



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:34 AM UTC

PDB ID : 5U8Q / pdb_00005u8q
Title : Structure of the ectodomain of the human Type 1 insulin-like growth factor receptor in complex with IGF-I
Authors : Lawrence, M.; Xu, Y.
Deposited on : 2016-12-14
Resolution : 3.27 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

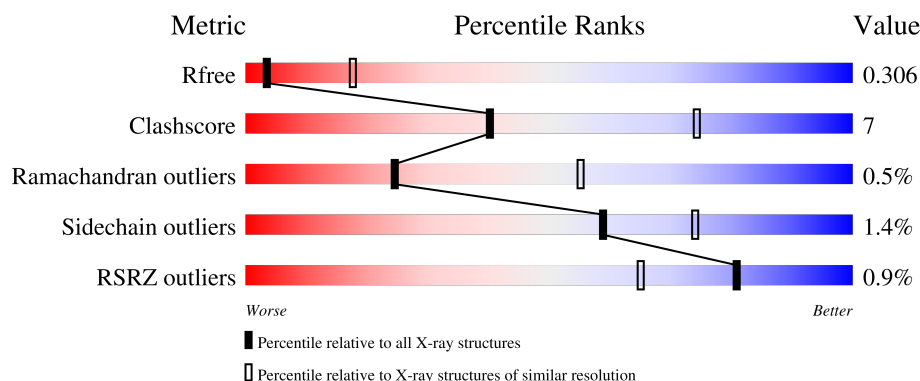
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	885	
2	B	70	
3	H	126	
4	L	108	
5	C	2	

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Mol	Chain	Length	Quality of chain
5	E	2	 100%
6	D	4	 50% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8704 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6427	4066	1112	1202	47			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	MET	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	ARG	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	ARG	deletion	UNP P08069
A	?	-	ASN	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	ALA	deletion	UNP P08069
A	?	-	ALA	deletion	UNP P08069
A	?	-	ASP	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	TYR	deletion	UNP P08069
A	?	-	ASN	deletion	UNP P08069
A	?	-	ILE	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	ASP	deletion	UNP P08069
A	738	ALA	PRO	conflict	UNP P08069
A	739	GLY	GLU	conflict	UNP P08069
A	740	ASN	GLU	conflict	UNP P08069
A	741	ASN	LEU	conflict	UNP P08069

- Molecule 2 is a protein called Insulin-like growth factor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	48	Total	C	N	O	S	0	0	0
			375	235	63	70	7			

- Molecule 3 is a protein called Fv 24-60 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	118	Total	C	N	O	S	0	0	0
			915	581	150	181	3			

- Molecule 4 is a protein called Fv 24-60 light chain.

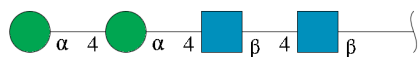
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	107	Total	C	N	O	S	0	0	0
			820	511	140	166	3			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



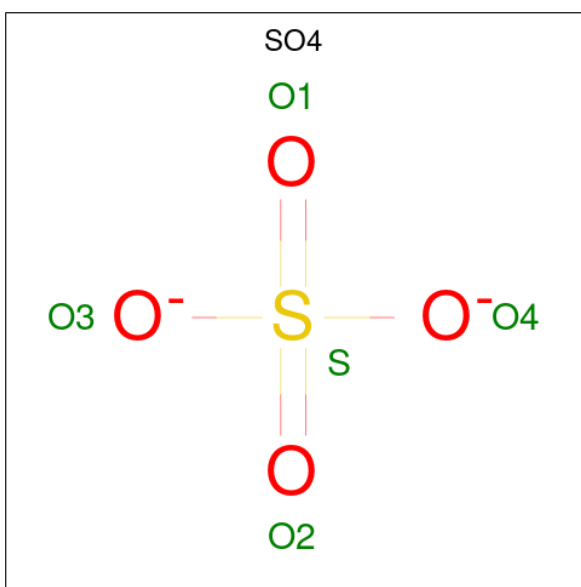
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



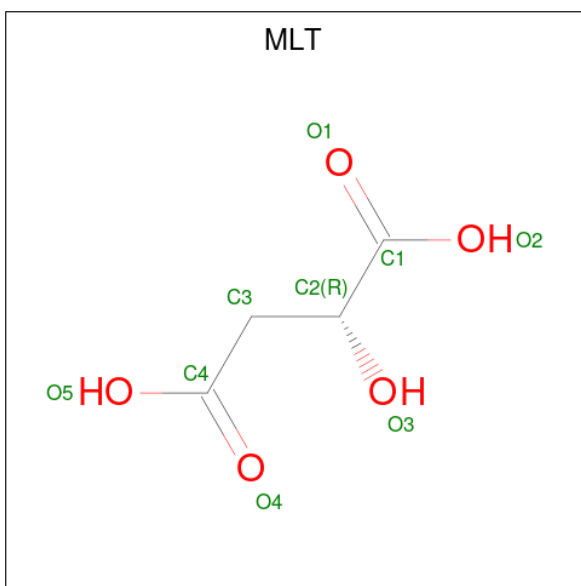
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

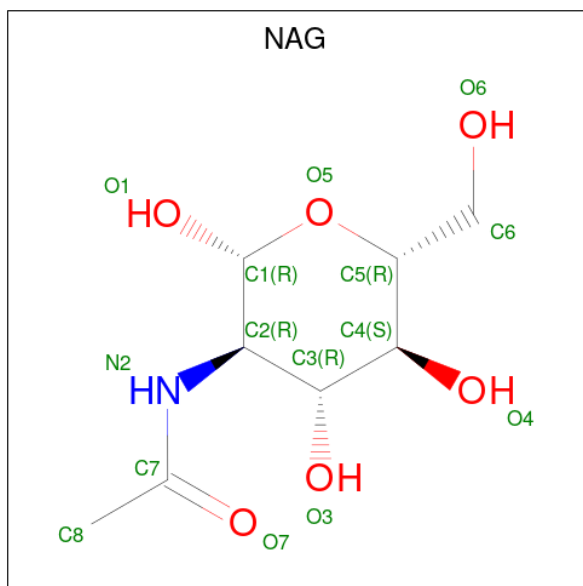
- Molecule 8 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

