	1.50	2 (18%)	15,15,17	0.97	0
2	GLC	G	3	2	11,11,12	1.71	2 (18%)	15,15,17	0.98	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	H	1	2	12,12,12	1.28	1 (8%)	17,17,17	1.10	0
2	GLC	H	2	2	11,11,12	1.60	2 (18%)	15,15,17	0.95	1 (6%)
2	GLC	H	3	2	11,11,12	1.77	2 (18%)	15,15,17	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	GLC	O5-C1	4.89	1.51	1.43
2	H	3	GLC	O5-C1	4.67	1.51	1.43
2	E	3	GLC	O5-C1	4.46	1.51	1.43
2	G	3	GLC	O5-C1	4.44	1.51	1.43
2	H	2	GLC	O5-C1	3.66	1.49	1.43
2	F	2	GLC	O5-C1	3.55	1.49	1.43
2	G	2	GLC	O5-C1	3.30	1.49	1.43
2	E	2	GLC	O5-C1	3.18	1.49	1.43
2	E	1	GLC	O5-C1	2.95	1.50	1.42
2	H	2	GLC	O5-C5	2.89	1.49	1.43
2	F	2	GLC	O5-C5	2.88	1.49	1.43
2	G	1	GLC	O5-C1	2.83	1.49	1.42
2	E	2	GLC	O5-C5	2.80	1.48	1.43
2	H	1	GLC	O5-C1	2.79	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	GLC	O5-C1	2.75	1.49	1.42
2	F	3	GLC	O5-C5	2.69	1.48	1.43
2	G	2	GLC	O5-C5	2.61	1.48	1.43
2	H	3	GLC	O5-C5	2.57	1.48	1.43
2	G	3	GLC	O5-C5	2.44	1.48	1.43
2	E	3	GLC	O5-C5	2.23	1.47	1.43
2	F	2	GLC	C2-C3	-2.16	1.49	1.52
2	F	3	GLC	C2-C3	-2.08	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GLC	O5-C1-C2	3.80	116.98	110.30
2	E	1	GLC	C1-C2-C3	3.57	117.64	110.36
2	E	3	GLC	C1-C2-C3	3.33	114.50	109.64
2	E	2	GLC	C1-O5-C5	-2.96	108.22	112.19
2	F	3	GLC	C1-O5-C5	2.89	116.06	112.19
2	G	3	GLC	C1-C2-C3	2.52	113.32	109.64
2	E	3	GLC	C1-O5-C5	-2.42	108.94	112.19
2	F	3	GLC	C1-C2-C3	2.21	112.87	109.64
2	H	2	GLC	C3-C4-C5	2.15	114.13	110.23
2	F	2	GLC	C3-C4-C5	2.06	113.96	110.23

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	2	GLC	C4-C5-C6-O6
2	F	3	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

