



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:38 AM UTC

PDB ID : 8FPA / pdb_00008fpa
Title : Structure of a chimeric antibody (Fab) fragment bound to de-N-acetyl
polysialic acid (dPSA)
Authors : Beernink, P.T.; Agirre, J.; Beernink, B.P.; Moe, G.R.
Deposited on : 2023-01-04
Resolution : 1.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

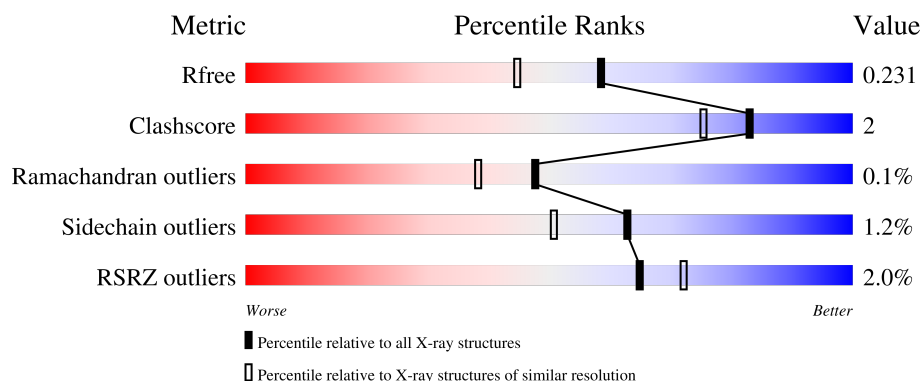
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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.



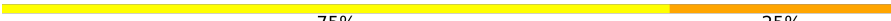
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	226	<div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	C	226	<div> <div>88%</div> <div>8%</div> <div>..</div> </div>
2	B	219	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	D	219	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>
3	E	4	<div> <div>75%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	B	307	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13690 atoms, of which 6431 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 Chimeric antibody Fab fragment, Fd chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	H	N	O	S	0	3	0
			3197	1038	1550	275	328	6			
1	C	219	Total	C	H	N	O	S	0	1	0
			3183	1034	1542	275	326	6			

- Molecule 2 is a protein called Humanized antibody Fab fragment, light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	216	Total	C	H	N	O	S	0	2	0
			3265	1055	1595	278	332	5			
2	D	211	Total	C	H	N	O	S	0	1	0
			3193	1033	1562	271	322	5			

- Molecule 3 is an oligosaccharide called 5-amino-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-9)-3,5-dideoxy-5-propanamido-D-glycero-D-galacto-non-2-ulosonic acid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	4	Total	C	H	N	O	0	0	0
			135	45	54	4	32			
3	F	4	Total	C	H	N	O	0	0	0
			135	45	54	4	32			

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



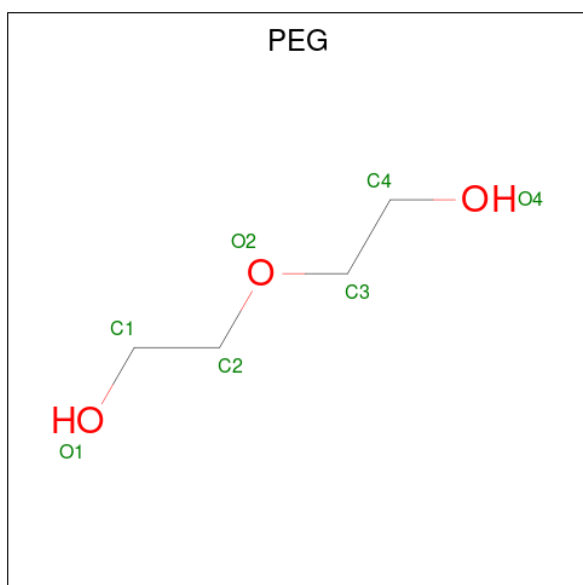
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	B	1	Total	C	H	O	0	0
			11	3	5	3		
5	C	1	Total	C	H	O	0	0
			11	3	5	3		
5	D	1	Total	C	H	O	0	0
			11	3	5	3		
5	D	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			15	4	8	3		
6	A	1	Total	C	H	O	0	0
			15	4	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			15	4	8	3		

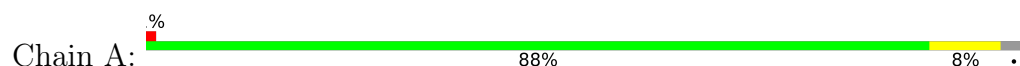
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	101	Total	O	0	0
			101	101		
7	B	113	Total	O	0	0
			113	113		
7	C	99	Total	O	0	0
			99	99		
7	D	94	Total	O	0	0
			94	94		

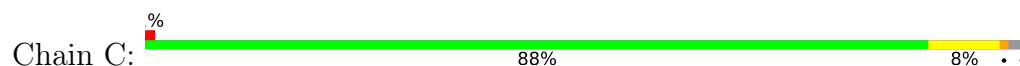
3 Residue-property plots [i](#)

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.

