



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:49 AM UTC

PDB ID : 3OL2 / pdb_00003ol2
Title : Receptor-ligand structure of Human Semaphorin 4D with Plexin B1.
Authors : Janssen, B.J.C.; Robinson, R.A.; Perez-Branguli, F.; Bell, C.H.; Mitchell, C.J.; Siebold, C.; Jones, E.Y.
Deposited on : 2010-08-25
Resolution : 2.99 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

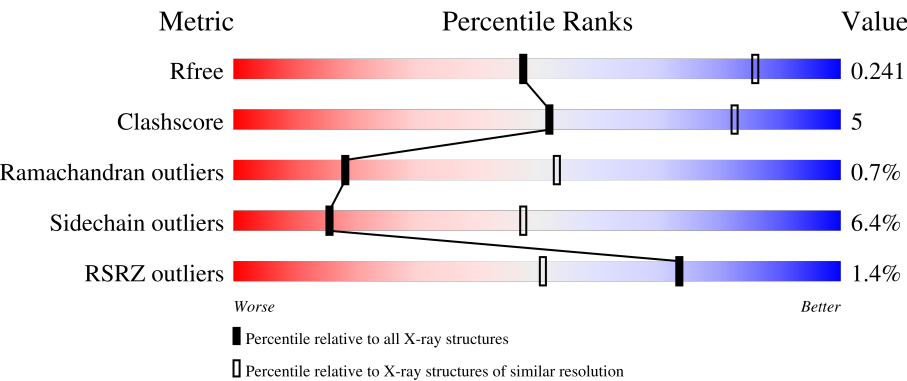
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	663	% 77%14%• 7%
2	B	528	2% 72%18%• 6%
3	C	3	33%33%33%
3	E	3	33%67%
3	H	3	33%33%33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	2	 100%
4	F	2	 100%
4	G	2	 50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8828 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 Semaphorin-4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4866	3100	840	903	23			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	LYS	-	expression tag	UNP Q92854
A	679	HIS	-	expression tag	UNP Q92854
A	680	HIS	-	expression tag	UNP Q92854
A	681	HIS	-	expression tag	UNP Q92854
A	682	HIS	-	expression tag	UNP Q92854
A	683	HIS	-	expression tag	UNP Q92854
A	684	HIS	-	expression tag	UNP Q92854

- Molecule 2 is a protein called Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	496	Total	C	N	O	S	0	0	0
			3747	2354	652	719	22			

There are 12 discrepancies between the modelled and reference sequences:

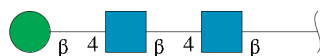
Chain	Residue	Modelled	Actual	Comment	Reference
B	17	GLU	-	cloning artifact	UNP O43157
B	18	THR	-	cloning artifact	UNP O43157
B	19	GLY	-	cloning artifact	UNP O43157
B	536	GLY	-	expression tag	UNP O43157
B	537	THR	-	expression tag	UNP O43157
B	538	LYS	-	expression tag	UNP O43157
B	539	HIS	-	expression tag	UNP O43157
B	540	HIS	-	expression tag	UNP O43157
B	541	HIS	-	expression tag	UNP O43157

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	542	HIS	-	expression tag	UNP O43157
B	543	HIS	-	expression tag	UNP O43157
B	544	HIS	-	expression tag	UNP O43157

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



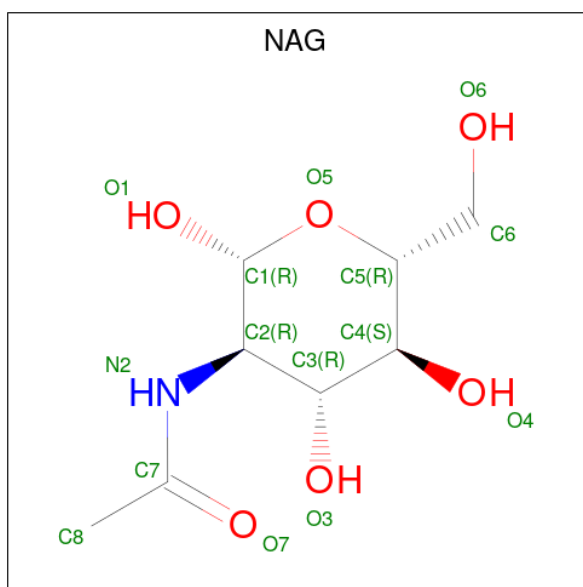
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