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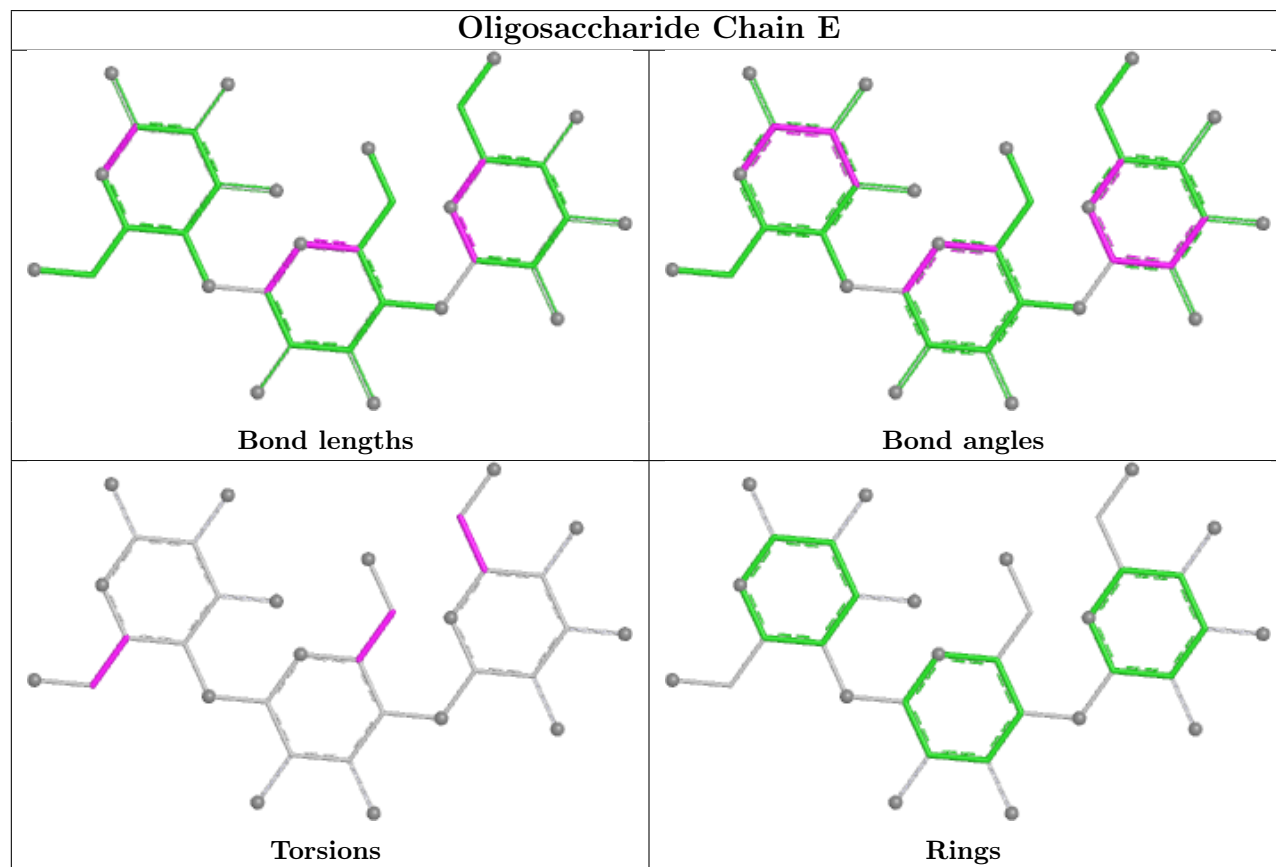
Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6

There are no ring outliers.