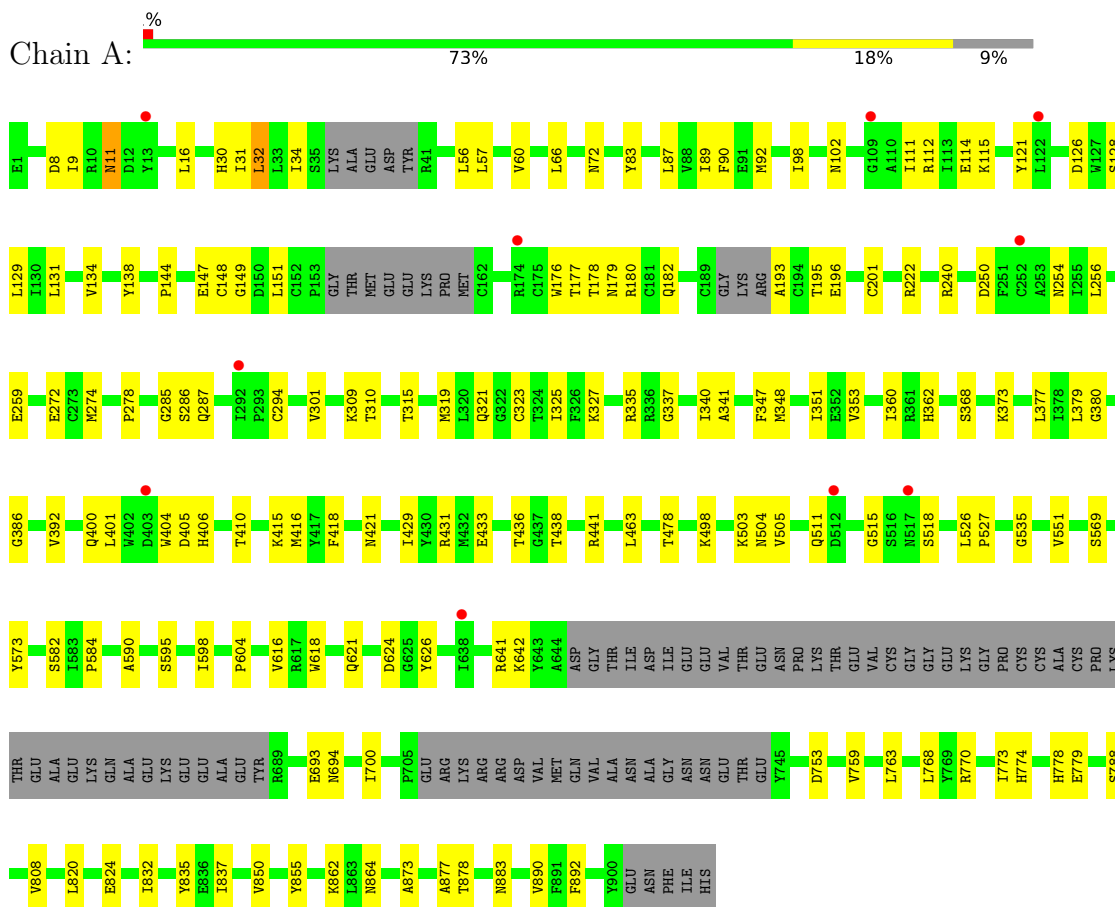


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

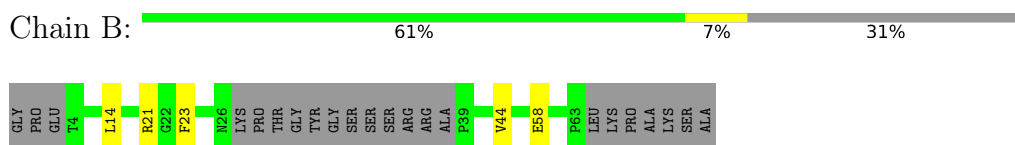
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

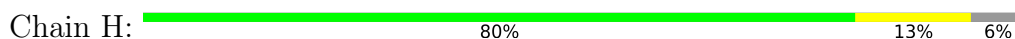
• Molecule 1: Insulin-like growth factor 1 receptor

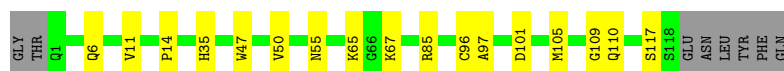


• Molecule 2: Insulin-like growth factor I



• Molecule 3: Fv 24-60 heavy chain





- Molecule 4: Fv 24-60 light chain

Chain L: 80% 18% ..



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



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

Chain D: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.69Å 197.66Å 117.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.17 – 3.27 22.17 – 3.27	Depositor EDS
% Data completeness (in resolution range)	98.6 (22.17-3.27) 98.7 (22.17-3.27)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.30Å)	Xtriage
Refinement program	phenix.refine 1.11.1-2575_1692, PHENIX 1.11.1-2575_1692	Depositor
R, R_{free}	0.260 , 0.303 0.261 , 0.306	Depositor DCC
R_{free} test set	1524 reflections (4.72%)	wwPDB-V
Wilson B-factor (Å ²)	111.0	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 126.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8704	wwPDB-V
Average B, all atoms (Å ²)	177.0	wwPDB-V

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, MLT, NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/6582	0.29	0/8931
2	B	0.08	0/381	0.27	0/511
3	H	0.08	0/936	0.24	0/1270
4	L	0.10	0/838	0.33	0/1136
All	All	0.09	0/8737	0.29	0/11848

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	6427	0	6220	87	0
2	B	375	0	347	5	0
3	H	915	0	888	11	0
4	L	820	0	792	13	0
5	C	28	0	25	1	0
5	E	28	0	25	0	0
6	D	50	0	43	0	0
7	A	10	0	0	0	0
8	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	42	0	39	0	0
All	All	8704	0	8383	112	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 7.