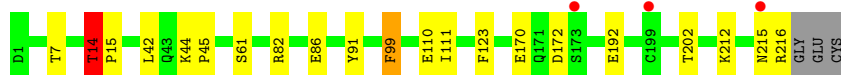
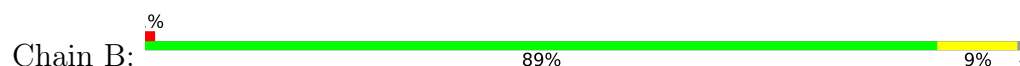
- Molecule 1: Chimeric antibody Fab fragment, Fd chain



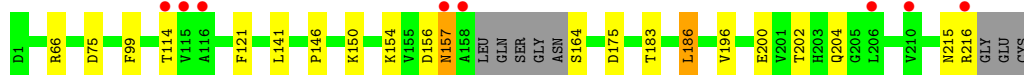
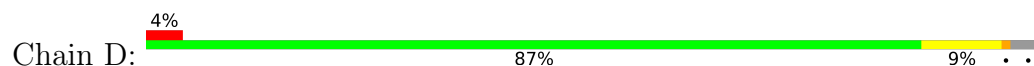
- Molecule 1: Chimeric antibody Fab fragment, Fd chain



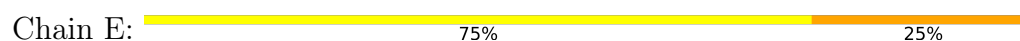
- Molecule 2: Humanized antibody Fab fragment, light chain



- Molecule 2: Humanized antibody Fab fragment, light chain



- Molecule 3: 5-amino-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-9)-3,5-dideoxy-5-propanamido-D-glycero-D-galacto-non-2-ulosonic acid



- Molecule 3: 5-amino-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-8)-3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-9)-3,5-dideoxy-5-propanamido-D-glycero-D-galacto-non-2-ulosonic acid

Chain F:

75%

25%

Y801
1802
1803
Y984

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.58Å 71.44Å 91.50Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	74.49 – 1.83 74.49 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.49-1.83) 99.8 (74.49-1.83)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.83Å)	Xtriage
Refinement program	Servalcat 0.4.105	Depositor
R, R_{free}	0.186 , 0.230 0.185 , 0.231	Depositor DCC
R_{free} test set	1458 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13690	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: Y98, ACY, GOL, PEG, Y8W, 18D

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	0.83	0/1695	1.22	4/2310 (0.2%)
1	C	0.81	0/1683	1.23	8/2294 (0.3%)
2	B	0.84	0/1712	1.27	11/2327 (0.5%)
2	D	0.78	0/1669	1.22	6/2266 (0.3%)
All	All	0.82	0/6759	1.23	29/9197 (0.3%)

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
1	C	0	1
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	ASP	CA-CB-CG	9.32	121.92	112.60
2	B	82	ARG	CB-CA-C	-8.18	98.89	110.34
2	B	212	LYS	CB-CA-C	6.78	122.12	109.71
2	D	99	PHE	CB-CA-C	-6.67	99.46	109.26
2	B	7	THR	CA-CB-OG1	-6.60	99.70	109.60
2	B	99	PHE	CB-CA-C	-6.53	99.66	108.87
2	B	110	GLU	CB-CG-CD	6.38	123.45	112.60
1	C	172	PHE	CA-CB-CG	-6.31	107.49	113.80
1	C	28	THR	CA-CB-OG1	-6.24	100.23	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	ASP	CA-CB-CG	6.06	118.66	112.60
2	B	123	PHE	CA-C-O	6.00	124.27	119.59
1	C	76	ASN	CB-CA-C	5.99	122.16	110.67
2	D	156	ASP	CB-CA-C	5.97	120.83	112.11
1	A	116	THR	OG1-CB-CG2	-5.97	97.36	109.30
2	B	202	THR	CA-CB-OG1	-5.87	100.80	109.60
2	D	175	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	50	TYR	CA-CB-CG	5.71	124.18	113.90
1	A	107	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	70	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	70	PHE	CA-CB-CG	5.51	119.31	113.80
1	C	50	TYR	CA-CB-CG	5.40	123.62	113.90
2	B	99	PHE	CA-CB-CG	-5.33	108.47	113.80
2	D	114	THR	CA-CB-OG1	-5.19	101.81	109.60
2	B	215	ASN	CB-CA-C	-5.18	100.75	109.72
1	C	171	THR	CA-CB-OG1	-5.13	101.90	109.60
2	D	75	ASP	CA-CB-CG	5.09	117.69	112.60
2	D	121	PHE	CA-CB-CG	5.07	118.87	113.80
1	C	58	TYR	CB-CA-C	-5.05	104.56	111.73
2	B	14	THR	CB-CA-C	5.02	116.64	109.26

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ARG	Sidechain
1	C	103	ARG	Sidechain
2	D	216	ARG	Sidechain
2	D	66	ARG	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	1647	1550	1619	7	0
1	C	1641	1542	1609	7	0
2	B	1670	1595	1657	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1631	1562	1621	7	0
3	E	81	54	36	1	0
3	F	81	54	36	1	0
4	A	8	0	6	0	0
4	B	4	0	3	2	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	A	6	5	8	0	0
5	B	36	30	48	1	0
5	C	6	5	8	0	0
5	D	12	10	16	0	0
6	A	14	16	20	1	0
6	D	7	8	10	1	0
7	A	101	0	0	0	0
7	B	113	0	0	0	0
7	C	99	0	0	0	0
7	D	94	0	0	0	0
All	All	7259	6431	6703	33	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 2.