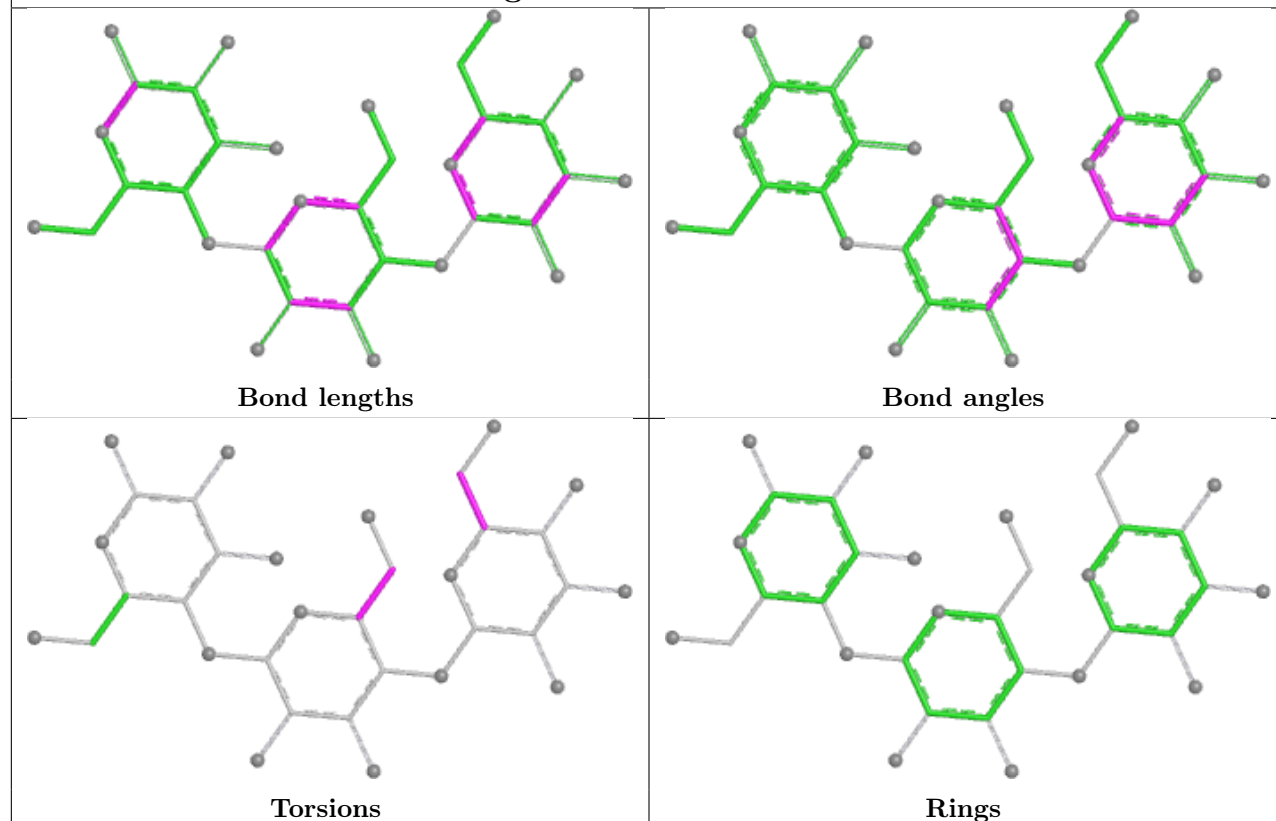
7 monomers are involved in 8 short contacts:

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

