



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:50 PM UTC

PDB ID : 6W9G / pdb_00006w9g
Title : Crystal Structure of the Fab fragment of humanized 5c8 antibody containing the fluorescent non-canonical amino acid L-(7-hydroxycoumarin-4-yl)ethylglycine in complex with CD40L at pH 6.8
Authors : Henderson, J.N.; Simmons, C.R.; Mills, J.H.
Deposited on : 2020-03-23
Resolution : 1.82 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

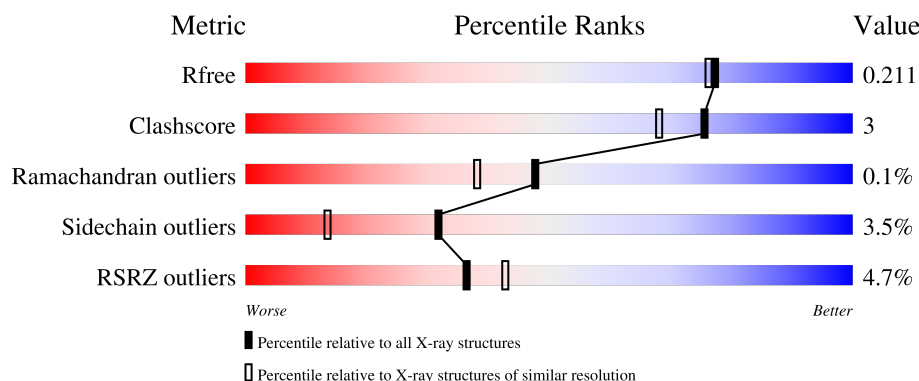
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	146	4% 82% 10% 6%
1	B	146	2% 82% 11% 6%
1	C	146	2% 81% 14% 5%
2	H	226	12% 88% 5% 6%
2	K	226	4% 88% 6%

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Mol	Chain	Length	Quality of chain
2	X	226	5% 88% 5% 7%
3	L	218	5% 93% 5% ••
3	M	218	% 94% 5% ••
3	Y	218	3% 93% 6% •
4	D	6	50% 50%
4	E	6	83% 17%
4	F	6	33% 67%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14802 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CD40 ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	10	0
			1096	701	185	205	5			
1	B	137	Total	C	N	O	S	0	9	0
			1095	698	189	204	4			
1	C	139	Total	C	N	O	S	0	14	0
			1130	725	188	212	5			

- Molecule 2 is a protein called 5c8* Fab (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	2	0
			1559	985	250	317	7			
2	K	213	Total	C	N	O	S	0	7	0
			1620	1023	262	328	7			
2	X	211	Total	C	N	O	S	0	1	0
			1562	985	253	317	7			

- Molecule 3 is a protein called 5c8* Fab (light chain).

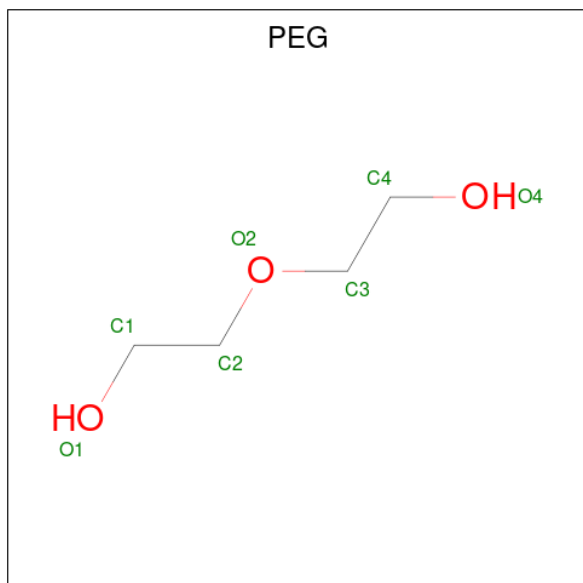
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	5	0
			1669	1053	276	335	5			
3	M	216	Total	C	N	O	S	0	2	0
			1660	1044	273	338	5			
3	Y	216	Total	C	N	O	S	0	4	0
			1685	1062	277	341	5			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	6	0
			86	48	3	35			
4	E	6	Total	C	N	O	0	6	0
			86	48	3	35			
4	F	6	Total	C	N	O	0	6	0
			86	48	3	35			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



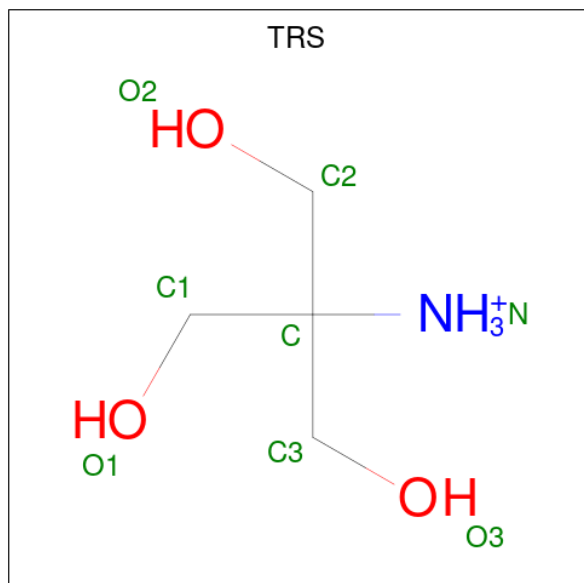
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	L	1	Total	C	O	0	0
			7	4	3		
5	Y	1	Total	C	O	0	0
			7	4	3		

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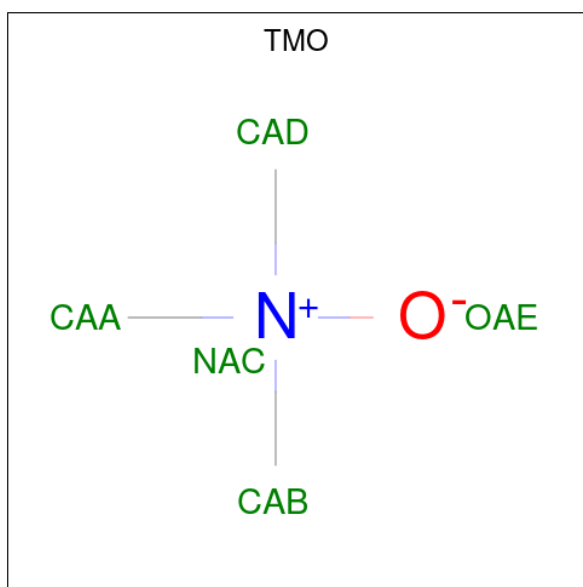
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	Y	1	Total	C	O	0	0
			7	4	3		
5	Y	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 7 is trimethylamine oxide (CCD ID: TMO) (formula: C_3H_9NO).



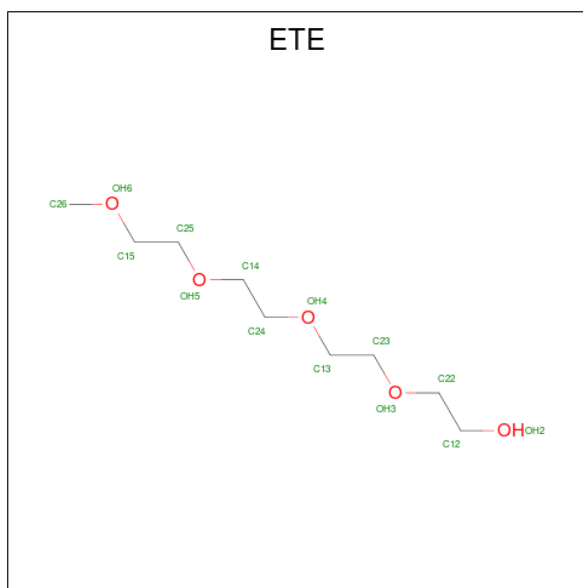
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			5	3	1	1		
7	B	1	Total	C	N	O	0	0
			5	3	1	1		
7	C	1	Total	C	N	O	0	0
			5	3	1	1		
7	H	1	Total	C	N	O	0	0
			5	3	1	1		
7	H	1	Total	C	N	O	0	0
			5	3	1	1		
7	L	1	Total	C	N	O	0	0
			5	3	1	1		
7	L	1	Total	C	N	O	0	0
			5	3	1	1		
7	L	1	Total	C	N	O	0	0
			5	3	1	1		
7	L	1	Total	C	N	O	0	0
			5	3	1	1		
7	K	1	Total	C	N	O	0	0
			5	3	1	1		
7	K	1	Total	C	N	O	0	0
			5	3	1	1		
7	K	1	Total	C	N	O	0	0
			5	3	1	1		
7	K	1	Total	C	N	O	0	0
			5	3	1	1		
7	M	1	Total	C	N	O	0	0
			5	3	1	1		