All (33) 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)
6:D:303:PEG:H41	3:F:1:Y8W:O5	1.99	0.62
2:D:154:LYS:HB3	2:D:157:ASN:HA	1.82	0.61
1:A:85:MET:HE2	1:A:88:LEU:HD21	1.86	0.57
2:B:192:GLU:O	2:B:216:ARG:NH2	2.38	0.56
2:B:99:PHE:CZ	5:B:306:GOL:H32	2.42	0.53
1:C:199:THR:HG23	1:C:216:LYS:HE3	1.91	0.52
2:D:154:LYS:NZ	2:D:200:GLU:OE1	2.40	0.51
2:D:196:VAL:HG22	2:D:215:ASN:OD1	2.12	0.49
2:B:15:PRO:HG3	2:B:111:ILE:HG23	1.93	0.49
1:A:199:THR:HG23	1:A:216:LYS:HE3	1.95	0.48
2:B:14:THR:HB	4:B:307:ACY:H2	1.95	0.48
1:C:30:THR:HG22	1:C:76:ASN:HB3	1.96	0.48
1:C:149:LYS:NZ	1:C:177:GLN:OE1	2.48	0.47
1:A:30:THR:HG22	1:A:76:ASN:HB3	1.96	0.46
1:A:156:VAL:CG2	1:A:184:LEU:HD13	2.45	0.45
2:B:15:PRO:HG3	2:B:111:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:LYS:HB3	2:D:202:THR:OG1	2.15	0.45
1:C:85:MET:HE2	1:C:88:LEU:HD21	2.00	0.44
2:D:164:SER:HA	2:D:183:THR:O	2.18	0.43
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.52	0.43
3:E:1:Y8W:C8	3:E:1:Y8W:O2	2.64	0.43
1:C:30:THR:N	1:C:31:PRO:CD	2.82	0.43
2:B:45:PRO:HB3	2:B:170:GLU:HG3	2.02	0.42
1:C:69:ARG:HH11	1:C:69:ARG:HD2	1.68	0.42
2:D:146:PRO:HG3	2:D:204:GLN:NE2	2.35	0.42
6:A:304:PEG:H32	6:A:304:PEG:H12	1.93	0.41
2:B:44:LYS:NZ	2:B:86:GLU:O	2.48	0.41
1:A:30:THR:N	1:A:31:PRO:CD	2.84	0.41
2:D:186:LEU:HD12	2:D:186:LEU:N	2.35	0.41
1:A:6:GLU:HA	1:A:21:SER:O	2.22	0.40
1:C:17:SER:HA	1:C:85:MET:O	2.21	0.40
1:A:17[B]:SER:HA	1:A:85:MET:O	2.21	0.40
2:B:14:THR:HB	4:B:307:ACY:CH3	2.52	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	220/226 (97%)	218 (99%)	2 (1%)	0	100	100
1	C	218/226 (96%)	212 (97%)	6 (3%)	0	100	100
2	B	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
2	D	208/219 (95%)	203 (98%)	4 (2%)	1 (0%)	24	12
All	All	862/890 (97%)	844 (98%)	17 (2%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	157	ASN

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	186/190 (98%)	183 (98%)	3 (2%)	55	39
1	C	184/190 (97%)	182 (99%)	2 (1%)	65	54
2	B	195/196 (100%)	193 (99%)	2 (1%)	68	58
2	D	190/196 (97%)	188 (99%)	2 (1%)	65	54
All	All	755/772 (98%)	746 (99%)	9 (1%)	63	51

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	50	TYR
1	A	155	PRO
2	B	14	THR
2	B	61	SER
1	C	50	TYR
1	C	192	SER
2	D	141	LEU
2	D	186	LEU

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

Mol	Chain	Res	Type
1	A	170	HIS
2	B	17	GLN
2	B	142	ASN
1	C	56	ASN
1	C	78	GLN
2	D	194	HIS
2	D	204	GLN

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$
3	Y8W	E	1	3	21,21,21	2.36	4 (19%)	24,28,28	2.12	8 (33%)
3	18D	E	2	3	21,21,22	1.06	1 (4%)	22,29,32	1.69	7 (31%)
3	18D	E	3	3	21,21,22	0.92	0	22,29,32	1.51	3 (13%)
3	Y98	E	4	3	17,17,18	1.24	2 (11%)	19,24,27	1.77	4 (21%)
3	Y8W	F	1	3	21,21,21	2.48	4 (19%)	24,28,28	1.63	4 (16%)
3	18D	F	2	3	21,21,22	0.77	0	22,29,32	1.57	4 (18%)
3	18D	F	3	3	21,21,22	0.90	1 (4%)	22,29,32	1.45	4 (18%)
3	Y98	F	4	3	17,17,18	1.21	2 (11%)	19,24,27	1.71	4 (21%)