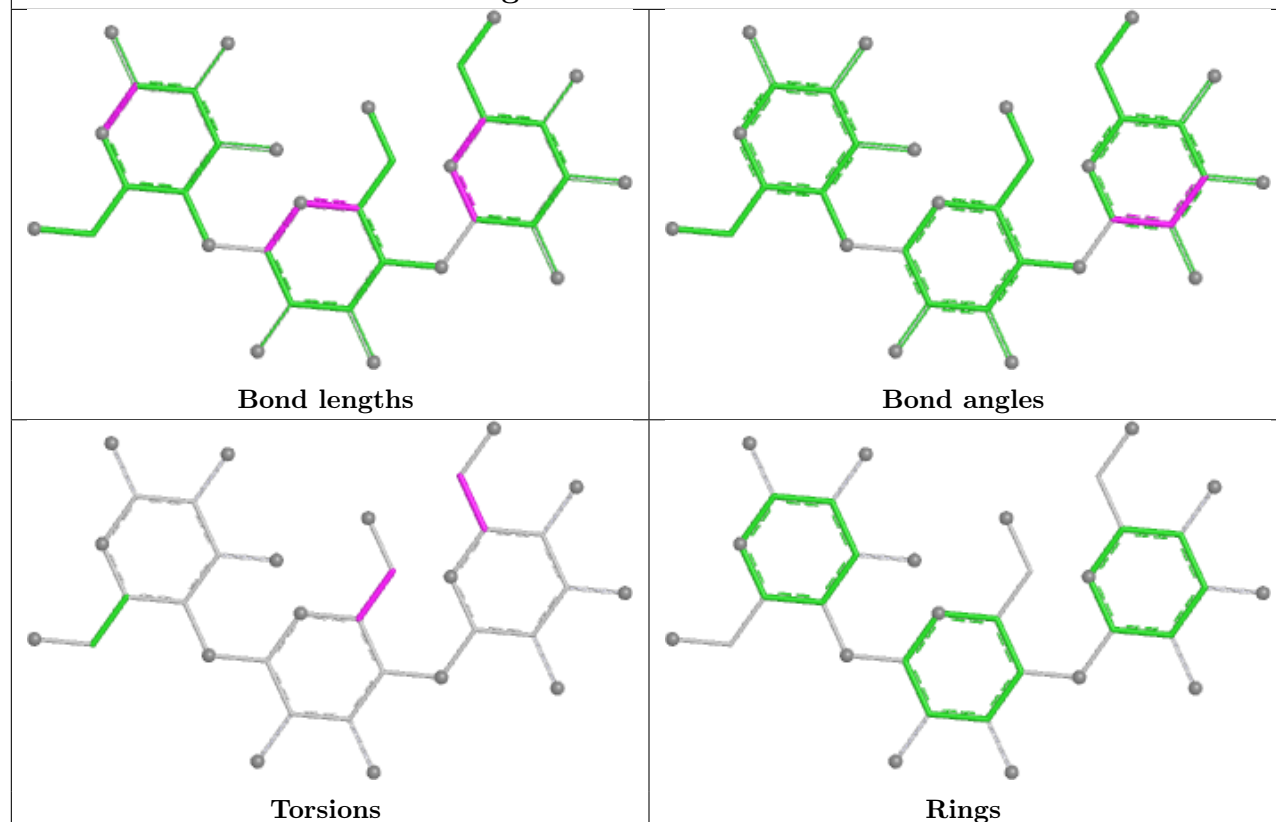
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