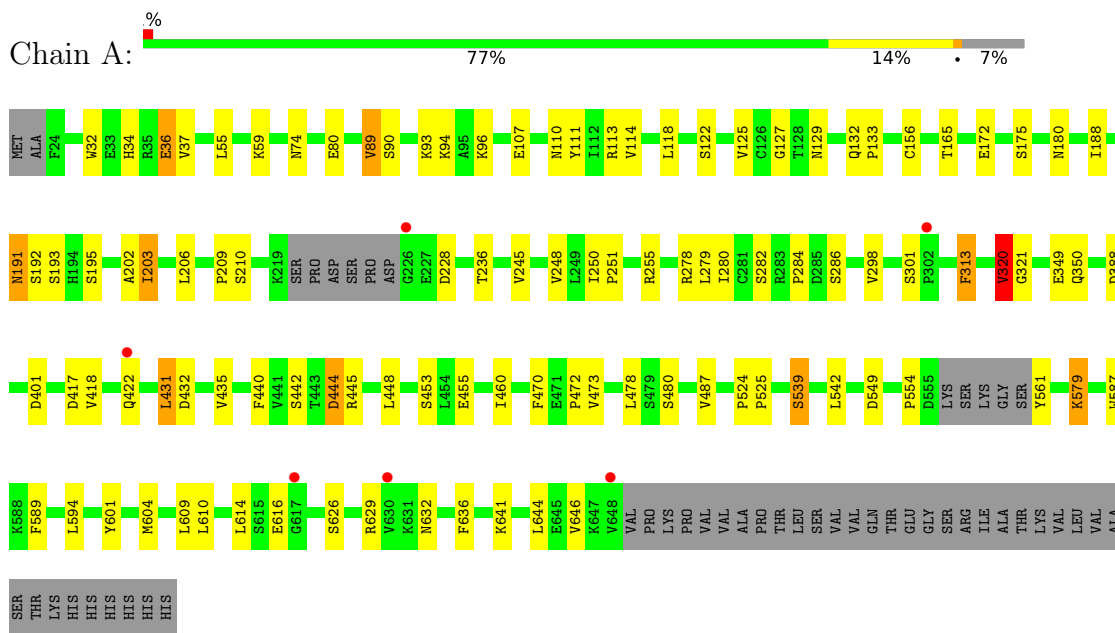


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

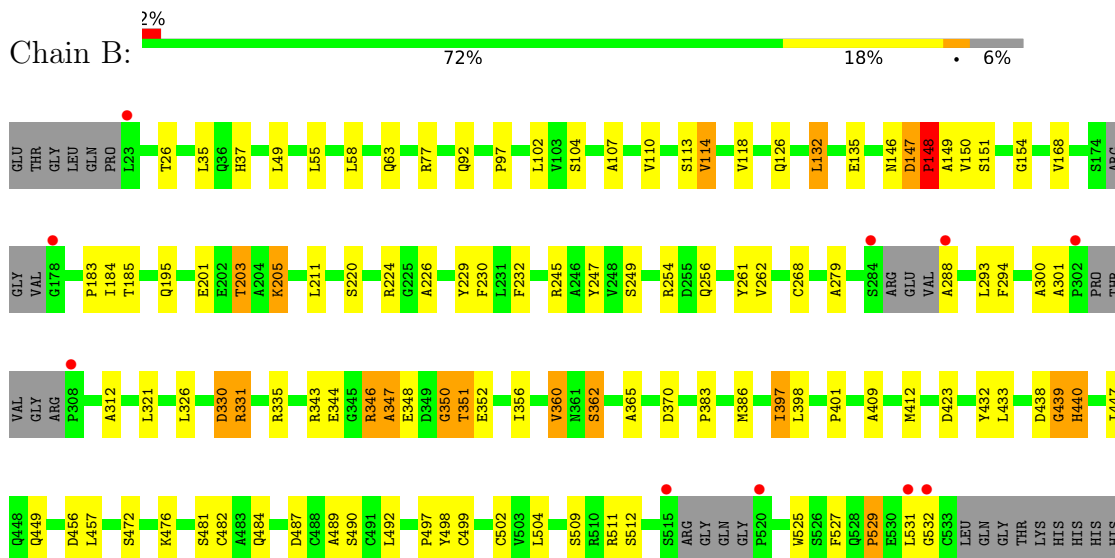
3 Residue-property plots [i](#)