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	Y8W	E	1	3	-	4/32/32/32	-
3	18D	E	2	3	-	7/20/36/40	0/1/1/1
3	18D	E	3	3	-	3/20/36/40	0/1/1/1
3	Y98	E	4	3	-	6/14/30/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y8W	F	1	3	-	6/32/32/32	-
3	18D	F	2	3	-	5/20/36/40	0/1/1/1
3	18D	F	3	3	-	3/20/36/40	0/1/1/1
3	Y98	F	4	3	-	6/14/30/34	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	Y8W	C7-C8	-9.24	1.39	1.53
3	E	1	Y8W	C7-C8	-8.97	1.40	1.53
3	E	2	18D	C3-C2	-3.29	1.47	1.52
3	E	1	Y8W	C5-C4	2.98	1.57	1.53
3	F	1	Y8W	C11-C10	-2.98	1.48	1.53
3	F	3	18D	C2-C1	2.85	1.55	1.52
3	E	4	Y98	C7-C6	2.84	1.56	1.52
3	F	1	Y8W	O6-C8	2.79	1.29	1.22
3	E	1	Y8W	O6-C8	2.69	1.29	1.22
3	F	4	Y98	C7-C6	2.59	1.56	1.52
3	E	4	Y98	O1A-C1	2.58	1.29	1.22
3	F	4	Y98	O1B-C1	-2.24	1.23	1.30
3	E	1	Y8W	O1-C3	2.20	1.27	1.23
3	F	1	Y8W	C9-C4	2.07	1.57	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	Y8W	C6-C7-C8	5.08	124.93	115.89
3	E	1	Y8W	C6-C7-C8	4.81	124.46	115.89
3	E	3	18D	C11-C10-N5	4.70	121.92	115.78
3	E	1	Y8W	C2-C3-N1	4.47	121.62	115.78
3	E	4	Y98	C4-C5-N5	-4.29	102.25	111.11
3	F	4	Y98	O6-C2-C3	3.98	115.91	110.56
3	E	1	Y8W	O3-C7-C6	-3.77	113.55	121.40
3	F	3	18D	O1B-C1-C2	3.69	122.30	112.71
3	E	2	18D	O1B-C1-C2	3.54	121.91	112.71
3	F	2	18D	O1B-C1-C2	3.50	121.81	112.71
3	F	2	18D	C9-C8-C7	3.50	119.30	112.17
3	E	1	Y8W	C6-C5-C4	-3.49	108.20	113.00
3	E	4	Y98	O6-C2-C3	3.32	115.03	110.56
3	F	1	Y8W	C2-C3-N1	3.24	120.01	115.78
3	E	2	18D	C9-C8-C7	3.14	118.56	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	18D	O1A-C1-C2	-3.03	116.30	122.85
3	E	2	18D	O9-C9-C8	-3.03	104.79	111.16
3	E	1	Y8W	O5-C8-O6	-2.95	116.87	123.90
3	F	1	Y8W	O3-C7-C6	-2.93	115.29	121.40
3	E	3	18D	C9-C8-C7	2.61	117.48	112.17
3	E	4	Y98	O1B-C1-C2	2.60	119.47	112.71
3	E	1	Y8W	O1-C3-N1	-2.47	118.76	122.95
3	E	1	Y8W	O6-C8-C7	2.39	124.78	121.81
3	F	3	18D	O1B-C1-O1A	-2.31	118.84	124.08
3	E	2	18D	C5-N5-C10	2.25	126.22	122.90
3	E	2	18D	O8-C8-C9	-2.23	103.95	109.03
3	E	3	18D	O8-C8-C7	-2.23	104.02	109.25
3	E	2	18D	O6-C2-C1	2.21	111.90	107.72
3	F	3	18D	O8-C8-C7	-2.19	104.12	109.25
3	F	2	18D	O8-C8-C9	-2.17	104.08	109.03
3	F	4	Y98	O6-C2-C1	2.17	111.82	107.72
3	F	3	18D	C5-N5-C10	2.14	126.06	122.90
3	E	4	Y98	O1A-C1-C2	-2.13	118.24	122.85
3	F	1	Y8W	O1-C3-C2	-2.13	116.38	122.13
3	E	1	Y8W	O9-C11-C12	-2.12	104.21	109.03
3	F	4	Y98	C6-C5-N5	2.09	115.24	110.92
3	F	2	18D	O10-C10-N5	2.07	126.46	122.95
3	F	4	Y98	C9-C8-C7	2.02	116.28	112.17

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	Y8W	C6-C7-C8-O5
3	E	1	Y8W	C5-C6-C7-O3
3	E	1	Y8W	C5-C6-C7-C8
3	E	1	Y8W	O2-C5-C6-C7
3	E	4	Y98	C7-C8-C9-O9
3	E	4	Y98	O8-C8-C9-O9
3	E	4	Y98	C6-C7-C8-O8
3	E	4	Y98	O7-C7-C8-O8
3	F	1	Y8W	O3-C7-C8-O6
3	F	1	Y8W	C6-C7-C8-O6
3	F	1	Y8W	C6-C7-C8-O5
3	F	1	Y8W	C5-C6-C7-C8
3	F	1	Y8W	O2-C5-C6-C7
3	F	4	Y98	C6-C7-C8-O8