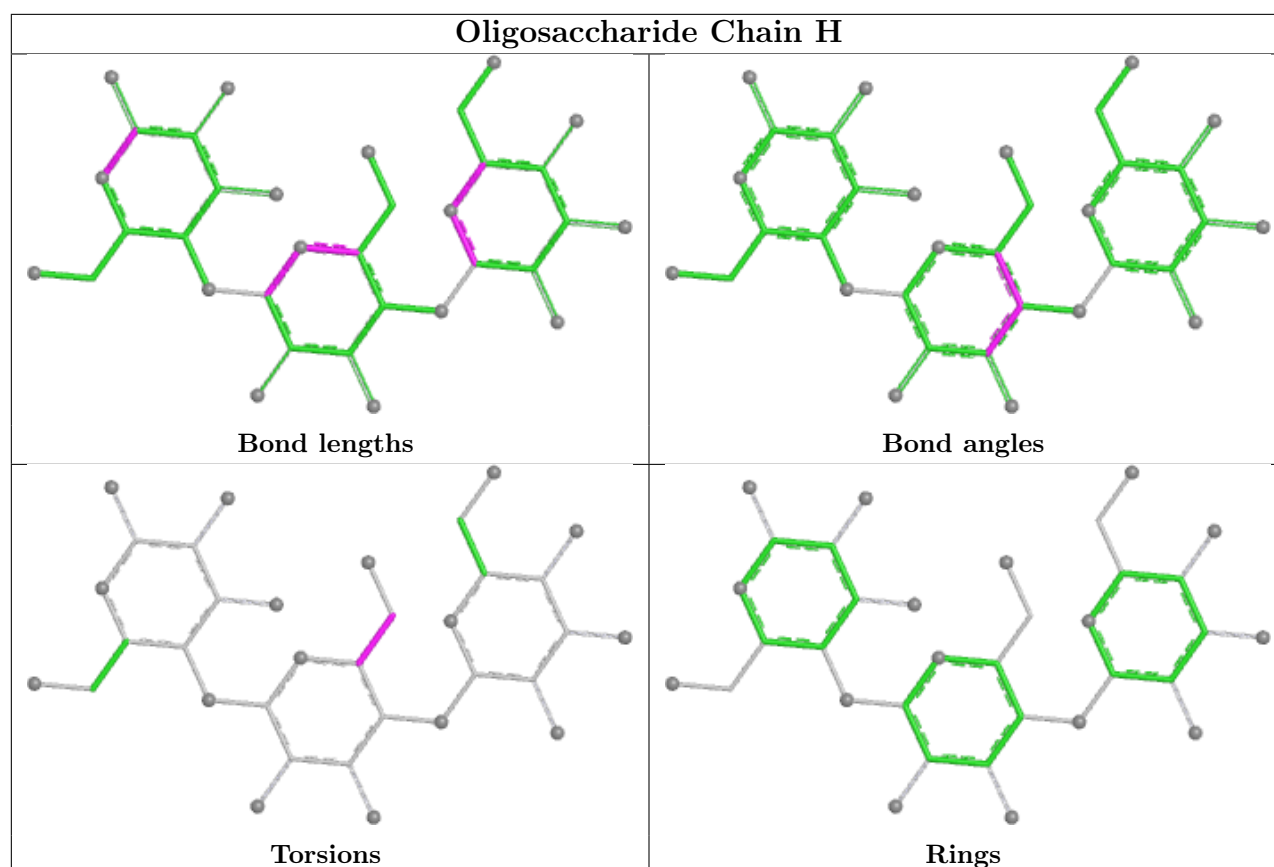


Oligosaccharide Chain F



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	C	501	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	505	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	B	501	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	506	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	503	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.06	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	C	501	SO4	2	0
3	C	504	SO4	1	0
3	B	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 [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	456/463 (98%)	-0.81	0 100 100	41, 70, 109, 197	0
1	B	456/463 (98%)	-0.77	0 100 100	45, 73, 117, 228	0
1	C	457/463 (98%)	-0.63	1 (0%) 91 90	48, 86, 139, 246	0
1	D	458/463 (98%)	-0.76	0 100 100	52, 83, 130, 212	0
All	All	1827/1852 (98%)	-0.74	1 (0%) 92 91	41, 77, 126, 246	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	ALA	2.2

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.