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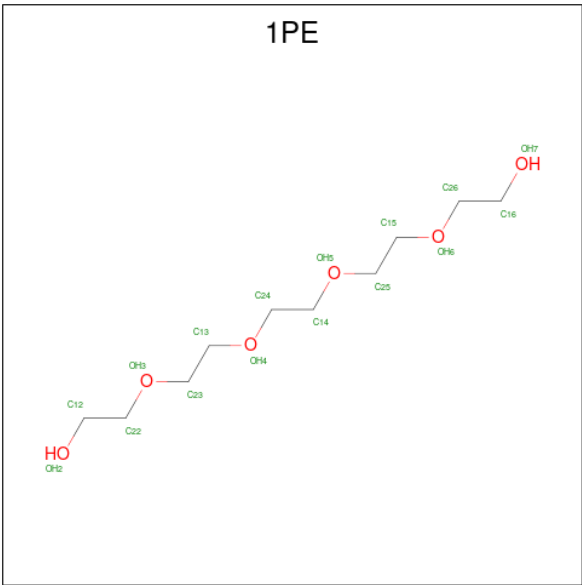
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			5	3	1	1		
7	M	1	Total	C	N	O	0	0
			5	3	1	1		
7	M	1	Total	C	N	O	0	0
			5	3	1	1		
7	X	1	Total	C	N	O	0	0
			5	3	1	1		
7	X	1	Total	C	N	O	0	0
			5	3	1	1		
7	Y	1	Total	C	N	O	0	0
			5	3	1	1		
7	Y	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 8 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		
8	B	1	Total	C	O	0	0
			14	9	5		
8	M	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			16	10	6		

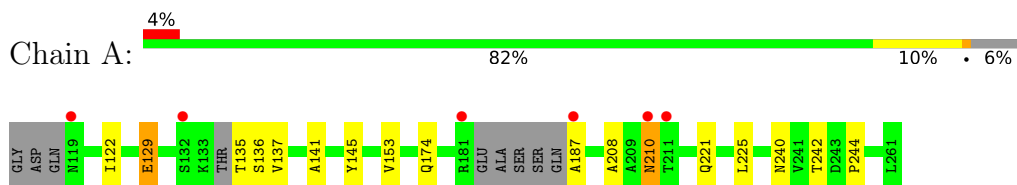
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	115	Total	O	0	18
			115	115		
10	B	117	Total	O	0	16
			117	117		
10	C	96	Total	O	0	14
			96	96		
10	H	87	Total	O	0	2
			87	87		
10	L	191	Total	O	0	4
			191	191		
10	K	133	Total	O	0	2
			133	133		
10	M	202	Total	O	0	0
			202	202		
10	X	102	Total	O	0	4
			102	102		
10	Y	195	Total	O	0	2
			195	195		

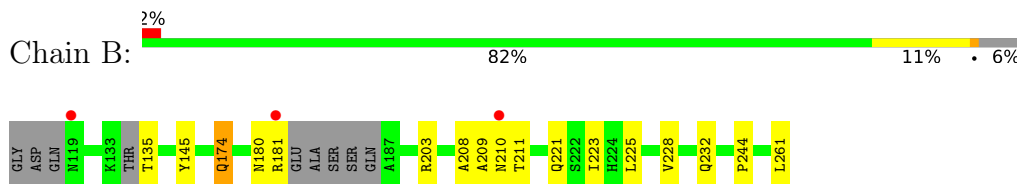
3 Residue-property plots [i](#)

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.

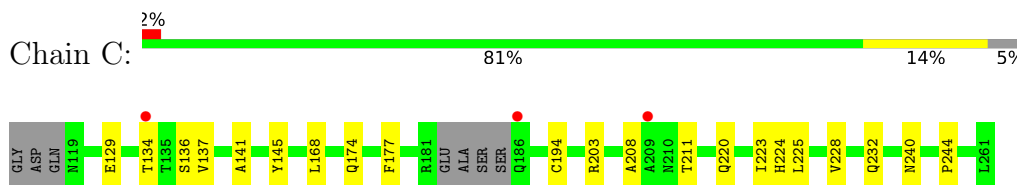
- Molecule 1: CD40 ligand



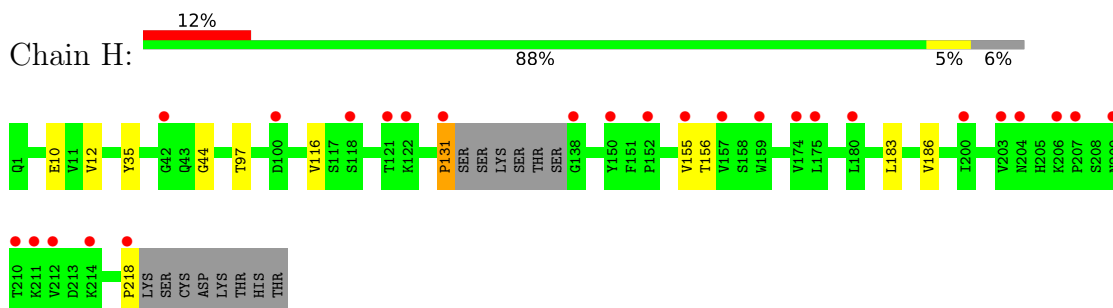
- Molecule 1: CD40 ligand



- Molecule 1: CD40 ligand

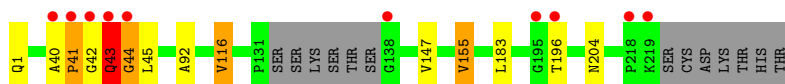


- Molecule 2: 5c8* Fab (heavy chain)

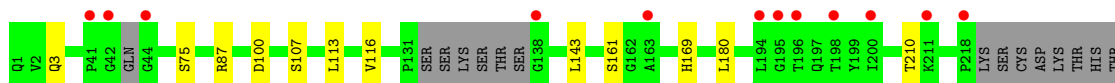
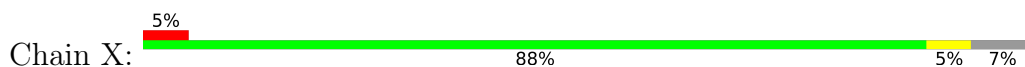


- Molecule 2: 5c8* Fab (heavy chain)





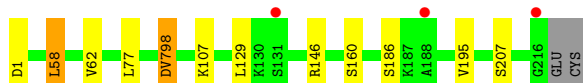
- Molecule 2: 5c8* Fab (heavy chain)



- Molecule 3: 5c8* Fab (light chain)



- Molecule 3: 5c8* Fab (light chain)



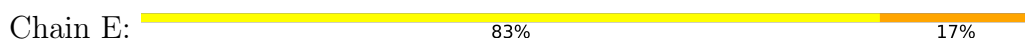
- Molecule 3: 5c8* Fab (light chain)



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.68Å 131.20Å 97.56Å 90.00° 108.82° 90.00°	Depositor
Resolution (Å)	48.47 – 1.82 48.47 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.47-1.82) 97.1 (48.47-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.207 0.187 , 0.211	Depositor DCC
R_{free} test set	11697 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14802	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: MAN, PEG, BMA, NAG, TMO, DV7, ETE, 1PE, TRS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.08	1/1144 (0.1%)	1.01	2/1548 (0.1%)
1	B	1.07	0/1143	1.11	2/1546 (0.1%)
1	C	1.01	1/1194 (0.1%)	1.02	2/1620 (0.1%)
2	H	0.96	0/1601	0.99	1/2187 (0.0%)
2	K	0.94	1/1663 (0.1%)	0.95	1/2268 (0.0%)
2	X	0.93	1/1600 (0.1%)	0.96	0/2181
3	L	0.94	0/1703	0.99	0/2318
3	M	1.02	0/1684	1.04	0/2293
3	Y	1.00	0/1700	1.03	4/2313 (0.2%)
All	All	0.99	4/13432 (0.0%)	1.01	12/18274 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1
3	M	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	TYR	CA-CB	5.23	1.59	1.52
2	K	45	LEU	N-CA	-5.20	1.39	1.46
1	A	145	TYR	CA-CB	5.19	1.59	1.52
2	X	100	ASP	C-O	5.18	1.30	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	136	VAL	CB-CA-C	8.01	122.49	110.63
1	A	187	ALA	CA-C-N	-6.81	113.78	120.52
1	A	187	ALA	C-N-CA	-6.81	113.78	120.52
3	Y	14	SER	CA-C-N	-6.42	113.17	119.78
3	Y	14	SER	C-N-CA	-6.42	113.17	119.78
2	H	131	PRO	CA-N-CD	-5.89	103.75	112.00
3	Y	112	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	C	228[A]	VAL	CB-CA-C	-5.39	104.22	110.91
1	C	228[B]	VAL	CB-CA-C	-5.39	104.22	110.91
1	B	228[A]	VAL	CB-CA-C	-5.06	103.96	110.84
1	B	228[B]	VAL	CB-CA-C	-5.06	103.96	110.84
2	K	116	VAL	CB-CA-C	5.01	118.04	110.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	44[B]	GLY	Peptide
3	M	160	SER	Peptide
3	M	98[A]	DV7	Peptide

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	1096	0	1093	10	0
1	B	1095	0	1098	12	0
1	C	1130	0	1145	15	0
2	H	1559	0	1480	4	0
2	K	1620	0	1560	20	0
2	X	1562	0	1494	2	0
3	L	1669	0	1580	8	0
3	M	1660	0	1552	5	0
3	Y	1685	0	1572	6	0
4	D	86	0	74	4	0
4	E	86	0	74	1	0
4	F	86	0	74	3	0
5	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	7	0	10	0	0
5	C	14	0	20	0	0
5	L	7	0	10	0	0
5	Y	21	0	30	0	0
6	A	16	0	24	0	0
7	A	5	0	9	0	0
7	B	5	0	9	0	0
7	C	5	0	9	0	0
7	H	10	0	18	0	0
7	K	20	0	36	0	0
7	L	20	0	36	0	0
7	M	20	0	36	0	0
7	X	10	0	18	0	0
7	Y	10	0	18	1	0
8	A	13	0	17	0	0
8	B	14	0	20	0	0
8	M	10	0	13	0	0
9	C	16	0	22	0	0
10	A	115	0	0	0	0
10	B	117	0	0	2	0
10	C	96	0	0	0	0
10	H	87	0	0	0	0
10	K	133	0	0	1	0
10	L	191	0	0	4	0
10	M	202	0	0	4	0
10	X	102	0	0	0	0
10	Y	195	0	0	1	0
All	All	14802	0	13161	81	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 3.