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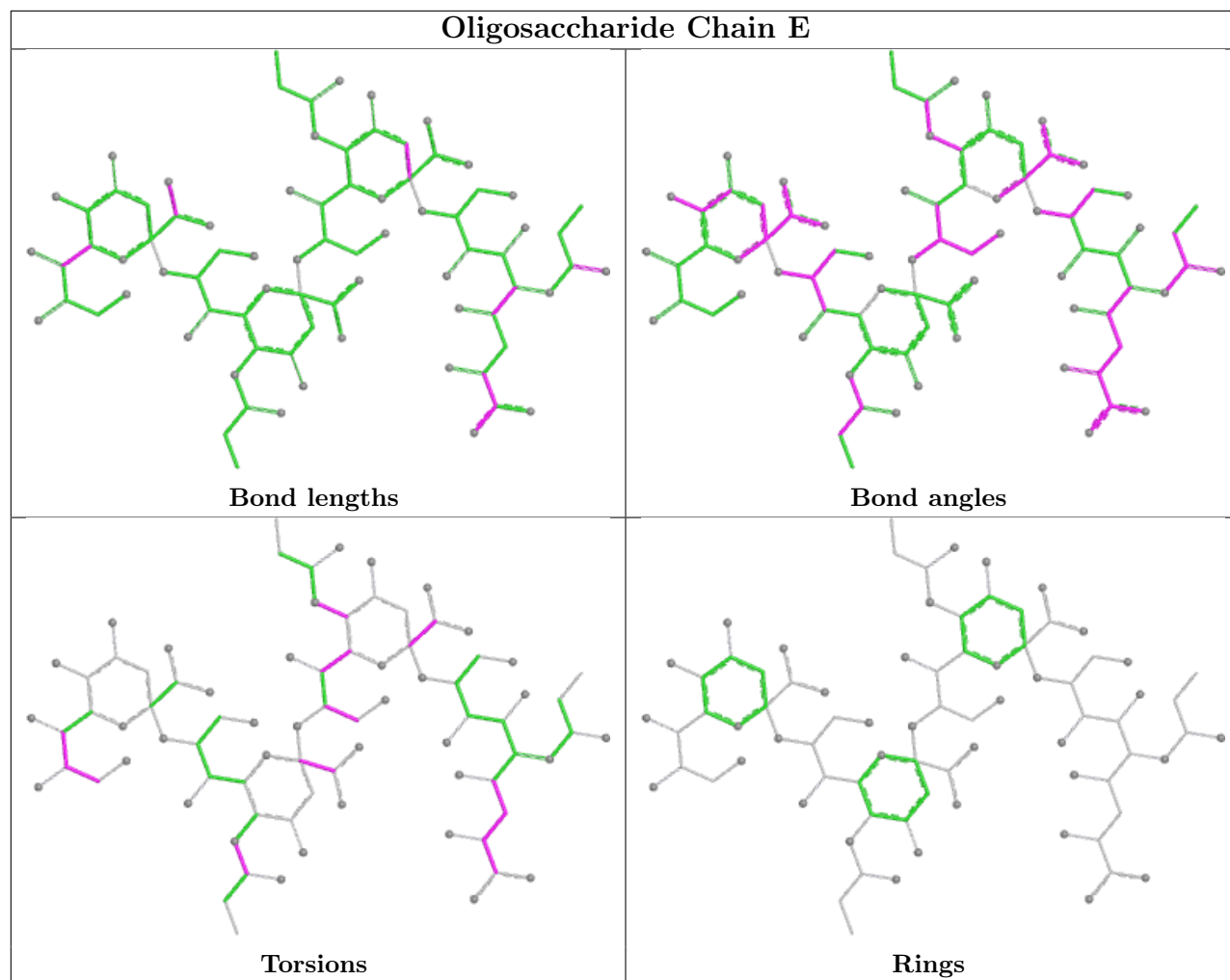
Mol	Chain	Res	Type	Atoms
3	F	4	Y98	O7-C7-C8-O8
3	F	4	Y98	O8-C8-C9-O9
3	E	4	Y98	O7-C7-C8-C9
3	F	4	Y98	O7-C7-C8-C9
3	E	4	Y98	C6-C7-C8-C9
3	F	4	Y98	C6-C7-C8-C9
3	E	3	18D	C11-C10-N5-C5
3	E	3	18D	O10-C10-N5-C5
3	E	2	18D	C7-C8-C9-O9
3	F	4	Y98	C7-C8-C9-O9
3	E	2	18D	O8-C8-C9-O9
3	F	2	18D	O8-C8-C9-O9
3	F	3	18D	O8-C8-C9-O9
3	E	2	18D	C4-C5-N5-C10
3	F	2	18D	C4-C5-N5-C10
3	F	2	18D	C7-C8-C9-O9
3	F	1	Y8W	C5-C6-C7-O3
3	E	2	18D	O6-C6-C7-O7
3	F	2	18D	O6-C6-C7-O7
3	F	3	18D	C7-C8-C9-O9
3	E	2	18D	O1A-C1-C2-O6
3	E	2	18D	C5-C6-C7-O7
3	E	2	18D	C6-C5-N5-C10
3	E	3	18D	O1A-C1-C2-O6
3	F	3	18D	O1A-C1-C2-O6
3	F	2	18D	C6-C5-N5-C10