All (112) 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:A:511:GLN:H	1:A:515:GLY:HA3	1.58	0.69
1:A:114:GLU:HG2	1:A:115:LYS:HG3	1.75	0.68
1:A:433:GLU:HA	1:A:436:THR:HB	1.75	0.67
1:A:337:GLY:HA3	1:A:340:ILE:HD11	1.78	0.66
1:A:144:PRO:HG2	1:A:147:GLU:HB2	1.78	0.64
1:A:348:MET:HA	1:A:351:ILE:HD13	1.81	0.63
1:A:9:ILE:HD13	1:A:16:LEU:HA	1.81	0.62
1:A:274:MET:HE1	1:A:278:PRO:HD3	1.82	0.61
1:A:240:ARG:HD2	1:A:272:GLU:HG2	1.82	0.61
1:A:256:LEU:O	3:H:55:ASN:ND2	2.34	0.61
1:A:360:ILE:HB	1:A:392:VAL:HG12	1.83	0.60
3:H:67:LYS:NZ	3:H:85:ARG:O	2.33	0.60
1:A:808:VAL:HB	1:A:890:VAL:HG11	1.83	0.60
1:A:87:LEU:HB3	1:A:111:ILE:HD12	1.86	0.58
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.85	0.58
3:H:47:TRP:HZ2	3:H:50:VAL:HG23	1.69	0.58
1:A:193:ALA:HB1	1:A:201:CYS:HB2	1.87	0.57
1:A:112:ARG:NH1	1:A:114:GLU:OE1	2.38	0.57
1:A:148:CYS:SG	1:A:149:GLY:N	2.78	0.56
4:L:10:THR:HG22	4:L:103:LYS:HB3	1.86	0.56
1:A:340:ILE:HB	1:A:511:GLN:HG3	1.86	0.56
1:A:129:LEU:HD11	1:A:182:GLN:HE21	1.71	0.56
1:A:598:ILE:HG22	1:A:759:VAL:HG22	1.88	0.56
4:L:90:GLN:OE1	4:L:92:ASN:ND2	2.39	0.55
2:B:21:ARG:NH1	2:B:58:GLU:OE1	2.34	0.55
1:A:878:THR:HA	1:A:883:ASN:HA	1.89	0.54
3:H:97:ALA:HB1	3:H:105:MET:HB3	1.90	0.54
4:L:7:SER:HB2	4:L:8:PRO:HD3	1.90	0.54
1:A:112:ARG:HG3	1:A:138:TYR:HB3	1.90	0.53
1:A:31:ILE:HB	1:A:57:LEU:HD23	1.90	0.53
1:A:66:LEU:HD12	1:A:98:ILE:HG23	1.91	0.53
1:A:301:VAL:HG11	1:A:327:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:LYS:HG3	4:L:55:ILE:HD11	1.91	0.53
1:A:353:VAL:HG22	1:A:377:LEU:HB2	1.91	0.52
4:L:29:ILE:HG13	4:L:31:ASN:O	2.10	0.51
1:A:526:LEU:HD12	1:A:527:PRO:HD2	1.92	0.51
1:A:778:HIS:CD2	1:A:779:GLU:HG2	2.46	0.51
1:A:503:LYS:O	1:A:505:VAL:N	2.42	0.51
3:H:47:TRP:CZ2	3:H:50:VAL:HG23	2.45	0.51
1:A:89:ILE:HG23	1:A:92:MET:HG3	1.93	0.51
1:A:595:SER:HA	1:A:763:LEU:HB2	1.92	0.51
1:A:503:LYS:O	1:A:573:TYR:OH	2.22	0.50
1:A:11:ASN:CG	2:B:23:PHE:H	2.19	0.50
1:A:753:ASP:OD1	1:A:753:ASP:N	2.40	0.50
1:A:582:SER:HB3	1:A:604:PRO:HB2	1.93	0.50
1:A:584:PRO:HG2	1:A:773:ILE:HG22	1.92	0.50
1:A:285:GLY:O	1:A:287:GLN:N	2.45	0.49
1:A:392:VAL:HG23	1:A:421:ASN:HD21	1.78	0.49
2:B:14:LEU:HB3	2:B:23:PHE:HE2	1.78	0.49
1:A:774:HIS:CE1	1:A:788:SER:HB3	2.48	0.49
1:A:90:PHE:HD1	1:A:114:GLU:HB3	1.78	0.48
1:A:694:ASN:HA	2:B:44:VAL:HG21	1.96	0.48
1:A:32:LEU:HD11	1:A:56:LEU:HD22	1.96	0.47
1:A:34:ILE:HB	1:A:60:VAL:HG13	1.95	0.47
3:H:6:GLN:H	3:H:110:GLN:HE22	1.60	0.47
1:A:405:ASP:OD1	1:A:431:ARG:NE	2.48	0.47
1:A:250:ASP:O	1:A:254:ASN:ND2	2.42	0.47
1:A:478:THR:HG22	1:A:535:GLY:HA3	1.97	0.47
1:A:72:ASN:HA	1:A:102:ASN:HD22	1.80	0.47
3:H:35:HIS:NE2	3:H:101:ASP:O	2.45	0.47
1:A:126:ASP:OD1	1:A:128:SER:OG	2.26	0.46
1:A:335:ARG:HH11	1:A:362:HIS:HB3	1.80	0.46
1:A:624:ASP:OD1	1:A:641:ARG:NH1	2.48	0.46
1:A:401:LEU:HD11	1:A:429:ILE:HG22	1.98	0.46
1:A:8:ASP:HA	1:A:30:HIS:HB2	1.97	0.46
3:H:35:HIS:HB2	3:H:97:ALA:HB3	1.98	0.46
1:A:177:THR:HG23	1:A:180:ARG:H	1.81	0.45
1:A:325:ILE:HG23	1:A:353:VAL:HB	1.98	0.45
1:A:222:ARG:HH11	5:C:2:NAG:H82	1.81	0.45
1:A:590:ALA:HB3	1:A:598:ILE:HD11	1.98	0.45
1:A:177:THR:HG23	1:A:179:ASN:H	1.81	0.45
4:L:14:THR:HG23	4:L:107:LYS:HB3	1.97	0.45
3:H:96:CYS:O	3:H:109:GLY:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:THR:HG22	1:A:441:ARG:HD2	1.98	0.45
2:B:14:LEU:HB3	2:B:23:PHE:CE2	2.51	0.45
1:A:121:TYR:OH	1:A:151:LEU:O	2.32	0.45
1:A:618:TRP:HA	1:A:770:ARG:O	2.17	0.45
1:A:551:VAL:N	1:A:569:SER:OG	2.42	0.44
1:A:177:THR:OG1	1:A:178:THR:N	2.50	0.44
1:A:368:SER:HA	1:A:400:GLN:O	2.18	0.44
1:A:377:LEU:HD23	1:A:410:THR:HB	1.98	0.44
4:L:92:ASN:OD1	4:L:93:SER:N	2.51	0.44
1:A:128:SER:HA	1:A:134:VAL:HG21	2.00	0.44
1:A:873:ALA:HB2	1:A:892:PHE:HE1	1.82	0.44
1:A:835:TYR:HB2	1:A:850:VAL:HB	2.00	0.43
1:A:309:LYS:HZ1	1:A:319:MET:HB2	1.83	0.43
1:A:498:LYS:HD2	1:A:518:SER:HB2	1.99	0.43
1:A:323:CYS:HB2	1:A:351:ILE:HD11	2.00	0.43
1:A:176:TRP:CD1	1:A:182:GLN:HA	2.54	0.43
1:A:820:LEU:HD12	1:A:837:ILE:HD13	2.00	0.43
1:A:195:THR:OG1	1:A:196:GLU:N	2.51	0.43
1:A:341:ALA:HB2	1:A:511:GLN:HE21	1.84	0.43
1:A:824:GLU:HB2	1:A:855:TYR:CE1	2.54	0.43
1:A:32:LEU:HD23	1:A:700:ILE:HG23	2.01	0.42
1:A:259:GLU:OE2	3:H:65:LYS:NZ	2.51	0.42
1:A:832:ILE:HD12	1:A:877:ALA:HB1	2.02	0.42
4:L:49:LYS:HE2	4:L:55:ILE:HG13	2.01	0.41
1:A:321:GLN:HB2	1:A:347:PHE:HD1	1.85	0.41
1:A:386:GLY:O	1:A:415:LYS:NZ	2.41	0.41
3:H:14:PRO:HD3	3:H:117:SER:O	2.20	0.41
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.56	0.41
4:L:61:ARG:HD2	4:L:77:SER:O	2.20	0.41
1:A:621:GLN:HB2	1:A:768:LEU:HB3	2.03	0.41
4:L:90:GLN:HE22	4:L:92:ASN:CG	2.29	0.41
1:A:416:MET:HB3	1:A:418:PHE:HE1	1.85	0.41
1:A:616:VAL:HG12	1:A:773:ILE:HG12	2.03	0.41
1:A:404:TRP:CD1	1:A:406:HIS:HD1	2.39	0.41
1:A:642:LYS:HB3	1:A:642:LYS:HE2	1.86	0.41
1:A:463:LEU:HB2	1:A:569:SER:HB3	2.02	0.41
1:A:862:LYS:HE3	1:A:864:ASN:HB3	2.02	0.41
1:A:274:MET:HE3	1:A:274:MET:HB2	1.88	0.40
4:L:103:LYS:NZ	4:L:105:GLU:HB3	2.36	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	789/885 (89%)	723 (92%)	61 (8%)	5 (1%)	21	51
2	B	44/70 (63%)	40 (91%)	4 (9%)	0	100	100
3	H	116/126 (92%)	111 (96%)	5 (4%)	0	100	100
4	L	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
All	All	1054/1189 (89%)	973 (92%)	76 (7%)	5 (0%)	24	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	SER
1	A	11	ASN
1	A	379	LEU
1	A	380	GLY
1	A	504	ASN