All (81) 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)
2:K:43[B]:GLN:HG3	2:K:44[B]:GLY:H	0.92	1.06
2:K:43[B]:GLN:CG	2:K:44[B]:GLY:N	2.12	1.06
2:K:43[B]:GLN:HG3	2:K:44[B]:GLY:N	1.62	1.03
2:K:43[B]:GLN:CG	2:K:44[B]:GLY:H	1.65	1.01
2:K:40[B]:ALA:O	2:K:42[B]:GLY:N	2.03	0.90
3:L:146[A]:ARG:HH11	3:L:146[A]:ARG:HG2	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:OD1	1:A:221:GLN:NE2	2.18	0.77
2:K:40[A]:ALA:O	2:K:43[A]:GLN:HB2	1.87	0.75
2:K:40[A]:ALA:C	2:K:43[A]:GLN:HB2	2.11	0.74
3:M:146:ARG:NH2	10:M:402:HOH:O	2.20	0.74
3:M:186:SER:OG	3:M:186:SER:CA	2.37	0.73
1:C:208:ALA:HB2	1:C:225[A]:LEU:HD21	1.77	0.67
3:L:146[A]:ARG:HG2	3:L:146[A]:ARG:NH1	2.07	0.65
2:K:43[B]:GLN:HG2	2:K:44[B]:GLY:N	2.08	0.64
1:B:221[A]:GLN:NE2	1:C:211:THR:OG1	2.31	0.64
2:K:42[B]:GLY:O	2:K:43[B]:GLN:HB3	1.99	0.62
1:B:174[B]:GLN:NE2	10:B:403:HOH:O	2.34	0.61
2:K:40[A]:ALA:HB1	2:K:41[A]:PRO:HD2	1.82	0.60
1:A:208:ALA:HB2	1:A:225:LEU:HD21	1.84	0.60
2:K:40[B]:ALA:C	2:K:42[B]:GLY:H	2.07	0.59
1:B:203[B]:ARG:NH2	10:B:401:HOH:O	2.28	0.59
2:K:40[A]:ALA:O	2:K:43[A]:GLN:CB	2.51	0.58
2:K:40[A]:ALA:HB1	2:K:41[A]:PRO:CD	2.34	0.58
1:A:225:LEU:CD2	1:C:174[A]:GLN:HE22	2.18	0.57
2:H:131:PRO:HG2	2:H:218:PRO:HA	1.85	0.56
1:B:211:THR:O	1:B:221[B]:GLN:NE2	2.28	0.56
3:Y:98[B]:DV7:OI	4:D:2[B]:NAG:H81	2.06	0.55
2:K:40[A]:ALA:HB3	2:K:43[A]:GLN:HG2	1.89	0.54
3:Y:167[A]:VAL:HG22	3:Y:179:LEU:HD12	1.89	0.53
3:L:107:LYS:NZ	10:L:404[A]:HOH:O	2.41	0.53
4:D:2[B]:NAG:H62	4:D:3[B]:BMA:C1	2.39	0.52
1:A:137:VAL:HG22	1:A:240:ASN:OD1	2.10	0.52
2:K:40[A]:ALA:HB3	2:K:43[A]:GLN:CG	2.40	0.51
3:M:107:LYS:NZ	10:M:405:HOH:O	2.44	0.51
1:B:208:ALA:HB2	1:B:225:LEU:HD21	1.94	0.50
1:C:129[A]:GLU:OE2	1:C:141:ALA:HB2	2.10	0.50
1:B:135:THR:O	1:B:244:PRO:HG2	2.12	0.50
1:B:145:TYR:OH	1:C:232[A]:GLN:NE2	2.44	0.50
3:M:1:ASP:OD1	10:M:401:HOH:O	2.19	0.49
2:X:169:HIS:CD2	3:Y:141:ASN:HD21	2.30	0.49
2:X:169:HIS:HD2	3:Y:141:ASN:HD21	1.61	0.48
1:C:203[B]:ARG:NH2	10:M:404:HOH:O	2.43	0.48
2:K:40[B]:ALA:C	2:K:42[B]:GLY:N	2.65	0.48
3:L:109:GLU:HG2	3:L:110:ILE:N	2.28	0.48
3:L:146[A]:ARG:NH2	10:L:405:HOH:O	2.47	0.47
1:A:122:ILE:HG23	1:A:153[A]:VAL:HG23	1.97	0.47
3:Y:98[B]:DV7:OI	4:D:2[B]:NAG:O7	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:41[B]:PRO:HD3	2:K:92:ALA:HA	1.95	0.47
2:H:44:GLY:HA3	10:L:455:HOH:O	2.14	0.47
1:C:194:CYS:SG	4:F:1[A]:NAG:H82	2.55	0.46
1:A:135:THR:O	1:A:244:PRO:HG2	2.16	0.46
1:B:180:ASN:O	1:B:181:ARG:HB2	2.15	0.46
2:H:183:LEU:C	2:H:183:LEU:HD12	2.41	0.46
1:A:129[B]:GLU:HG3	1:A:141:ALA:HB2	1.97	0.45
3:L:28[A]:ARG:HB3	3:L:28[A]:ARG:NH1	2.31	0.45
1:C:208:ALA:CB	1:C:225[A]:LEU:HD21	2.44	0.45
3:M:58:LEU:HD22	3:M:62:VAL:HB	1.99	0.45
1:B:174[A]:GLN:HE21	1:B:174[A]:GLN:HB2	1.52	0.44
1:C:208:ALA:HB2	1:C:225[A]:LEU:CD2	2.48	0.43
1:C:137:VAL:HG22	1:C:240:ASN:OD1	2.18	0.43
4:F:2[B]:NAG:H62	4:F:3[B]:BMA:C1	2.47	0.43
1:A:136:SER:CB	4:D:1[B]:NAG:H83	2.48	0.43
2:K:147:VAL:HG11	2:K:155:VAL:HG11	2.01	0.42
1:A:122:ILE:CG2	1:A:153[A]:VAL:HG23	2.50	0.42
1:A:225:LEU:HD23	1:C:174[A]:GLN:OE1	2.20	0.42
4:F:3[B]:BMA:H61	4:F:4[B]:MAN:C5	2.49	0.41
3:L:155:ASP:HA	3:L:195:VAL:HG13	2.02	0.41
7:Y:304:TMO:HAAA	10:Y:414:HOH:O	2.20	0.41
2:K:1:GLN:N	10:K:405:HOH:O	2.53	0.41
1:C:136:SER:HA	1:C:244:PRO:HG3	2.02	0.41
3:L:43:LYS:NZ	10:L:407:HOH:O	2.48	0.41
1:C:174[B]:GLN:OE1	1:C:224:HIS:ND1	2.54	0.41
2:H:35:TYR:HB2	2:H:97:THR:HG23	2.04	0.40
1:B:209:ALA:C	1:B:210:ASN:OD1	2.65	0.40
1:C:177:PHE:O	1:C:220:GLN:HA	2.21	0.40
2:K:183:LEU:HD12	2:K:183:LEU:C	2.46	0.40
4:E:2[B]:NAG:H62	4:E:3[B]:BMA:C1	2.51	0.40
1:B:232[A]:GLN:CD	1:B:232[A]:GLN:H	2.29	0.40
3:Y:136:VAL:HG22	3:Y:152:TRP:CH2	2.56	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	141/146 (97%)	139 (99%)	2 (1%)	0	100	100
1	B	140/146 (96%)	139 (99%)	1 (1%)	0	100	100
1	C	149/146 (102%)	146 (98%)	3 (2%)	0	100	100
2	H	210/226 (93%)	207 (99%)	3 (1%)	0	100	100
2	K	216/226 (96%)	207 (96%)	5 (2%)	4 (2%)	6	1
2	X	206/226 (91%)	200 (97%)	6 (3%)	0	100	100
3	L	216/218 (99%)	211 (98%)	5 (2%)	0	100	100
3	M	214/218 (98%)	208 (97%)	6 (3%)	0	100	100
3	Y	216/218 (99%)	210 (97%)	6 (3%)	0	100	100
All	All	1708/1770 (96%)	1667 (98%)	37 (2%)	4 (0%)	48	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	43[A]	GLN
2	K	43[B]	GLN
2	K	41[A]	PRO
2	K	41[B]	PRO

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	121/122 (99%)	115 (95%)	6 (5%)	22	6
1	B	122/122 (100%)	118 (97%)	4 (3%)	33	15
1	C	128/122 (105%)	124 (97%)	4 (3%)	35	17
2	H	171/194 (88%)	165 (96%)	6 (4%)	32	13
2	K	179/194 (92%)	173 (97%)	6 (3%)	32	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	174/194 (90%)	164 (94%)	10 (6%)	18	4
3	L	184/191 (96%)	177 (96%)	7 (4%)	29	11
3	M	182/191 (95%)	176 (97%)	6 (3%)	33	15
3	Y	185/191 (97%)	178 (96%)	7 (4%)	29	11
All	All	1446/1521 (95%)	1390 (96%)	56 (4%)	32	11