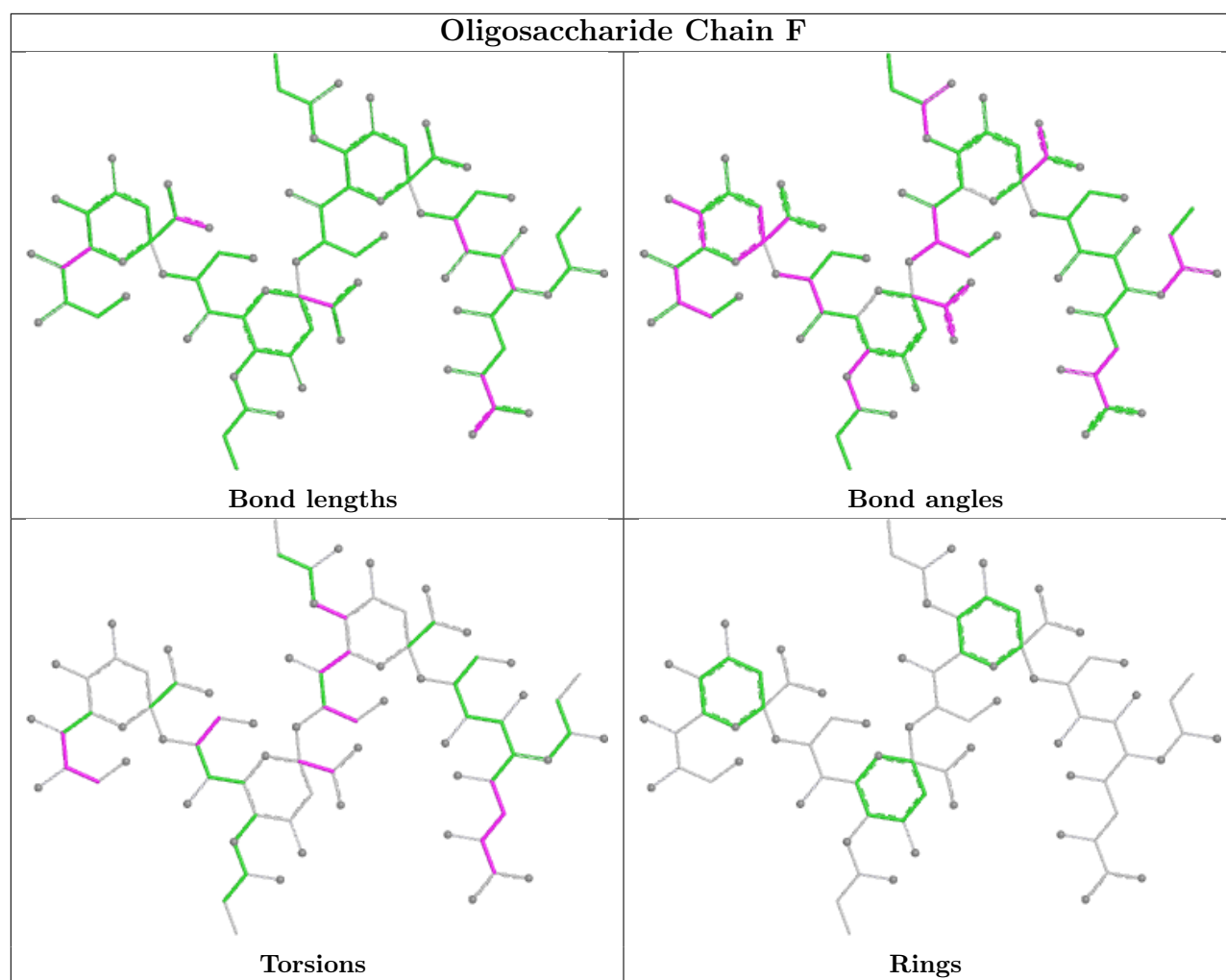
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	Y8W	1	0
3	F	1	Y8W	1	0

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





5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
5	GOL	A	303	-	5,5,5	0.13	0	5,5,5	0.61	0
4	ACY	B	307	-	3,3,3	0.63	0	3,3,3	1.29	0
5	GOL	C	301	-	5,5,5	0.40	0	5,5,5	0.40	0
5	GOL	B	305	-	5,5,5	0.27	0	5,5,5	0.50	0
5	GOL	B	303	-	5,5,5	0.17	0	5,5,5	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	301	-	5,5,5	0.19	0	5,5,5	0.86	0
5	GOL	B	306	-	5,5,5	0.25	0	5,5,5	0.56	0
4	ACY	D	304	-	3,3,3	1.08	0	3,3,3	0.39	0
5	GOL	B	304	-	5,5,5	0.18	0	5,5,5	0.46	0
5	GOL	D	302	-	5,5,5	0.20	0	5,5,5	0.36	0
5	GOL	D	301	-	5,5,5	0.28	0	5,5,5	0.95	0
4	ACY	C	302	-	3,3,3	0.95	0	3,3,3	1.45	0
5	GOL	B	302	-	5,5,5	0.14	0	5,5,5	0.29	0
6	PEG	A	304	-	6,6,6	0.56	0	5,5,5	0.56	0
6	PEG	D	303	-	6,6,6	0.35	0	5,5,5	0.37	0
4	ACY	A	302	-	3,3,3	0.89	0	3,3,3	1.18	0
6	PEG	A	305	-	6,6,6	0.30	0	5,5,5	0.22	0
4	ACY	A	301	-	3,3,3	0.88	0	3,3,3	1.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	303	-	-	1/4/4/4	-
5	GOL	C	301	-	-	2/4/4/4	-
5	GOL	B	305	-	-	2/4/4/4	-
5	GOL	B	303	-	-	2/4/4/4	-
5	GOL	B	301	-	-	0/4/4/4	-
5	GOL	B	306	-	-	2/4/4/4	-
5	GOL	D	302	-	-	0/4/4/4	-
5	GOL	B	304	-	-	2/4/4/4	-
5	GOL	D	301	-	-	3/4/4/4	-
5	GOL	B	302	-	-	2/4/4/4	-
6	PEG	A	304	-	-	2/4/4/4	-
6	PEG	D	303	-	-	2/4/4/4	-
6	PEG	A	305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	GOL	O1-C1-C2-C3
5	B	305	GOL	C1-C2-C3-O3
5	B	306	GOL	O1-C1-C2-C3
5	C	301	GOL	C1-C2-C3-O3
5	B	305	GOL	O2-C2-C3-O3
5	B	303	GOL	C1-C2-C3-O3
5	B	304	GOL	O1-C1-C2-C3
5	D	301	GOL	C1-C2-C3-O3
6	A	305	PEG	O1-C1-C2-O2
5	B	302	GOL	O1-C1-C2-O2
5	B	306	GOL	O1-C1-C2-O2
5	C	301	GOL	O2-C2-C3-O3
6	A	304	PEG	O1-C1-C2-O2
6	D	303	PEG	O2-C3-C4-O4
6	A	305	PEG	O2-C3-C4-O4
6	A	304	PEG	C1-C2-O2-C3
5	A	303	GOL	O1-C1-C2-O2
5	D	301	GOL	O1-C1-C2-O2
6	D	303	PEG	C1-C2-O2-C3
5	B	303	GOL	O2-C2-C3-O3
5	B	304	GOL	O1-C1-C2-O2
5	D	301	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	307	ACY	2	0
5	B	306	GOL	1	0
6	A	304	PEG	1	0
6	D	303	PEG	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, 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	219/226 (96%)	-0.13	3 (1%) 73 81	16, 33, 52, 72	3 (1%)
1	C	219/226 (96%)	0.10	3 (1%) 73 81	17, 37, 58, 77	1 (0%)
2	B	216/219 (98%)	-0.04	3 (1%) 73 81	18, 36, 57, 69	2 (0%)
2	D	211/219 (96%)	0.36	8 (3%) 44 48	20, 41, 64, 95	1 (0%)
All	All	865/890 (97%)	0.07	17 (1%) 65 72	16, 36, 58, 95	7 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	173	SER	4.2
2	D	158	ALA	3.1
2	D	157	ASN	2.9
1	C	167	SER	2.7
1	A	42	GLY	2.7
1	C	219	PRO	2.7
2	D	116	ALA	2.6
2	D	206	LEU	2.4
2	B	199	CYS	2.4
1	A	219	PRO	2.3
1	C	166	THR	2.3
2	D	114	THR	2.3
1	A	139	GLY	2.2
2	D	115	VAL	2.2
2	D	216	ARG	2.1
2	D	210	VAL	2.1
2	B	215	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