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	715/787 (91%)	706 (99%)	9 (1%)	61	75
2	B	41/57 (72%)	41 (100%)	0	100	100
3	H	100/107 (94%)	99 (99%)	1 (1%)	68	77
4	L	95/95 (100%)	92 (97%)	3 (3%)	34	60
All	All	951/1046 (91%)	938 (99%)	13 (1%)	59	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	83	TYR
1	A	131	LEU
1	A	294	CYS
1	A	310	THR
1	A	315	THR
1	A	373	LYS
1	A	626	TYR
1	A	693	GLU
3	H	11	VAL
4	L	29	ILE
4	L	33	LEU
4	L	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	94	ASN
1	A	102	ASN
1	A	223	HIS
1	A	269	HIS
1	A	464	HIS
1	A	827	ASN
3	H	57	ASN
4	L	38	GLN
4	L	90	GLN
4	L	92	ASN

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
5	NAG	C	1	1,5	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	C	2	5	14,14,15	0.28	0	17,19,21	0.54	0
6	NAG	D	1	1,6	14,14,15	0.44	0	17,19,21	0.40	0
6	NAG	D	2	6	14,14,15	0.31	0	17,19,21	0.47	0
6	MAN	D	3	6	11,11,12	0.94	0	15,15,17	1.13	2 (13%)
6	MAN	D	4	6	11,11,12	0.70	0	15,15,17	1.19	2 (13%)
5	NAG	E	1	1,5	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	E	2	5	14,14,15	0.24	0	17,19,21	0.44	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	NAG	C	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	MAN	D	3	6	-	0/2/19/22	0/1/1/1
6	MAN	D	4	6	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	4	MAN	C1-O5-C5	3.62	117.03	112.19
6	D	3	MAN	C1-O5-C5	2.72	115.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3	MAN	O2-C2-C3	-2.19	105.62	110.15
6	D	4	MAN	O2-C2-C3	-2.11	105.78	110.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