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129[A]	GLU
1	A	129[B]	GLU
1	A	174[A]	GLN
1	A	174[B]	GLN
1	A	210	ASN
1	A	242	THR
1	B	174[A]	GLN
1	B	174[B]	GLN
1	B	223	ILE
1	B	261	LEU
1	C	134	THR
1	C	168[A]	LEU
1	C	168[B]	LEU
1	C	223	ILE
2	H	10	GLU
2	H	12	VAL
2	H	116	VAL
2	H	155	VAL
2	H	156	THR
2	H	186	VAL
3	L	136	VAL
3	L	146[A]	ARG
3	L	146[B]	ARG
3	L	151	GLN
3	L	195	VAL
3	L	207	SER
3	L	215	ARG
2	K	43[A]	GLN
2	K	43[B]	GLN
2	K	116	VAL
2	K	155	VAL
2	K	196	THR

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Mol	Chain	Res	Type
2	K	204	ASN
3	M	58	LEU
3	M	77[A]	LEU
3	M	77[B]	LEU
3	M	129	LEU
3	M	195	VAL
3	M	207	SER
2	X	3	GLN
2	X	75	SER
2	X	87	ARG
2	X	107	SER
2	X	113	LEU
2	X	116	VAL
2	X	143	LEU
2	X	161	SER
2	X	180	LEU
2	X	210	THR
3	Y	131	SER
3	Y	133	THR
3	Y	136	VAL
3	Y	151	GLN
3	Y	156	ASN
3	Y	195	VAL
3	Y	207	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	221	GLN
2	H	176	GLN
3	L	164	GLN
3	L	214	ASN
2	K	59	ASN
3	M	164	GLN
2	X	3	GLN
2	X	39	GLN
2	X	209	ASN
3	Y	42	GLN
3	Y	141	ASN
3	Y	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	DV7	M	98[A]	3	18,19,20	0.84	1 (5%)	21,26,28	1.19	2 (9%)
3	DV7	Y	98[B]	-	18,19,20	1.00	1 (5%)	21,26,28	1.77	3 (14%)
3	DV7	Y	98[A]	-	18,19,20	0.96	0	21,26,28	1.36	1 (4%)

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	DV7	M	98[A]	3	-	2/6/7/9	0/2/2/2
3	DV7	Y	98[B]	-	-	0/6/7/9	0/2/2/2
3	DV7	Y	98[A]	-	-	2/6/7/9	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	98[B]	DV7	OH1-CZ1	-2.67	1.33	1.38
3	M	98[A]	DV7	CE2-CD	-2.06	1.42	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	98[B]	DV7	CG-CD-CE2	4.75	123.93	118.68
3	Y	98[A]	DV7	OH1-CZ1-OH2	-3.86	111.39	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	98[B]	DV7	OH1-CZ1-OH2	-3.82	111.44	116.40
3	M	98[A]	DV7	CB-CG-CD	-3.23	104.28	113.01
3	M	98[A]	DV7	OH1-CZ1-OH2	-2.34	113.37	116.40
3	Y	98[B]	DV7	CZ3-CE2-CZ2	-2.32	115.17	118.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	98[A]	DV7	CE2-CD-CG-CB
3	Y	98[A]	DV7	CE2-CD-CG-CB
3	M	98[A]	DV7	CA-CB-CG-CD
3	Y	98[A]	DV7	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	98[B]	DV7	2	0

5.5 Carbohydrates ⓘ

21 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	$\# Z > 2$
4	NAG	D	1[A]	1	14,14,15	0.47	0	17,19,21	2.12	7 (41%)
4	NAG	D	1[B]	4,1	14,14,15	0.85	0	17,19,21	2.15	4 (23%)
4	NAG	D	2[B]	4	14,14,15	0.49	0	17,19,21	1.43	4 (23%)
4	BMA	D	3[B]	4	11,11,12	0.40	0	15,15,17	1.22	1 (6%)
4	MAN	D	4[B]	4	11,11,12	0.37	0	15,15,17	1.25	2 (13%)
4	MAN	D	5[B]	4	11,11,12	0.39	0	15,15,17	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	D	6[B]	4	11,11,12	0.31	0	15,15,17	1.08	2 (13%)
4	NAG	E	1[A]	1	14,14,15	0.46	0	17,19,21	2.18	5 (29%)
4	NAG	E	1[B]	4,1	14,14,15	0.68	0	17,19,21	2.21	4 (23%)
4	NAG	E	2[B]	4	14,14,15	0.45	0	17,19,21	1.19	1 (5%)
4	BMA	E	3[B]	4	11,11,12	0.39	0	15,15,17	0.73	0
4	MAN	E	4[B]	4	11,11,12	0.40	0	15,15,17	1.25	1 (6%)
4	MAN	E	5[B]	4	11,11,12	0.29	0	15,15,17	1.57	3 (20%)
4	MAN	E	6[B]	4	11,11,12	0.50	0	15,15,17	1.55	2 (13%)
4	NAG	F	1[A]	1	14,14,15	0.60	0	17,19,21	1.91	6 (35%)
4	NAG	F	1[B]	4,1	14,14,15	0.62	0	17,19,21	1.97	4 (23%)
4	NAG	F	2[B]	4	14,14,15	0.44	0	17,19,21	1.44	2 (11%)
4	BMA	F	3[B]	4	11,11,12	0.34	0	15,15,17	1.41	3 (20%)
4	MAN	F	4[B]	4	11,11,12	0.34	0	15,15,17	1.10	1 (6%)
4	MAN	F	5[B]	4	11,11,12	0.31	0	15,15,17	1.34	2 (13%)
4	MAN	F	6[B]	4	11,11,12	0.63	0	15,15,17	1.55	2 (13%)

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
4	NAG	D	1[A]	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1[B]	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2[B]	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4[B]	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6[B]	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1[A]	1	-	1/6/23/26	0/1/1/1
4	NAG	E	1[B]	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2[B]	4	-	1/6/23/26	0/1/1/1
4	BMA	E	3[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6[B]	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1[A]	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1[B]	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	2[B]	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3[B]	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4[B]	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5[B]	4	-	2/2/19/22	0/1/1/1
4	MAN	F	6[B]	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1[B]	NAG	C1-O5-C5	7.80	122.64	112.19
4	D	1[B]	NAG	C1-O5-C5	5.98	120.20	112.19
4	F	1[B]	NAG	C1-O5-C5	5.84	120.01	112.19
4	D	1[A]	NAG	C1-O5-C5	4.86	118.70	112.19
4	E	1[A]	NAG	C1-C2-N2	4.66	117.77	110.43
4	F	1[A]	NAG	C1-C2-N2	4.11	116.90	110.43
4	E	1[A]	NAG	C6-C5-C4	-4.03	103.12	113.02
4	F	1[A]	NAG	C1-O5-C5	3.77	117.24	112.19
4	F	6[B]	MAN	O5-C5-C6	3.76	114.99	107.66
4	F	6[B]	MAN	C6-C5-C4	-3.73	103.87	113.02
4	E	6[B]	MAN	O5-C5-C6	3.71	114.88	107.66
4	E	4[B]	MAN	C1-O5-C5	-3.69	107.24	112.19
4	E	1[A]	NAG	O5-C5-C6	3.66	114.78	107.66
4	E	1[A]	NAG	C1-O5-C5	3.62	117.04	112.19
4	F	2[B]	NAG	C3-C4-C5	3.60	116.76	110.23
4	E	2[B]	NAG	C3-C4-C5	3.57	116.70	110.23
4	F	3[B]	BMA	C2-C3-C4	-3.42	104.85	110.86
4	D	1[B]	NAG	O5-C5-C6	-3.40	101.05	107.66
4	E	6[B]	MAN	C6-C5-C4	-3.37	104.73	113.02
4	D	1[A]	NAG	C1-C2-N2	3.33	115.67	110.43
4	F	4[B]	MAN	C1-O5-C5	3.32	116.64	112.19
4	E	5[B]	MAN	C2-C3-C4	-3.20	105.23	110.86
4	D	1[A]	NAG	O5-C5-C6	3.09	113.67	107.66
4	F	1[A]	NAG	O3-C3-C2	-3.00	103.16	109.40
4	D	2[B]	NAG	C1-O5-C5	2.91	116.09	112.19
4	D	3[B]	BMA	C1-C2-C3	2.86	113.81	109.64
4	D	1[A]	NAG	O5-C1-C2	-2.80	106.97	111.29
4	F	1[B]	NAG	C2-N2-C7	2.76	126.60	122.90
4	D	2[B]	NAG	C3-C4-C5	2.73	115.18	110.23
4	D	1[B]	NAG	C1-C2-N2	-2.72	106.14	110.43
4	F	5[B]	MAN	O2-C2-C3	-2.72	104.52	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5[B]	MAN	C2-C3-C4	-2.69	106.13	110.86
4	E	5[B]	MAN	C3-C4-C5	-2.66	105.40	110.23
4	D	1[A]	NAG	C6-C5-C4	-2.66	106.49	113.02
4	D	5[B]	MAN	C1-C2-C3	-2.65	105.78	109.64
4	E	1[A]	NAG	O5-C1-C2	-2.65	107.19	111.29
4	D	6[B]	MAN	C6-C5-C4	-2.59	106.65	113.02
4	F	1[A]	NAG	O5-C1-C2	-2.59	107.29	111.29
4	D	4[B]	MAN	O6-C6-C5	-2.57	102.60	111.33
4	F	5[B]	MAN	C1-O5-C5	-2.55	108.77	112.19
4	F	1[B]	NAG	C8-C7-N2	-2.50	111.97	116.12
4	E	5[B]	MAN	C1-C2-C3	-2.44	106.09	109.64
4	D	4[B]	MAN	C6-C5-C4	-2.37	107.19	113.02
4	F	1[A]	NAG	C6-C5-C4	-2.36	107.22	113.02
4	F	1[B]	NAG	O7-C7-N2	2.35	126.13	121.98
4	E	1[B]	NAG	O7-C7-N2	2.30	126.05	121.98
4	D	2[B]	NAG	O4-C4-C5	-2.21	103.88	109.32
4	F	2[B]	NAG	C1-O5-C5	-2.20	109.23	112.19
4	D	1[A]	NAG	C4-C3-C2	2.18	114.21	111.02
4	D	1[A]	NAG	C2-N2-C7	2.15	125.78	122.90
4	E	1[B]	NAG	C8-C7-N2	-2.12	112.60	116.12
4	F	1[A]	NAG	C4-C3-C2	2.11	114.11	111.02
4	F	3[B]	BMA	C6-C5-C4	-2.09	107.88	113.02
4	F	3[B]	BMA	O5-C5-C6	2.09	111.73	107.66
4	D	6[B]	MAN	O5-C5-C6	2.06	111.68	107.66
4	E	1[B]	NAG	O5-C1-C2	2.06	114.47	111.29
4	D	2[B]	NAG	O3-C3-C2	-2.05	105.15	109.40
4	D	1[B]	NAG	O5-C1-C2	2.02	114.42	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	5[B]	MAN	O5-C5-C6-O6
4	F	5[B]	MAN	C4-C5-C6-O6
4	D	1[B]	NAG	C8-C7-N2-C2
4	D	1[B]	NAG	O7-C7-N2-C2
4	D	6[B]	MAN	C4-C5-C6-O6
4	F	3[B]	BMA	C4-C5-C6-O6
4	F	3[B]	BMA	O5-C5-C6-O6
4	D	6[B]	MAN	O5-C5-C6-O6
4	D	1[A]	NAG	O5-C5-C6-O6
4	D	2[B]	NAG	C4-C5-C6-O6