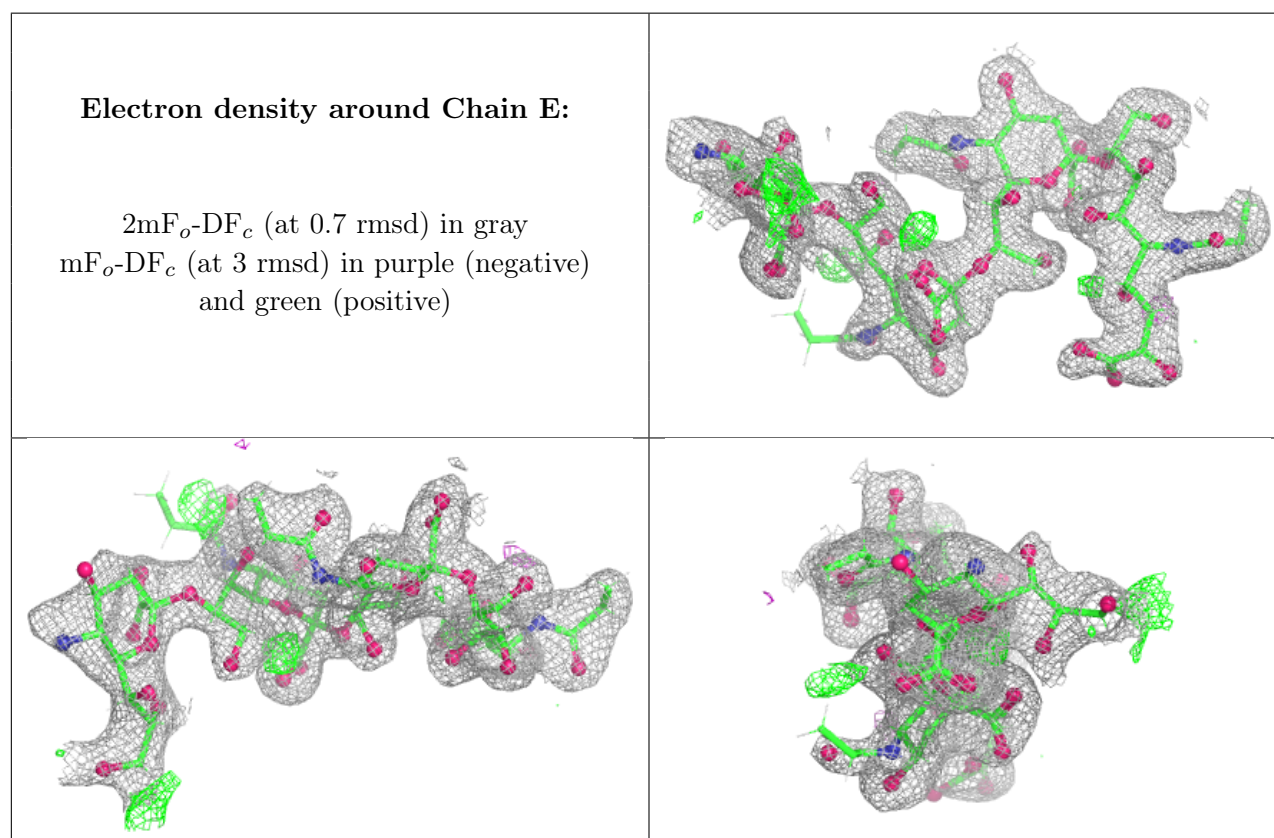
There are no non-standard protein/DNA/RNA residues in this entry.