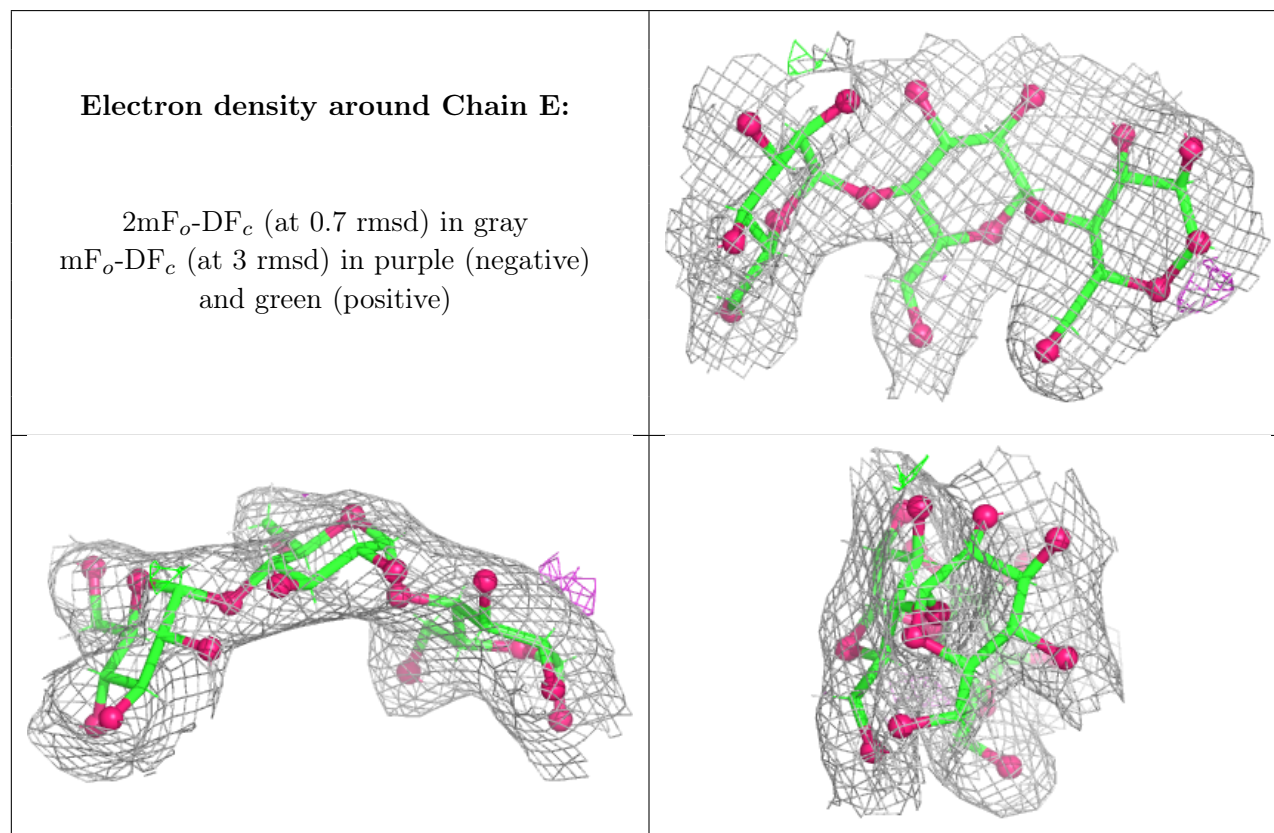
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	3	11/12	0.97	0.06	57,62,74,74	0
2	GLC	F	1	12/12	0.98	0.05	51,54,65,65	0
2	GLC	E	3	11/12	0.98	0.05	51,55,65,66	0
2	GLC	G	1	12/12	0.98	0.07	56,58,69,71	0
2	GLC	G	3	11/12	0.98	0.11	80,94,107,113	0
2	GLC	H	1	12/12	0.98	0.05	49,50,59,60	0

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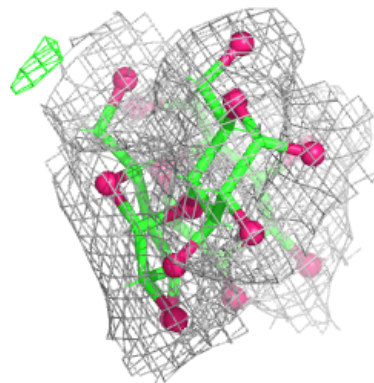
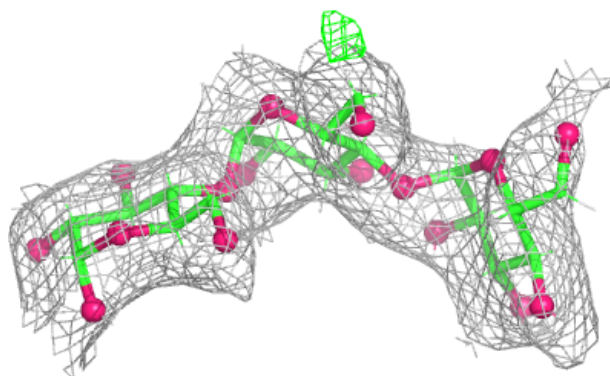
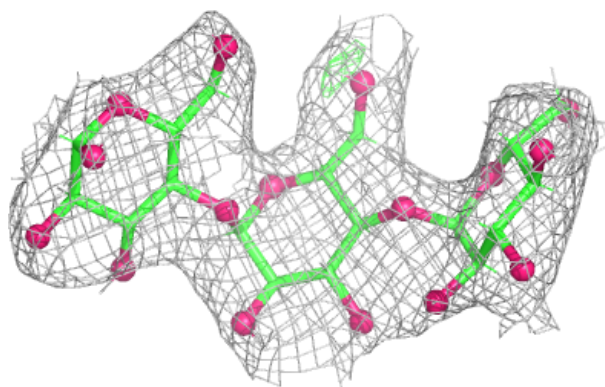
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	H	2	11/12	0.98	0.07	46,51,60,61	0
2	GLC	G	2	11/12	0.99	0.05	47,59,71,74	0
2	GLC	F	2	11/12	0.99	0.04	32,49,59,59	0
2	GLC	E	1	12/12	0.99	0.04	44,46,55,56	0
2	GLC	E	2	11/12	0.99	0.05	43,44,53,54	0
2	GLC	H	3	11/12	0.99	0.05	58,64,75,77	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.