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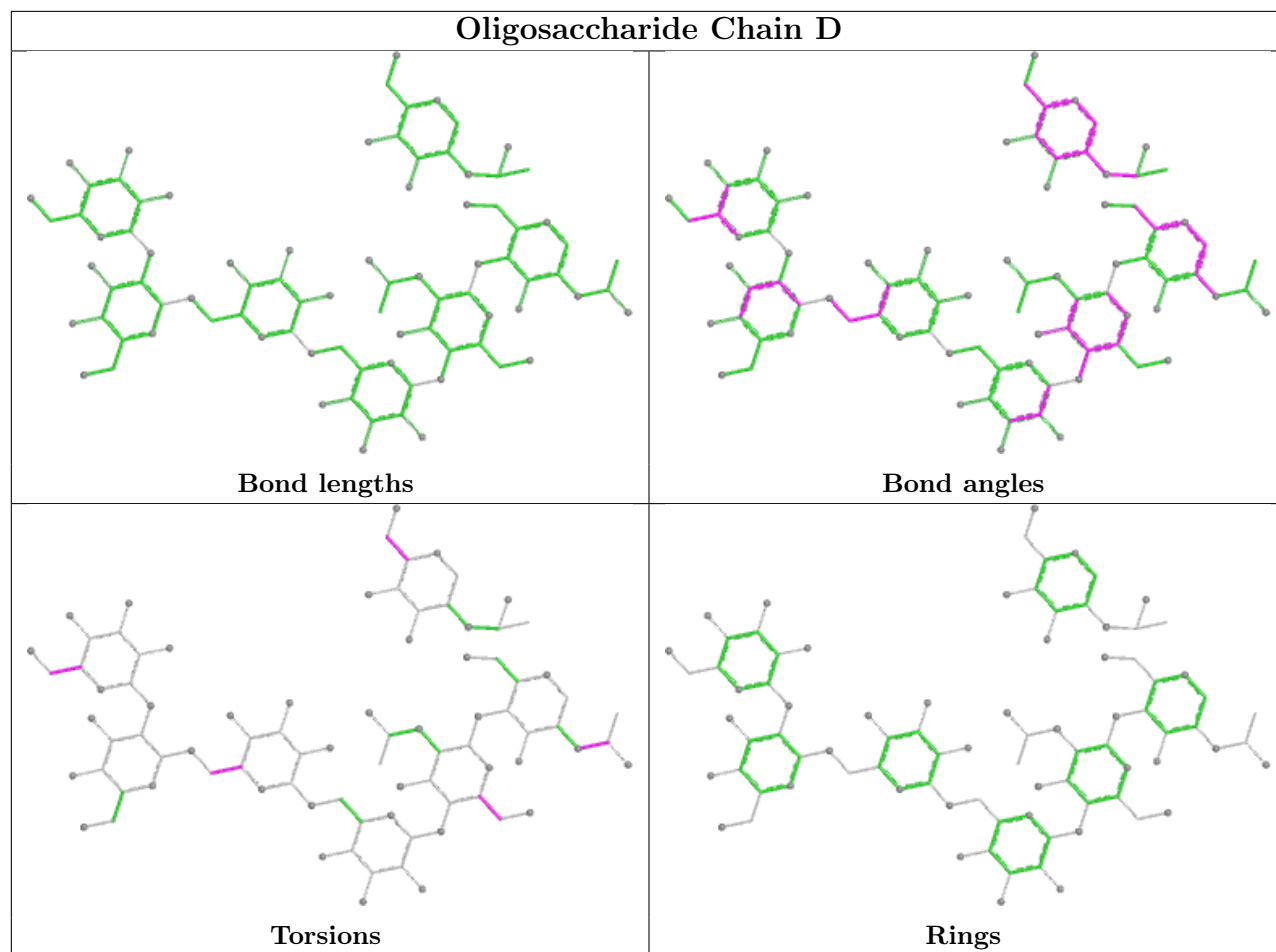
Mol	Chain	Res	Type	Atoms
4	E	1[A]	NAG	O5-C5-C6-O6
4	D	4[B]	MAN	C4-C5-C6-O6
4	E	1[B]	NAG	C3-C2-N2-C7
4	F	2[B]	NAG	C4-C5-C6-O6
4	E	2[B]	NAG	C4-C5-C6-O6
4	E	1[B]	NAG	C1-C2-N2-C7
4	F	1[B]	NAG	C1-C2-N2-C7
4	F	1[B]	NAG	C3-C2-N2-C7
4	F	2[B]	NAG	O5-C5-C6-O6
4	D	2[B]	NAG	O5-C5-C6-O6

There are no ring outliers.

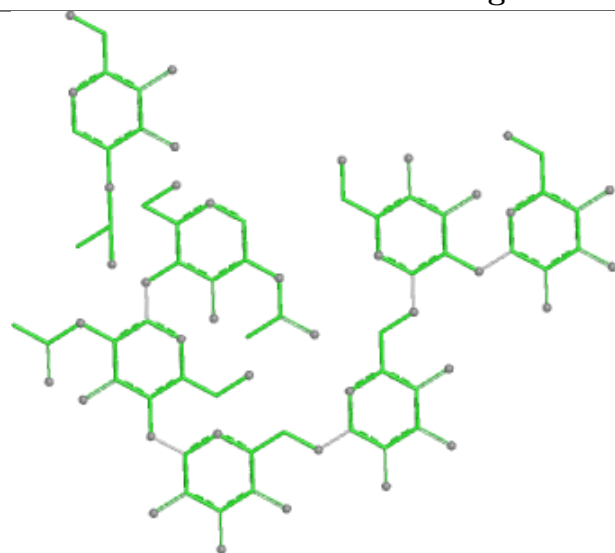
9 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3[B]	BMA	1	0
4	F	2[B]	NAG	1	0
4	E	3[B]	BMA	1	0
4	D	2[B]	NAG	3	0
4	F	4[B]	MAN	1	0
4	F	1[A]	NAG	1	0
4	F	3[B]	BMA	2	0
4	E	2[B]	NAG	1	0
4	D	1[B]	NAG	1	0

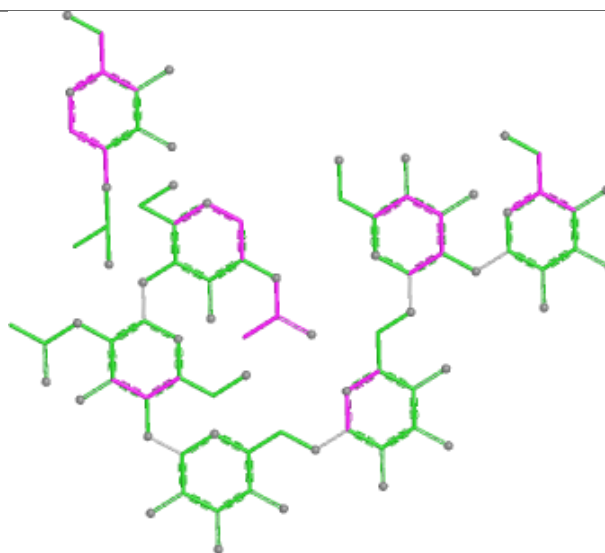
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