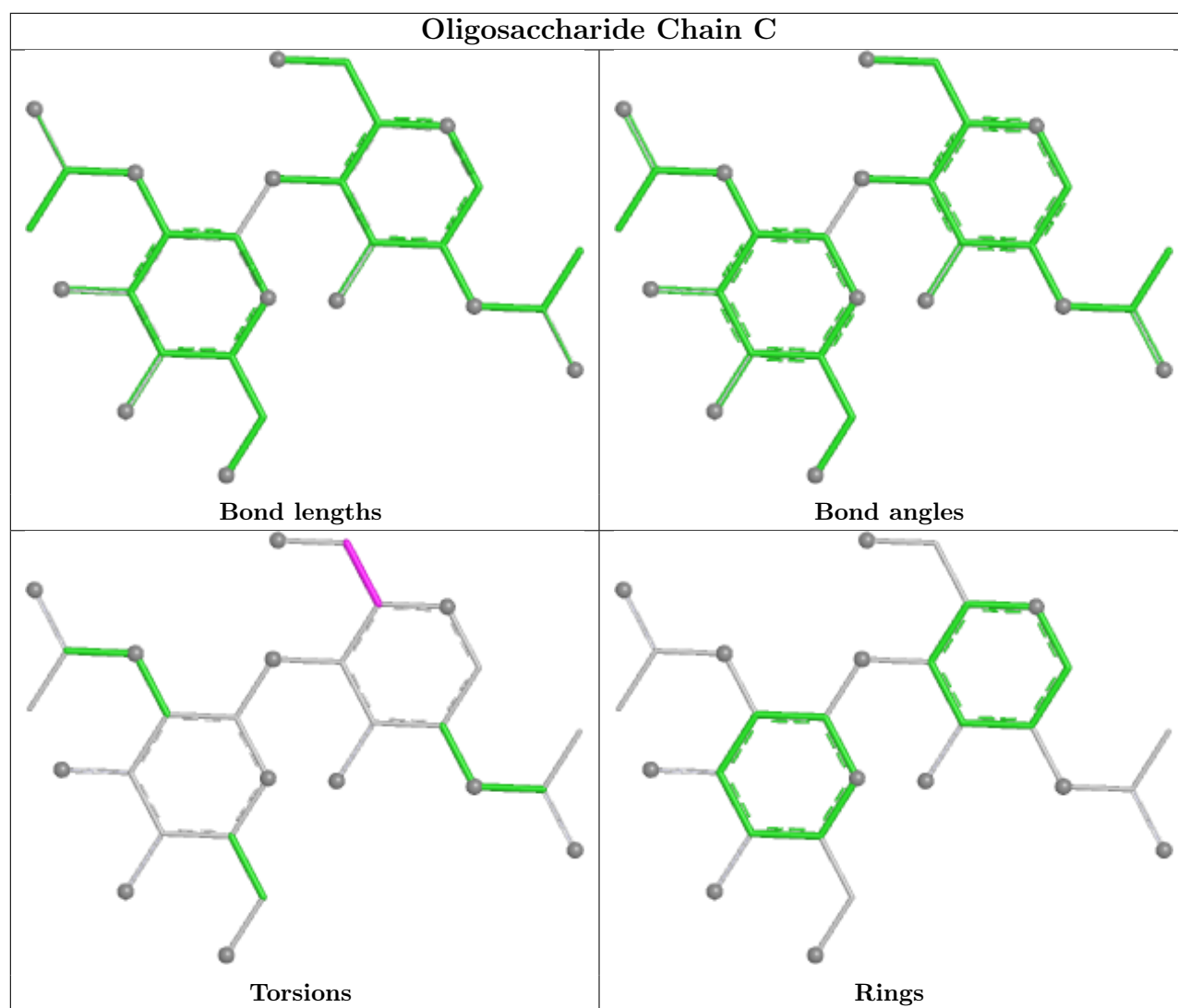
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
6	D	4	MAN	O5-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
6	D	4	MAN	C4-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6