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: Semaphorin-4D

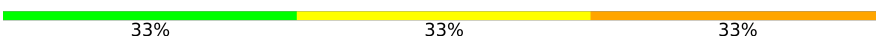


• Molecule 2: Plexin-B1





- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  33% 33% 33%

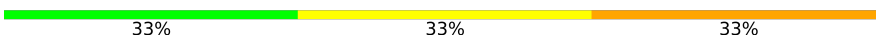


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

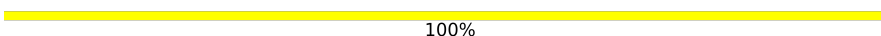


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 33% 33%

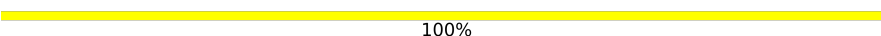


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



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

Chain F:  100%



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

Chain G:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	83.06Å 173.44Å 482.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 2.99 49.49 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.49-2.99) 99.2 (49.49-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.190 , 0.237 0.194 , 0.241	Depositor DCC
R_{free} test set	1760 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8828	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: NAG, BMA

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	0.81	2/4984 (0.0%)	1.34	40/6757 (0.6%)
2	B	0.91	0/3842	1.39	41/5247 (0.8%)
All	All	0.86	2/8826 (0.0%)	1.36	81/12004 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	VAL	CA-C	7.13	1.59	1.52
1	A	203	ILE	CA-CB	5.05	1.56	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	VAL	N-CA-C	9.39	122.22	113.20
2	B	350	GLY	CA-C-N	8.69	137.34	121.70
2	B	350	GLY	C-N-CA	8.69	137.34	121.70
1	A	431	LEU	CA-C-N	8.11	131.96	120.28
1	A	431	LEU	C-N-CA	8.11	131.96	120.28
2	B	365	ALA	N-CA-C	7.58	119.55	108.86
2	B	482	CYS	CA-C-N	7.24	130.30	120.38
2	B	482	CYS	C-N-CA	7.24	130.30	120.38
1	A	632	ASN	N-CA-C	-6.92	103.48	112.68
2	B	26	THR	CB-CA-C	6.71	120.35	109.07
2	B	499	CYS	N-CA-C	6.69	121.20	109.96
1	A	432	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	349	GLU	CA-C-N	6.53	133.44	121.70
1	A	349	GLU	C-N-CA	6.53	133.44	121.70
1	A	191	ASN	CA-CB-CG	6.45	119.05	112.60
2	B	509	SER	N-CA-C	6.44	116.78	108.34
1	A	89	VAL	N-CA-CB	6.41	117.71	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	LEU	CA-C-N	6.38	128.89	122.00
2	B	132	LEU	C-N-CA	6.38	128.89	122.00
2	B	147	ASP	CA-CB-CG	6.27	118.87	112.60
2	B	330	ASP	CA-CB-CG	6.27	118.87	112.60
2	B	126	GLN	CA-C-N	6.02	128.63	120.38