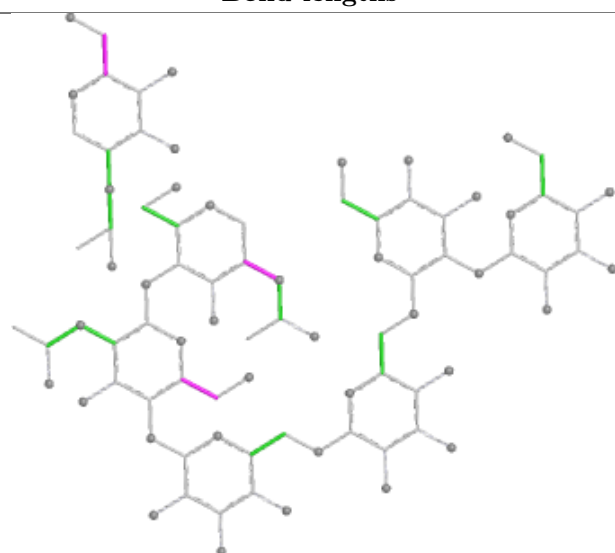
Oligosaccharide Chain E



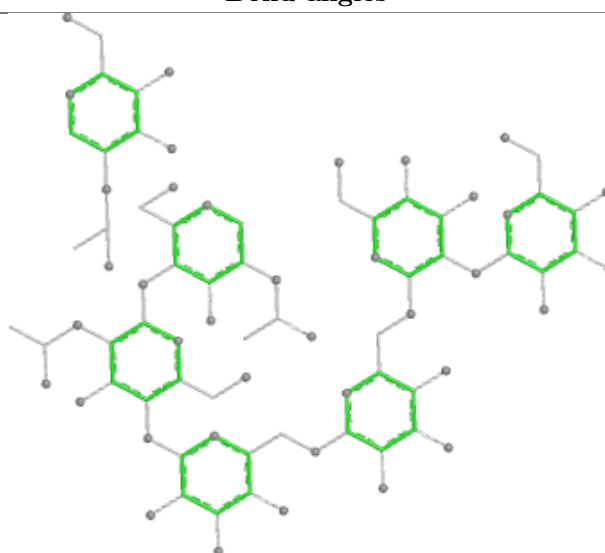
Bond lengths



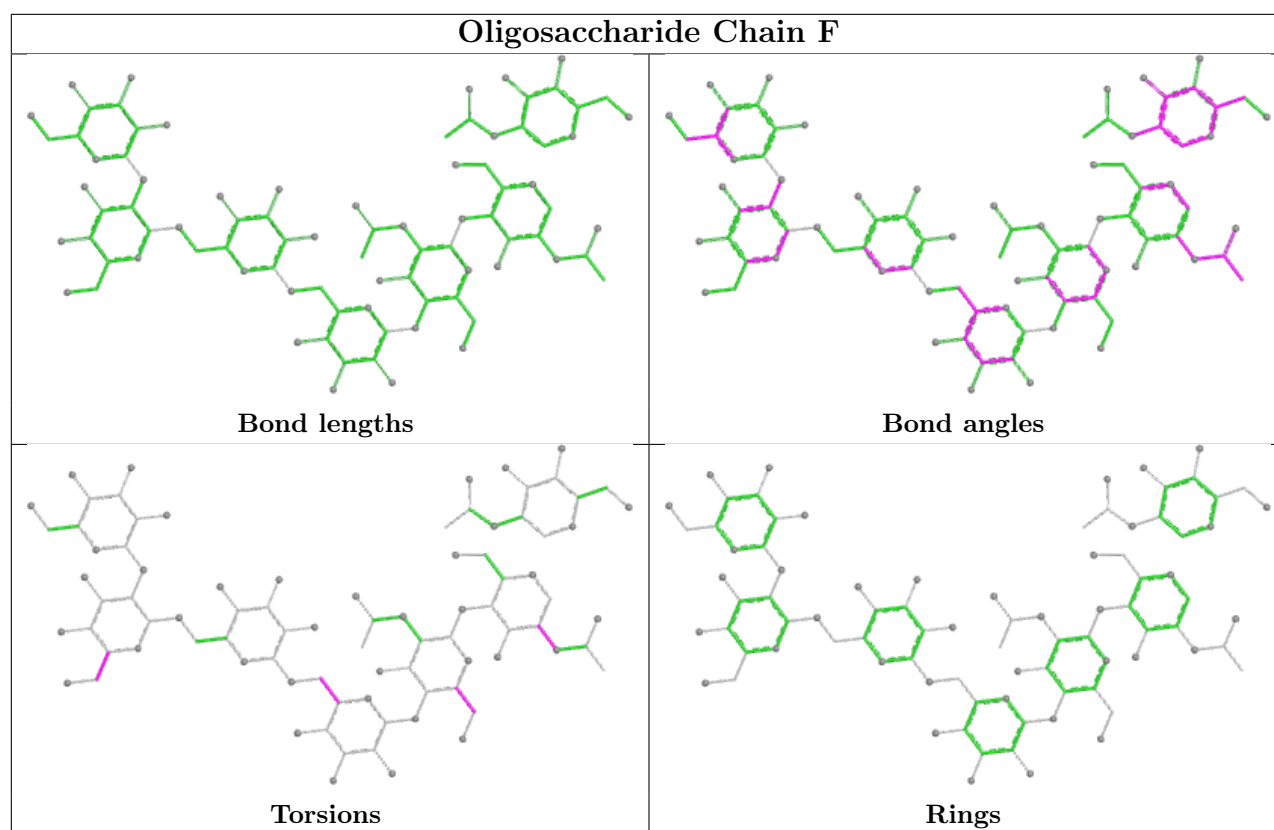
Bond angles



Torsions



Rings



5.6 Ligand geometry [i](#)

35 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	$\# Z > 2$
8	ETE	M	305	-	9,9,13	0.54	0	8,8,12	0.35	0
7	TMO	C	309	-	4,4,4	5.94	1 (25%)	6,6,6	0.30	0
7	TMO	M	301	-	4,4,4	6.36	1 (25%)	6,6,6	0.20	0
5	PEG	Y	301	-	6,6,6	0.49	0	5,5,5	0.24	0
7	TMO	K	301	-	4,4,4	6.53	1 (25%)	6,6,6	0.17	0
8	ETE	B	309	-	13,13,13	0.57	0	12,12,12	0.66	0
6	TRS	A	308	-	7,7,7	0.44	0	9,9,9	0.59	0
7	TMO	Y	305	-	4,4,4	6.26	1 (25%)	6,6,6	0.23	0
7	TMO	H	301	-	4,4,4	5.92	1 (25%)	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TMO	A	310	-	4,4,4	6.32	1 (25%)	6,6,6	0.22	0
7	TMO	L	303	-	4,4,4	6.29	1 (25%)	6,6,6	0.24	0
7	TMO	H	302	-	4,4,4	6.32	1 (25%)	6,6,6	0.18	0
7	TMO	M	303	-	4,4,4	6.14	1 (25%)	6,6,6	0.21	0
7	TMO	L	304	-	4,4,4	6.33	1 (25%)	6,6,6	0.17	0
7	TMO	K	304	-	4,4,4	6.24	1 (25%)	6,6,6	0.16	0
7	TMO	L	302	-	4,4,4	6.28	1 (25%)	6,6,6	0.17	0
6	TRS	A	309	-	7,7,7	0.52	0	9,9,9	0.47	0
5	PEG	C	307	-	6,6,6	0.49	0	5,5,5	0.17	0
7	TMO	L	305	-	4,4,4	6.13	1 (25%)	6,6,6	0.25	0
7	TMO	Y	304	-	4,4,4	6.34	1 (25%)	6,6,6	0.22	0
5	PEG	Y	302	-	6,6,6	0.62	0	5,5,5	0.35	0
7	TMO	X	301	-	4,4,4	6.33	1 (25%)	6,6,6	0.19	0
7	TMO	B	308	-	4,4,4	6.23	1 (25%)	6,6,6	0.32	0
5	PEG	C	308	-	6,6,6	0.51	0	5,5,5	0.40	0
8	ETE	A	311	-	12,12,13	0.61	0	11,11,12	0.75	0
7	TMO	K	302	-	4,4,4	6.24	1 (25%)	6,6,6	0.21	0
7	TMO	X	302	-	4,4,4	6.42	1 (25%)	6,6,6	0.16	0
9	1PE	C	310	-	15,15,15	0.51	0	14,14,14	0.37	0
5	PEG	B	307	-	6,6,6	0.57	0	5,5,5	0.38	0
7	TMO	M	304	-	4,4,4	6.32	1 (25%)	6,6,6	0.19	0
7	TMO	M	302	-	4,4,4	6.31	1 (25%)	6,6,6	0.23	0
5	PEG	A	307	-	6,6,6	0.47	0	5,5,5	0.51	0
7	TMO	K	303	-	4,4,4	6.40	1 (25%)	6,6,6	0.15	0
5	PEG	L	301	-	6,6,6	0.48	0	5,5,5	0.35	0
5	PEG	Y	303	-	6,6,6	0.48	0	5,5,5	0.57	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	PEG	C	307	-	-	2/4/4/4	-
8	ETE	M	305	-	-	3/7/7/11	-
9	1PE	C	310	-	-	9/13/13/13	-
5	PEG	Y	301	-	-	1/4/4/4	-
5	PEG	Y	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	B	307	-	-	2/4/4/4	-
8	ETE	B	309	-	-	7/11/11/11	-
6	TRS	A	308	-	-	3/9/9/9	-
5	PEG	Y	303	-	-	1/4/4/4	-
5	PEG	A	307	-	-	3/4/4/4	-
8	ETE	A	311	-	-	6/10/10/11	-
5	PEG	L	301	-	-	2/4/4/4	-
5	PEG	C	308	-	-	1/4/4/4	-
6	TRS	A	309	-	-	7/9/9/9	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	301	TMO	OAE-NAC	-13.05	1.24	1.42
7	X	302	TMO	OAE-NAC	-12.79	1.25	1.42
7	K	303	TMO	OAE-NAC	-12.74	1.25	1.42
7	M	301	TMO	OAE-NAC	-12.69	1.25	1.42
7	L	304	TMO	OAE-NAC	-12.65	1.25	1.42
7	Y	304	TMO	OAE-NAC	-12.65	1.25	1.42
7	X	301	TMO	OAE-NAC	-12.62	1.25	1.42
7	H	302	TMO	OAE-NAC	-12.62	1.25	1.42
7	M	302	TMO	OAE-NAC	-12.61	1.25	1.42
7	M	304	TMO	OAE-NAC	-12.55	1.25	1.42
7	A	310	TMO	OAE-NAC	-12.55	1.25	1.42
7	L	302	TMO	OAE-NAC	-12.53	1.25	1.42
7	L	303	TMO	OAE-NAC	-12.53	1.25	1.42
7	Y	305	TMO	OAE-NAC	-12.49	1.25	1.42
7	K	304	TMO	OAE-NAC	-12.47	1.25	1.42
7	B	308	TMO	OAE-NAC	-12.45	1.25	1.42
7	K	302	TMO	OAE-NAC	-12.44	1.25	1.42
7	M	303	TMO	OAE-NAC	-12.28	1.25	1.42
7	L	305	TMO	OAE-NAC	-12.22	1.25	1.42
7	C	309	TMO	OAE-NAC	-11.85	1.26	1.42
7	H	301	TMO	OAE-NAC	-11.80	1.26	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	308	TRS	C2-C-C1-O1
6	A	309	TRS	C1-C-C2-O2
6	A	309	TRS	C3-C-C2-O2
6	A	309	TRS	N-C-C2-O2
8	B	309	ETE	OH4-C13-C23-OH3
8	A	311	ETE	C14-C24-OH4-C13
8	A	311	ETE	C13-C23-OH3-C22
5	Y	303	PEG	O1-C1-C2-O2
5	Y	301	PEG	O2-C3-C4-O4