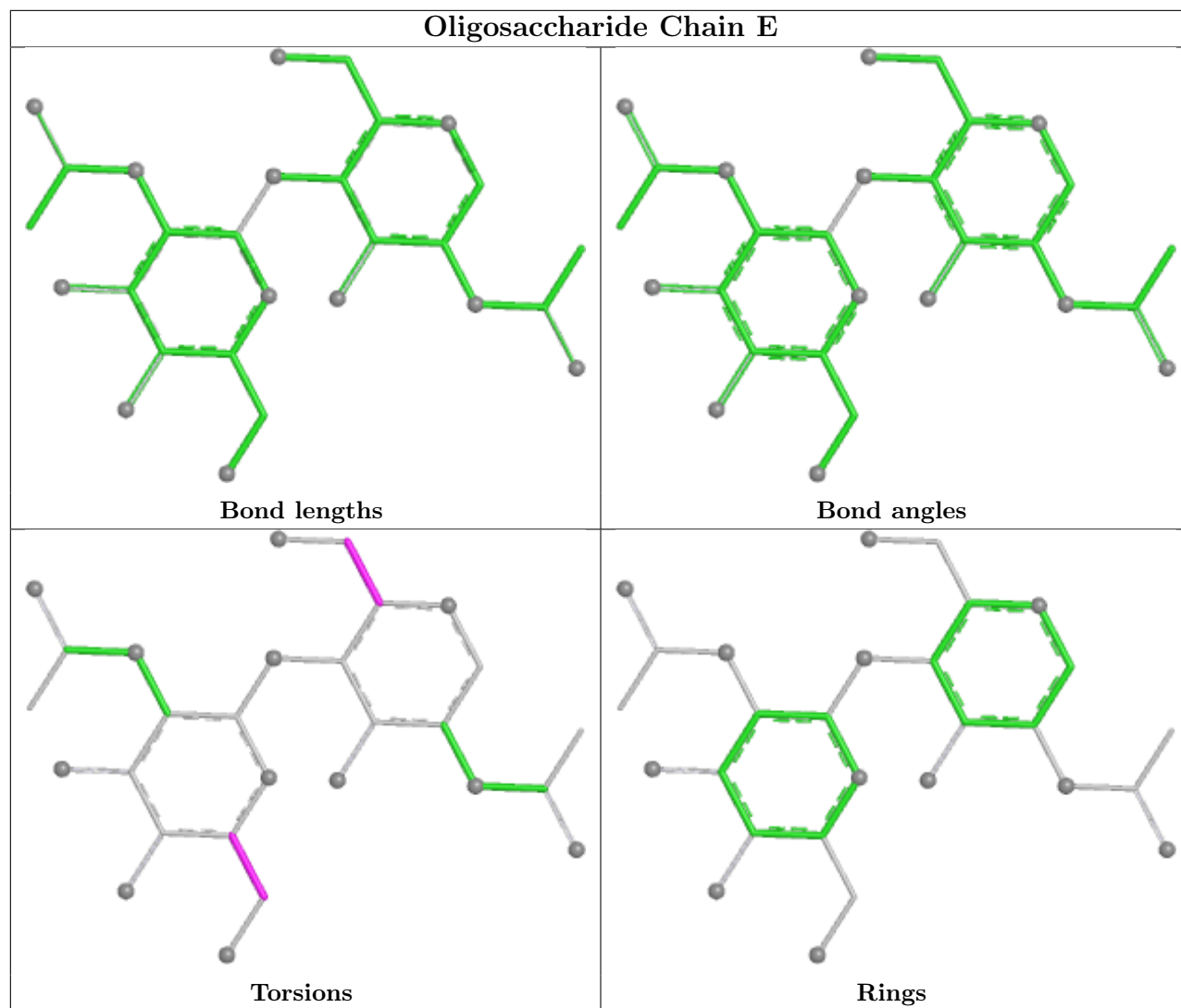
There are no ring outliers.

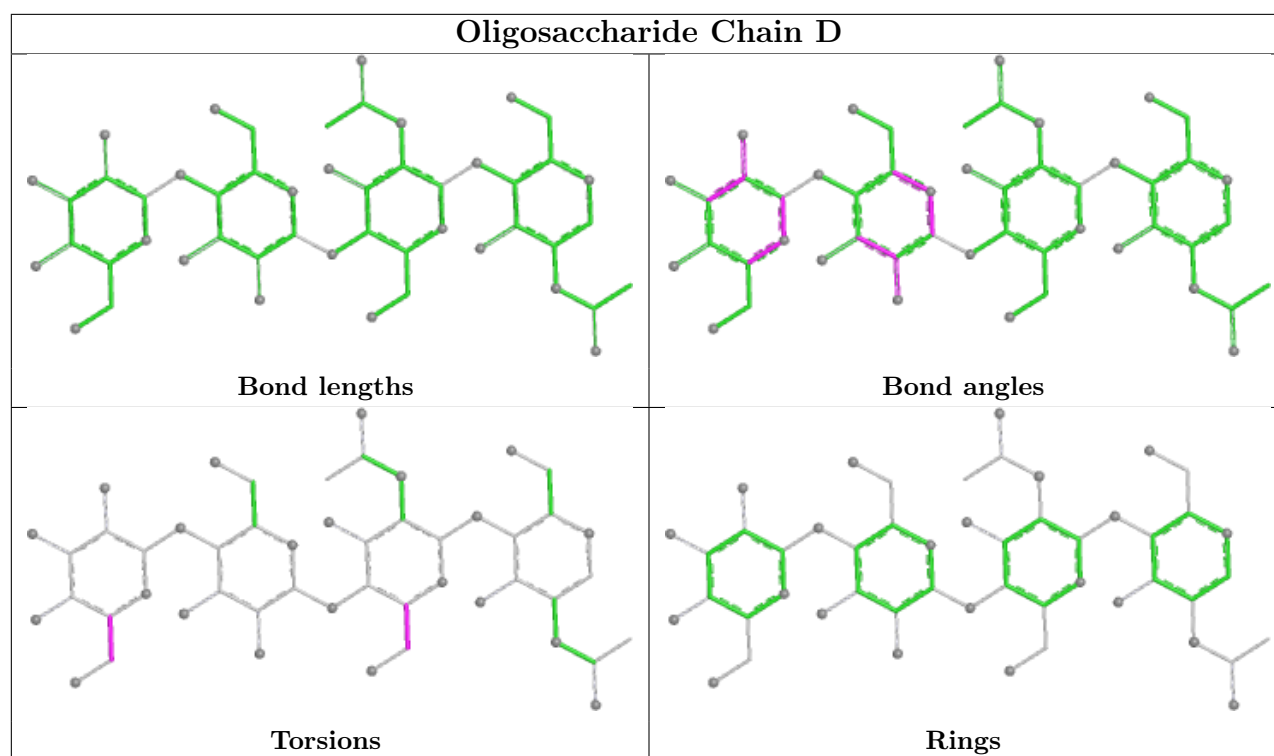
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	1	0