2	B	126	GLN	C-N-CA	6.02	128.63	120.38
2	B	288	ALA	CA-C-N	6.00	129.72	121.33
2	B	288	ALA	C-N-CA	6.00	129.72	121.33
1	A	388	ASP	CA-C-N	5.99	128.23	120.44
1	A	388	ASP	C-N-CA	5.99	128.23	120.44
2	B	397	ILE	CA-C-N	5.95	132.33	122.33
2	B	397	ILE	C-N-CA	5.95	132.33	122.33
2	B	360	VAL	N-CA-CB	5.95	118.41	110.26
2	B	148	PRO	N-CA-C	-5.94	100.24	112.47
2	B	502	CYS	CA-C-N	5.89	128.48	120.77
2	B	502	CYS	C-N-CA	5.89	128.48	120.77
2	B	203	THR	CB-CA-C	5.85	119.21	109.56
1	A	180	ASN	CA-C-N	5.80	127.98	120.44
1	A	180	ASN	C-N-CA	5.80	127.98	120.44
1	A	349	GLU	N-CA-C	5.75	119.17	111.24
1	A	36	GLU	N-CA-C	5.73	119.90	113.02
1	A	282	SER	CA-C-N	5.68	130.79	122.66
1	A	282	SER	C-N-CA	5.68	130.79	122.66
1	A	320	VAL	N-CA-CB	-5.67	104.00	112.67
1	A	320	VAL	CB-CA-C	5.60	116.24	110.70
1	A	313	PHE	CA-CB-CG	5.57	119.37	113.80
2	B	26	THR	N-CA-C	-5.57	106.85	113.97
1	A	228	ASP	CA-CB-CG	5.55	118.16	112.60
2	B	114	VAL	N-CA-CB	-5.53	102.10	111.23
1	A	460	ILE	CA-C-N	5.50	127.70	120.60
1	A	460	ILE	C-N-CA	5.50	127.70	120.60
1	A	480	SER	CA-C-N	5.47	128.47	120.71
1	A	480	SER	C-N-CA	5.47	128.47	120.71
2	B	511	ARG	CA-C-N	5.41	127.79	120.38
2	B	511	ARG	C-N-CA	5.41	127.79	120.38
2	B	447	ILE	N-CA-C	-5.40	106.42	111.45
1	A	202	ALA	CA-C-N	5.39	125.61	120.43
1	A	202	ALA	C-N-CA	5.39	125.61	120.43
1	A	96	LYS	CA-C-N	5.39	127.50	120.28
1	A	96	LYS	C-N-CA	5.39	127.50	120.28
2	B	498	TYR	CA-C-N	5.34	129.99	122.09
2	B	498	TYR	C-N-CA	5.34	129.99	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	PRO	N-CA-C	5.34	120.95	113.53
2	B	489	ALA	CA-C-N	5.32	127.41	120.28
2	B	489	ALA	C-N-CA	5.32	127.41	120.28
1	A	188	ILE	N-CA-C	-5.31	99.51	107.37
2	B	401	PRO	N-CA-C	5.28	120.46	113.86
2	B	107	ALA	N-CA-C	5.26	117.41	109.41
2	B	300	ALA	N-CA-C	5.23	118.47	110.20
1	A	455	GLU	CA-C-N	5.23	129.77	122.08
1	A	455	GLU	C-N-CA	5.23	129.77	122.08
2	B	476	LYS	CA-C-N	5.19	126.33	122.59
2	B	476	LYS	C-N-CA	5.19	126.33	122.59
1	A	129	ASN	CA-CB-CG	5.16	117.76	112.60
2	B	268	CYS	CA-C-N	5.13	130.94	121.70
2	B	268	CYS	C-N-CA	5.13	130.94	121.70
2	B	423	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	34	HIS	CA-C-N	5.07	127.07	120.28
1	A	34	HIS	C-N-CA	5.07	127.07	120.28
1	A	180	ASN	N-CA-C	5.06	115.73	108.74
2	B	37	HIS	N-CA-C	5.06	117.36	109.52
1	A	122	SER	N-CA-C	5.05	116.51	108.79
1	A	444	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	188	ILE	N-CA-CB	5.00	117.97	111.67

There are no chirality outliers.