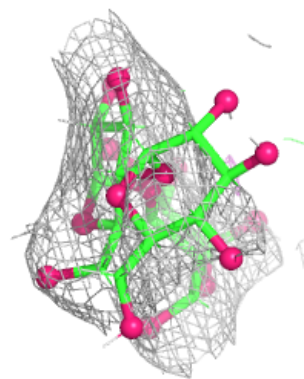
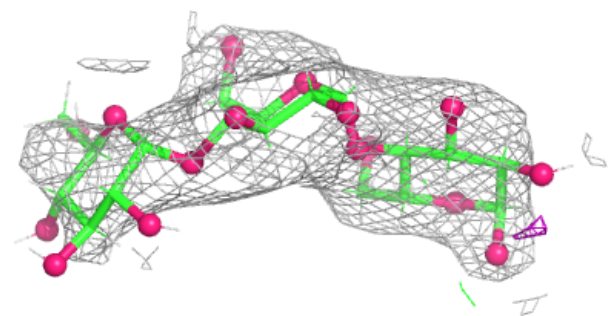
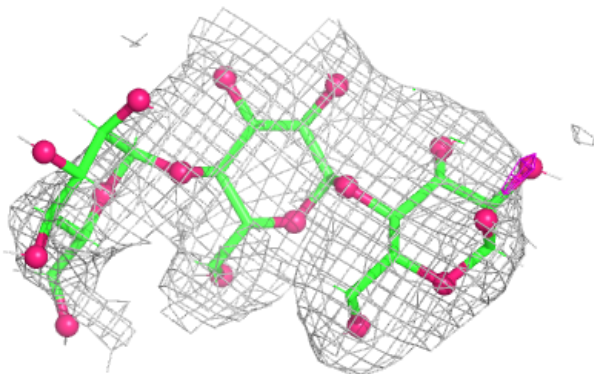