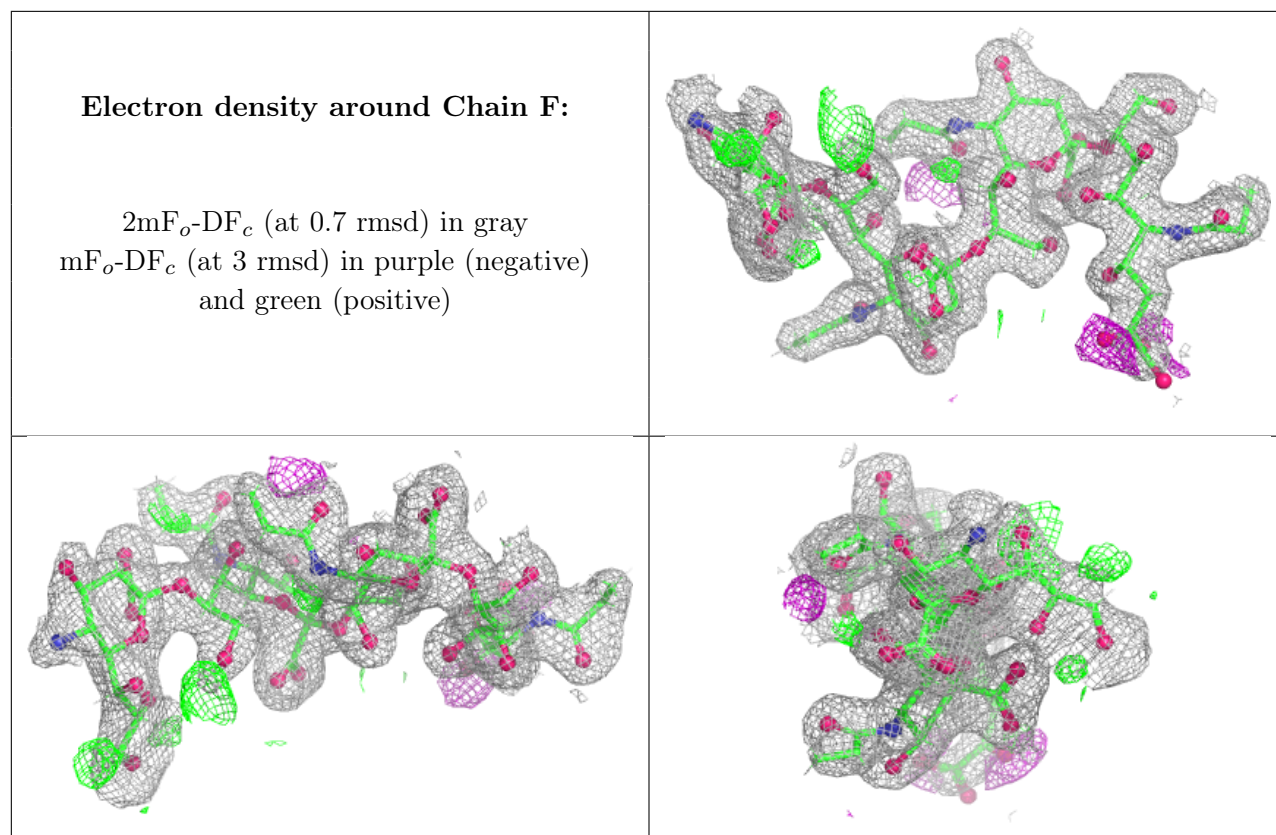
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
3	Y98	E	4	17/18	0.76	0.15	57,78,83,84	0
3	Y98	F	4	17/18	0.80	0.14	48,69,76,76	0
3	18D	E	3	21/22	0.87	0.12	46,54,85,85	0
3	18D	F	3	21/22	0.93	0.08	34,39,47,53	0
3	Y8W	F	1	22/22	0.94	0.12	29,36,58,78	0
3	18D	E	2	21/22	0.95	0.08	30,39,43,49	0
3	Y8W	E	1	22/22	0.95	0.08	28,39,74,88	0
3	18D	F	2	21/22	0.96	0.06	24,34,36,44	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.





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
6	PEG	D	303	7/7	0.84	0.15	53,55,66,77	0
6	PEG	A	304	7/7	0.85	0.17	43,57,69,69	0
4	ACY	D	304	4/4	0.85	0.21	47,52,64,72	0
4	ACY	B	307	4/4	0.86	0.18	54,57,71,72	0
5	GOL	C	301	6/6	0.87	0.13	40,44,47,58	0
5	GOL	D	301	6/6	0.87	0.17	42,58,65,70	0
4	ACY	A	301	4/4	0.87	0.19	32,41,41,52	0
4	ACY	A	302	4/4	0.87	0.19	55,61,63,83	0
5	GOL	B	303	6/6	0.88	0.14	38,49,57,60	0
5	GOL	B	302	6/6	0.89	0.12	46,51,54,61	0
4	ACY	C	302	4/4	0.90	0.17	38,53,54,55	0
5	GOL	B	305	6/6	0.90	0.13	44,51,60,64	0
6	PEG	A	305	7/7	0.91	0.13	57,62,69,70	0
5	GOL	B	304	6/6	0.91	0.11	43,49,55,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	D	302	6/6	0.92	0.10	31,39,43,43	0
5	GOL	A	303	6/6	0.94	0.10	35,49,54,61	0
5	GOL	B	306	6/6	0.95	0.10	31,44,44,67	0
5	GOL	B	301	6/6	0.96	0.07	30,33,35,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.