8	B	309	ETE	OH2-C12-C22-OH3
8	B	309	ETE	OH5-C14-C24-OH4
5	A	307	PEG	O2-C3-C4-O4
5	B	307	PEG	O1-C1-C2-O2
5	Y	302	PEG	O1-C1-C2-O2
6	A	308	TRS	C3-C-C1-O1
6	A	309	TRS	C3-C-C1-O1
5	C	307	PEG	O2-C3-C4-O4
8	M	305	ETE	OH5-C14-C24-OH4
8	B	309	ETE	C24-C14-OH5-C25
5	C	308	PEG	O2-C3-C4-O4
5	C	307	PEG	O1-C1-C2-O2
8	B	309	ETE	C15-C25-OH5-C14
9	C	310	1PE	OH2-C12-C22-OH3
9	C	310	1PE	OH7-C16-C26-OH6
6	A	309	TRS	N-C-C1-O1
8	A	311	ETE	OH4-C13-C23-OH3
9	C	310	1PE	C23-C13-OH4-C24
9	C	310	1PE	C12-C22-OH3-C23
5	B	307	PEG	C4-C3-O2-C2
5	Y	302	PEG	C1-C2-O2-C3
9	C	310	1PE	C24-C14-OH5-C25
9	C	310	1PE	C25-C15-OH6-C26
6	A	309	TRS	C2-C-C1-O1
8	M	305	ETE	C13-C23-OH3-C22
8	A	311	ETE	C15-C25-OH5-C14
8	A	311	ETE	OH6-C15-C25-OH5
8	M	305	ETE	OH2-C12-C22-OH3
8	A	311	ETE	C23-C13-OH4-C24
8	B	309	ETE	C14-C24-OH4-C13
5	A	307	PEG	C1-C2-O2-C3
6	A	308	TRS	N-C-C1-O1
6	A	309	TRS	C1-C-C3-O3
5	L	301	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	L	301	PEG	O2-C3-C4-O4
5	A	307	PEG	C4-C3-O2-C2
8	B	309	ETE	OH6-C15-C25-OH5
9	C	310	1PE	OH6-C15-C25-OH5
9	C	310	1PE	OH5-C14-C24-OH4
9	C	310	1PE	OH4-C13-C23-OH3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Y	304	TMO	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	137/146 (93%)	-0.13	6 (4%) 39 45	11, 22, 44, 56	10 (7%)
1	B	137/146 (93%)	-0.19	3 (2%) 62 69	12, 22, 39, 66	9 (6%)
1	C	139/146 (95%)	-0.14	3 (2%) 62 69	11, 22, 45, 64	15 (10%)
2	H	212/226 (93%)	0.69	26 (12%) 8 9	17, 43, 63, 74	2 (0%)
2	K	213/226 (94%)	0.13	10 (4%) 36 43	14, 34, 53, 75	7 (3%)
2	X	211/226 (93%)	0.35	12 (5%) 29 33	19, 39, 63, 76	1 (0%)
3	L	214/218 (98%)	0.01	11 (5%) 33 38	13, 27, 76, 86	4 (1%)
3	M	215/218 (98%)	-0.21	3 (1%) 73 79	10, 25, 58, 68	1 (0%)
3	Y	215/218 (98%)	-0.12	6 (2%) 55 60	13, 27, 64, 78	3 (1%)
All	All	1693/1770 (95%)	0.07	80 (4%) 36 43	10, 29, 62, 86	52 (3%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	THR	5.8
2	H	131	PRO	5.3
2	K	138	GLY	5.0
3	Y	216	GLY	4.7
2	K	219	LYS	4.4
2	X	138	GLY	4.3
3	M	216	GLY	4.0
1	A	211	THR	4.0
2	H	138	GLY	3.9
2	X	196	THR	3.6
2	X	42	GLY	3.5
2	H	42	GLY	3.4
2	H	212	VAL	3.4
2	H	203	VAL	3.3
3	L	158	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	119	ASN	3.1
2	K	196	THR	3.1
1	A	132	SER	3.1
2	H	218	PRO	3.1
2	X	218	PRO	3.0
1	A	181	ARG	3.0
2	H	207	PRO	2.8
2	K	43[A]	GLN	2.8
3	L	215	ARG	2.8
2	H	210	THR	2.8
2	K	41[A]	PRO	2.8
1	B	210	ASN	2.8
1	C	186	GLN	2.8
2	X	198	THR	2.8
2	H	100	ASP	2.7
1	B	181	ARG	2.7
2	K	42[A]	GLY	2.6
2	H	204	ASN	2.6
3	L	185	LEU	2.6
2	H	157	VAL	2.6
2	H	150	TYR	2.6
2	H	209	ASN	2.6
1	C	209	ALA	2.6
2	X	41	PRO	2.6
3	Y	130	LYS	2.6
2	K	218	PRO	2.5
3	L	130	LYS	2.5
3	M	131	SER	2.5
3	L	129	LEU	2.5
2	K	195	GLY	2.4
2	H	122	LYS	2.4
2	H	155	VAL	2.4
2	H	175	LEU	2.4
2	H	180	LEU	2.4
2	X	163	ALA	2.4
2	H	152	PRO	2.4
3	L	156	ASN	2.4
2	H	200	ILE	2.3
2	X	44	GLY	2.3
2	H	206	LYS	2.3
3	Y	129	LEU	2.3
2	H	159	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
3	M	188	ALA	2.3
3	L	132	GLY	2.3
1	A	119	ASN	2.3
2	K	44[A]	GLY	2.2
2	X	200	ILE	2.2
1	A	210	ASN	2.2
2	X	194	LEU	2.2
2	H	118	SER	2.2
2	X	195	GLY	2.2
3	L	126	ASP	2.2
2	H	214	LYS	2.2
2	H	121	THR	2.2
2	K	40[A]	ALA	2.2
2	H	211	LYS	2.2
3	Y	156	ASN	2.1
3	L	188	ALA	2.1
3	L	131	SER	2.1
2	X	211	LYS	2.1
1	A	187	ALA	2.1
3	Y	131	SER	2.0
3	Y	133	THR	2.0
2	H	174	VAL	2.0
3	L	195	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	DV7	M	98[A]	18/19	0.92	0.15	23,35,39,43	13
3	DV7	Y	98[A]	18/19	0.92	0.14	23,37,42,45	15
3	DV7	Y	98[B]	18/19	0.92	0.14	23,33,35,38	15
3	DV7	L	98[A]	18/19	0.93	0.14	23,32,36,38	13