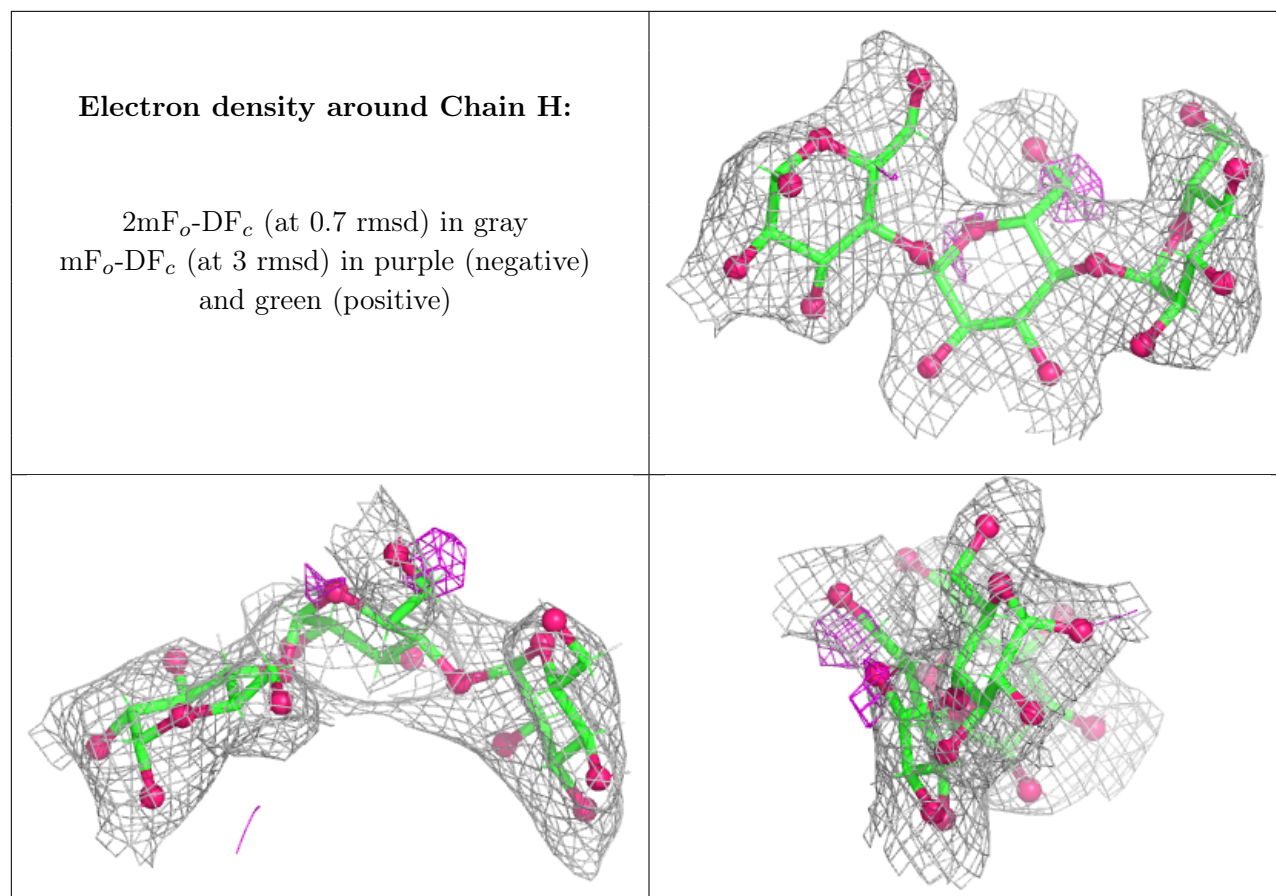
Electron density around Chain F:

$2mF_o - DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	504	5/5	0.94	0.07	108,109,109,109	0
3	SO4	B	503	5/5	0.96	0.07	75,75,75,75	0
3	SO4	A	505	5/5	0.97	0.06	80,81,81,81	0
3	SO4	B	502	5/5	0.97	0.06	78,79,79,79	0
3	SO4	A	503	5/5	0.97	0.07	69,69,69,70	0
3	SO4	B	506	5/5	0.97	0.10	89,89,89,89	0
3	SO4	C	503	5/5	0.97	0.07	79,79,80,80	0
3	SO4	A	504	5/5	0.97	0.06	106,106,106,106	0
3	SO4	D	503	5/5	0.97	0.08	119,119,119,120	0
3	SO4	D	505	5/5	0.97	0.06	94,95,95,95	0
3	SO4	D	502	5/5	0.98	0.04	73,73,73,74	0
3	SO4	B	505	5/5	0.98	0.09	86,87,87,87	0
3	SO4	D	504	5/5	0.98	0.05	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	504	5/5	0.98	0.07	128,128,128,128	0
3	SO4	A	502	5/5	0.99	0.04	80,80,80,80	0
3	SO4	D	501	5/5	0.99	0.05	63,64,64,64	0
3	SO4	A	501	5/5	0.99	0.07	89,89,90,91	0
3	SO4	C	501	5/5	0.99	0.07	88,88,89,90	0
3	SO4	C	502	5/5	0.99	0.04	104,104,104,104	0
3	SO4	B	501	5/5	0.99	0.04	46,55,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.