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







5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
9	NAG	A	1012	1	14,14,15	0.33	0	17,19,21	0.59	0
9	NAG	A	1004	1	14,14,15	0.27	0	17,19,21	0.57	0
8	MLT	A	1003	-	8,8,8	1.10	0	10,10,10	1.62	2 (20%)
7	SO4	A	1001	-	4,4,4	0.24	0	6,6,6	0.08	0
9	NAG	A	1007	1	14,14,15	0.37	0	17,19,21	0.60	0
7	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.08	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
9	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1012	1	-	2/6/23/26	0/1/1/1
8	MLT	A	1003	-	-	7/8/8/8	-
9	NAG	A	1007	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1003	MLT	O2-C1-C2	3.51	120.17	112.74
8	A	1003	MLT	O5-C4-C3	2.05	120.38	114.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1003	MLT	C1-C2-C3-C4
8	A	1003	MLT	O3-C2-C3-C4
9	A	1004	NAG	C3-C2-N2-C7
9	A	1012	NAG	C3-C2-N2-C7
8	A	1003	MLT	O2-C1-C2-C3
8	A	1003	MLT	C2-C3-C4-O5
9	A	1004	NAG	C1-C2-N2-C7
9	A	1012	NAG	C1-C2-N2-C7
8	A	1003	MLT	O1-C1-C2-C3
8	A	1003	MLT	C2-C3-C4-O4
8	A	1003	MLT	O2-C1-C2-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	801/885 (90%)	-0.07	10 (1%) 76 58	119, 174, 259, 316	0
2	B	48/70 (68%)	-0.32	0 100 100	140, 171, 205, 214	0
3	H	118/126 (93%)	-0.26	0 100 100	109, 147, 196, 222	0
4	L	107/108 (99%)	-0.01	0 100 100	102, 157, 202, 242	0
All	All	1074/1189 (90%)	-0.09	10 (0%) 81 65	102, 170, 251, 316	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ASP	4.2
1	A	252	CYS	2.6
1	A	174	ARG	2.5
1	A	13	TYR	2.4
1	A	638	ILE	2.4
1	A	517	ASN	2.3
1	A	292	ILE	2.2
1	A	122	LEU	2.1
1	A	109	GLY	2.1
1	A	403	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

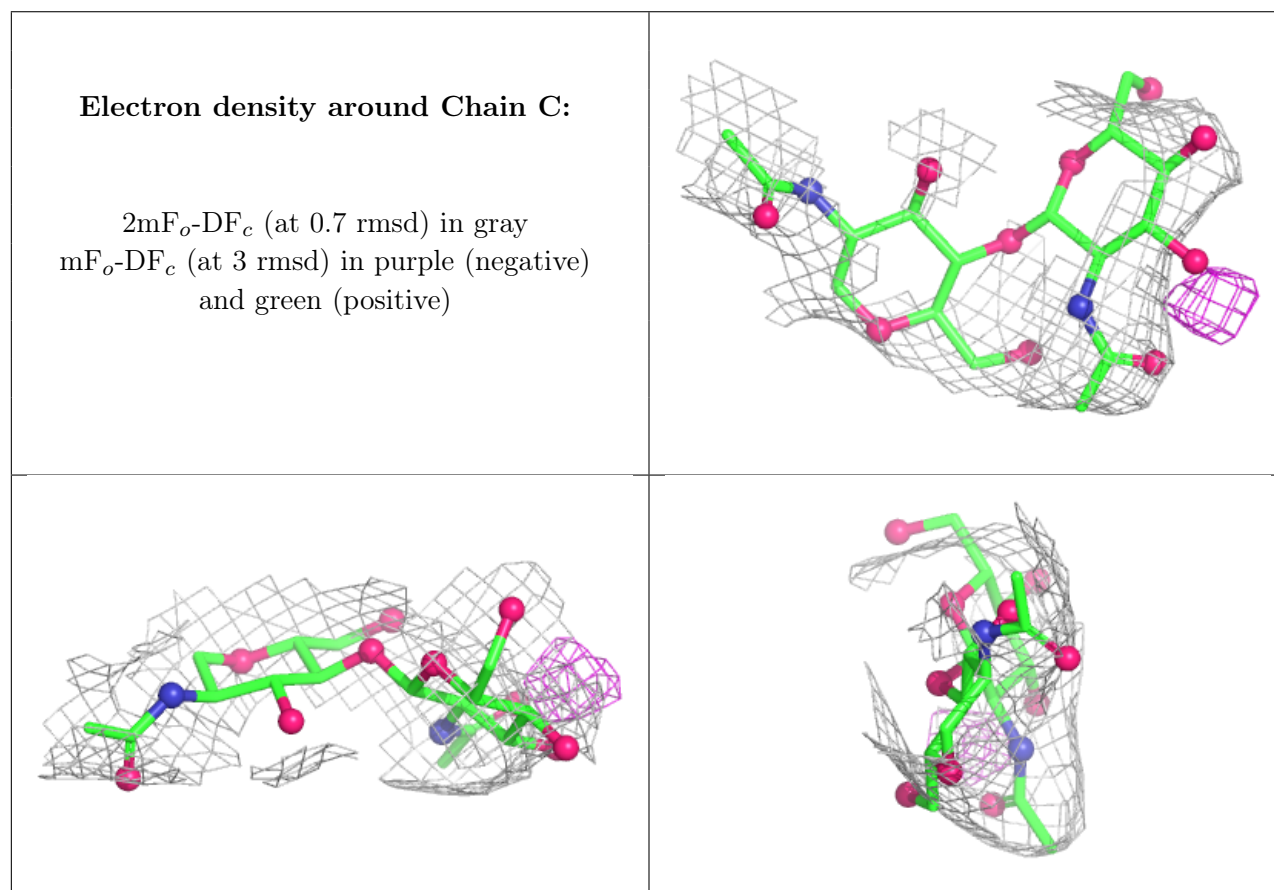
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