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,

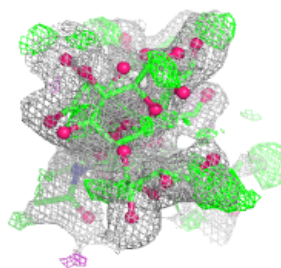
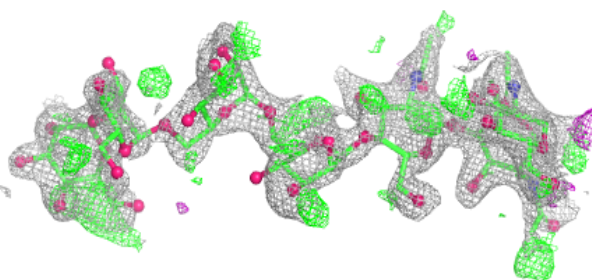
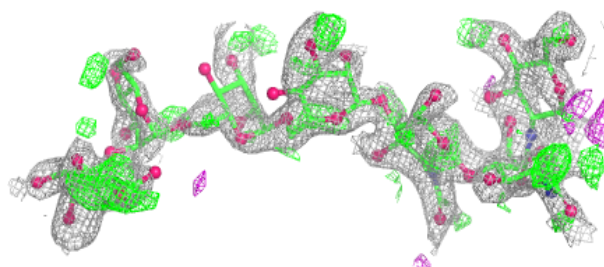
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	1[A]	14/15	-	-	37,39,40,40	14
4	NAG	D	1[B]	14/15	-	-	36,37,39,40	14
4	NAG	D	2[B]	14/15	-	-	36,37,38,39	14
4	BMA	D	3[B]	11/12	-	-	39,41,43,43	11
4	MAN	D	4[B]	11/12	-	-	44,47,50,51	11
4	MAN	D	5[B]	11/12	-	-	49,53,55,58	11
4	MAN	D	6[B]	11/12	-	-	43,49,53,54	11
4	NAG	E	1[A]	14/15	-	-	32,35,39,40	14
4	NAG	E	1[B]	14/15	-	-	29,31,38,38	14
4	NAG	E	2[B]	14/15	-	-	37,40,45,46	14
4	BMA	E	3[B]	11/12	-	-	47,52,56,58	11
4	MAN	E	4[B]	11/12	-	-	60,68,75,76	11
4	MAN	E	5[B]	11/12	-	-	72,80,91,92	11
4	MAN	E	6[B]	11/12	-	-	60,72,78,81	11
4	NAG	F	1[A]	14/15	-	-	36,40,45,45	14
4	NAG	F	1[B]	14/15	-	-	32,34,38,40	14
4	NAG	F	2[B]	14/15	-	-	33,35,37,38	14
4	BMA	F	3[B]	11/12	-	-	35,37,41,43	11
4	MAN	F	4[B]	11/12	-	-	36,38,44,48	11
4	MAN	F	5[B]	11/12	-	-	37,41,45,47	11
4	MAN	F	6[B]	11/12	-	-	32,33,35,35	11

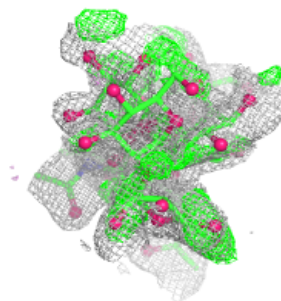
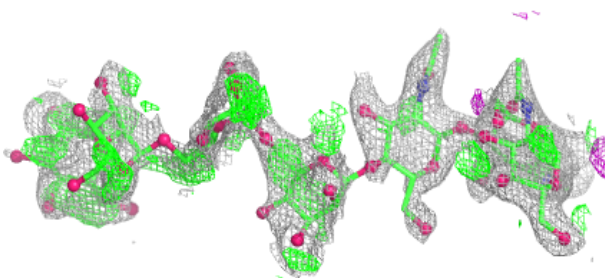
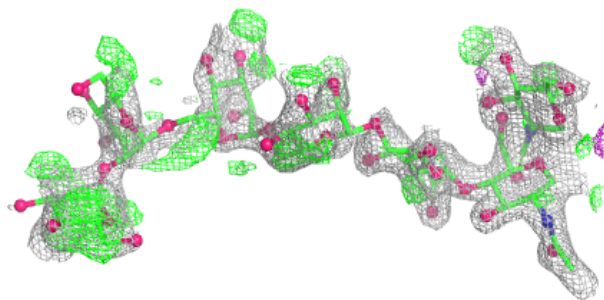
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

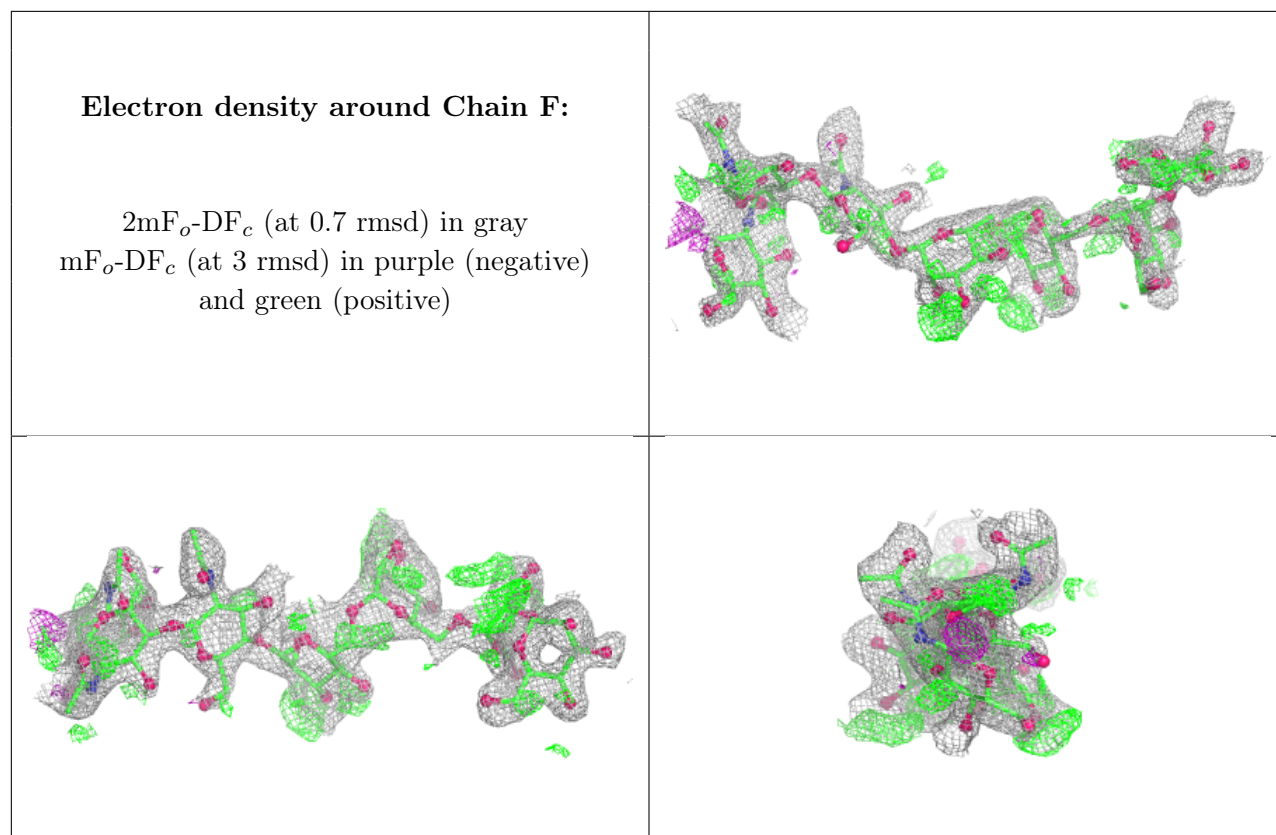
Electron density around Chain D:

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

**Electron density around Chain E:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TMO	L	304	5/5	0.73	0.29	74,75,76,77	0
7	TMO	K	304	5/5	0.75	0.28	65,65,69,71	0
7	TMO	M	303	5/5	0.78	0.27	68,70,73,74	0
8	ETE	B	309	14/14	0.80	0.20	62,64,68,71	0
5	PEG	Y	302	7/7	0.81	0.22	59,66,67,71	0
7	TMO	H	302	5/5	0.81	0.22	61,62,65,67	0
5	PEG	C	307	7/7	0.81	0.23	64,64,67,70	0
9	1PE	C	310	16/16	0.81	0.17	63,72,76,79	0
5	PEG	Y	303	7/7	0.82	0.20	64,66,68,69	0
6	TRS	A	309	8/8	0.82	0.27	79,84,86,87	0
8	ETE	A	311	13/14	0.83	0.16	53,62,65,66	0
6	TRS	A	308	8/8	0.83	0.22	57,61,63,67	0
5	PEG	B	307	7/7	0.83	0.20	57,61,64,64	0
5	PEG	A	307	7/7	0.84	0.16	59,61,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TMO	M	302	5/5	0.84	0.22	62,65,66,67	0
7	TMO	B	308	5/5	0.84	0.24	60,60,61,62	0
5	PEG	C	308	7/7	0.84	0.20	58,60,63,64	0
5	PEG	L	301	7/7	0.84	0.17	47,49,50,55	0
7	TMO	K	302	5/5	0.84	0.22	67,68,69,69	0
7	TMO	X	302	5/5	0.85	0.28	68,70,73,74	0
8	ETE	M	305	10/14	0.86	0.17	58,60,64,64	0
7	TMO	K	303	5/5	0.86	0.25	64,67,68,72	0
7	TMO	L	305	5/5	0.87	0.25	71,73,74,75	0
7	TMO	L	303	5/5	0.88	0.19	64,65,67,69	0
7	TMO	Y	305	5/5	0.88	0.20	63,64,66,67	0
7	TMO	M	304	5/5	0.88	0.18	50,52,53,57	0
5	PEG	Y	301	7/7	0.90	0.14	48,50,55,56	0
7	TMO	H	301	5/5	0.90	0.15	50,50,53,54	0
7	TMO	A	310	5/5	0.90	0.19	47,53,55,60	0
7	TMO	C	309	5/5	0.93	0.14	49,50,52,53	0
7	TMO	K	301	5/5	0.93	0.10	41,42,43,45	0
7	TMO	X	301	5/5	0.93	0.13	44,46,47,47	0
7	TMO	Y	304	5/5	0.95	0.13	46,46,47,51	0
7	TMO	M	301	5/5	0.95	0.11	40,41,42,42	0
7	TMO	L	302	5/5	0.96	0.10	40,41,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.