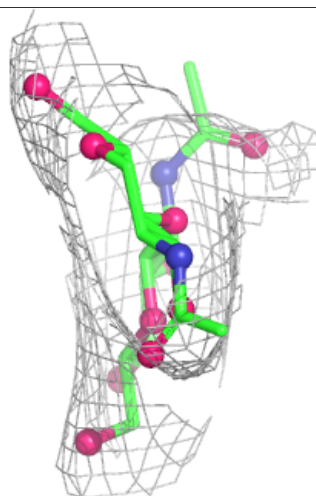
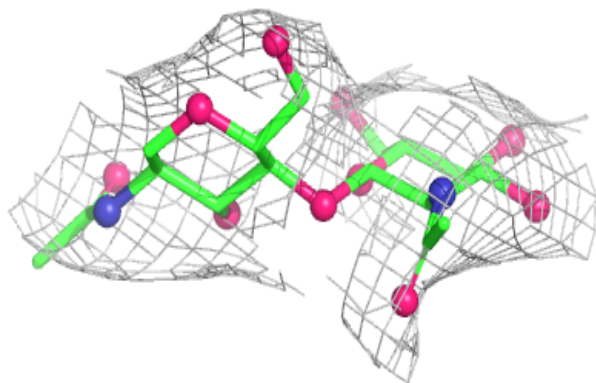
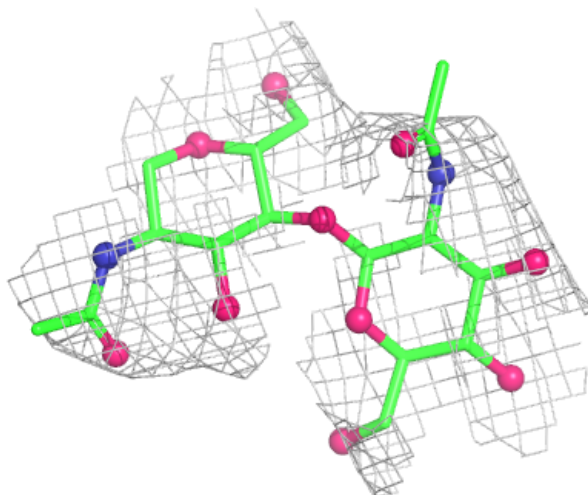
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	177,211,224,225	0
5	NAG	C	2	14/15	-	-	161,231,239,242	0
5	NAG	E	2	14/15	0.57	0.09	150,177,196,200	0
5	NAG	E	1	14/15	0.86	0.07	119,153,169,179	0
6	NAG	D	1	14/15	-	-	136,164,184,214	0
6	NAG	D	2	14/15	-	-	168,202,218,239	0
6	MAN	D	3	11/12	-	-	219,242,253,261	0
6	MAN	D	4	11/12	-	-	189,225,236,236	0

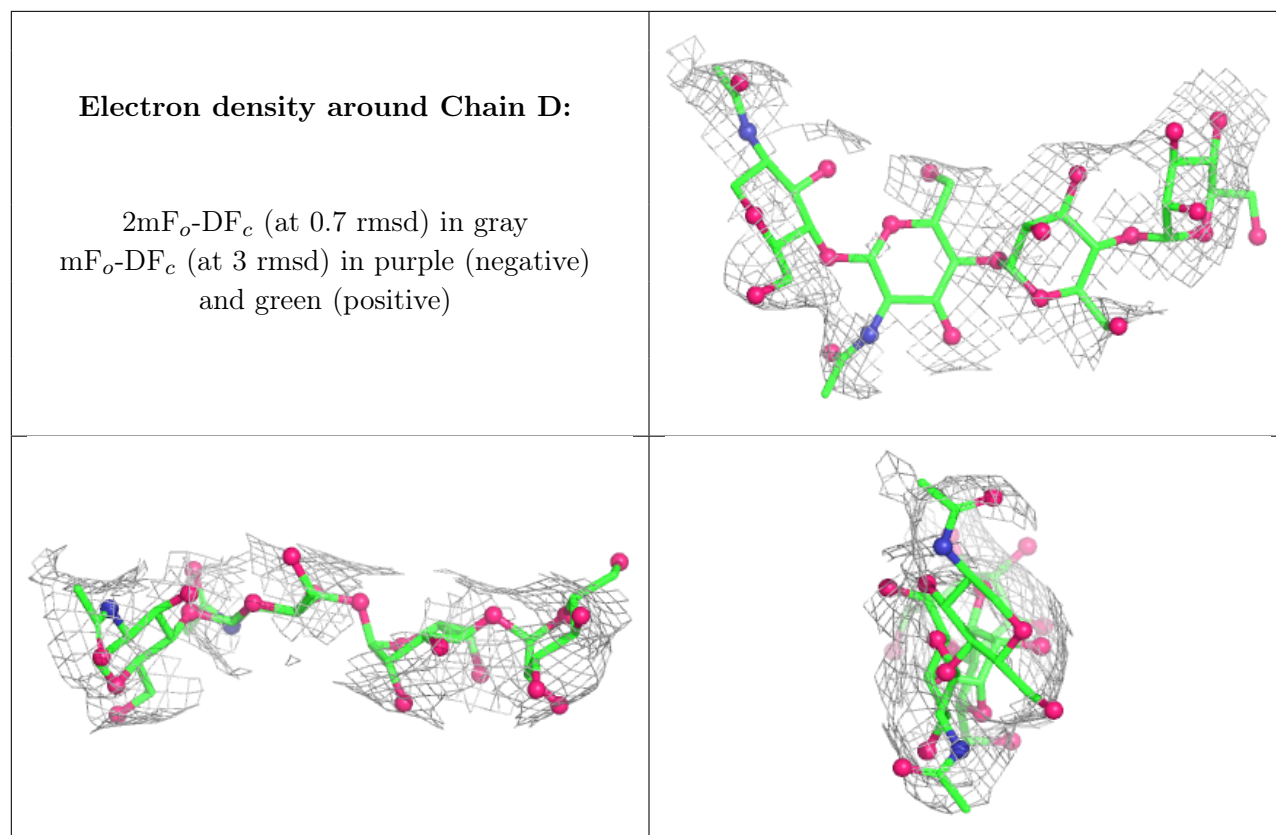
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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($\text{\AA}^2$)	Q<0.9
9	NAG	A	1012	14/15	0.35	0.11	159,188,214,215	0
9	NAG	A	1007	14/15	0.58	0.12	188,239,290,327	0
9	NAG	A	1004	14/15	0.64	0.12	172,207,225,227	0
7	SO4	A	1002	5/5	0.65	0.16	172,185,208,221	0
7	SO4	A	1001	5/5	0.70	0.13	163,205,216,216	0
8	MLT	A	1003	9/9	0.91	0.07	137,153,160,161	0

6.5 Other polymers [i](#)

There are no such residues in this entry.