There are no planarity outliers.

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	4866	0	4783	39	0
2	B	3747	0	3586	49	0
3	C	39	0	34	1	0
3	E	39	0	34	0	0
3	H	39	0	34	1	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	28	0	25	1	0
5	A	14	0	13	2	0
All	All	8828	0	8559	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (88) 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:B:350:GLY:HA2	2:B:351:THR:HG23	1.40	1.00
2:B:350:GLY:HA2	2:B:351:THR:CG2	2.17	0.72
2:B:232:PHE:HE2	2:B:249:SER:HB2	1.60	0.66
1:A:278:ARG:NH2	1:A:401:ASP:O	2.28	0.66
2:B:279:ALA:HB1	2:B:293:LEU:HD11	1.77	0.66
2:B:531:LEU:HB3	2:B:532:GLY:HA2	1.77	0.65
2:B:148:PRO:O	2:B:150:VAL:N	2.30	0.65
1:A:320:VAL:N	1:A:321:GLY:HA2	2.13	0.63
2:B:398:LEU:HA	2:B:439:GLY:HA3	1.81	0.62
2:B:148:PRO:C	2:B:150:VAL:H	2.07	0.61
2:B:147:ASP:C	2:B:148:PRO:O	2.42	0.60
1:A:440:PHE:HB3	1:A:448:LEU:HD11	1.83	0.59
1:A:255:ARG:HH11	1:A:255:ARG:HG3	1.67	0.59
2:B:481:SER:O	2:B:484:GLN:HG2	2.02	0.58
1:A:93:LYS:HE3	1:A:132:GLN:HE22	1.69	0.57
2:B:201:GLU:C	2:B:203:THR:H	2.14	0.56
1:A:172:GLU:HG2	1:A:192:SER:HA	1.86	0.56
2:B:432:TYR:HB2	2:B:497:PRO:HG3	1.88	0.56
1:A:604:MET:HB2	1:A:610:LEU:HD13	1.86	0.56
1:A:80:GLU:HG2	5:A:3000:NAG:H82	1.87	0.56
1:A:193:SER:HB2	4:G:1:NAG:H4	1.88	0.56
2:B:356:ILE:HD11	2:B:383:PRO:HB2	1.88	0.55
2:B:55:LEU:HD11	2:B:110:VAL:HG11	1.89	0.54
2:B:330:ASP:HB2	3:H:1:NAG:H82	1.89	0.53
1:A:524:PRO:HD2	1:A:525:PRO:HD2	1.91	0.53
2:B:301:ALA:HB2	2:B:312:ALA:HA	1.91	0.52
2:B:531:LEU:HB3	2:B:532:GLY:CA	2.42	0.50
1:A:539:SER:HA	1:A:542:LEU:HD12	1.92	0.50
2:B:346:ARG:HA	2:B:352:GLU:H	1.76	0.50
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.27	0.49
1:A:278:ARG:HD2	1:A:280:ILE:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HB3	1:A:209:PRO:HG3	1.94	0.48
2:B:226:ALA:HB1	2:B:254:ARG:HH12	1.78	0.48
1:A:111:TYR:CE1	3:C:1:NAG:H82	2.49	0.48
1:A:594:LEU:HD11	1:A:601:TYR:CZ	2.48	0.48
2:B:49:LEU:HD13	2:B:58:LEU:HD13	1.95	0.48
2:B:102:LEU:HD11	2:B:154:GLY:HA3	1.96	0.47
2:B:224:ARG:HD3	2:B:326:LEU:HD13	1.96	0.47
2:B:35:LEU:HD22	2:B:49:LEU:HD23	1.96	0.47
2:B:487:ASP:OD1	2:B:490:SER:HB2	2.15	0.47
2:B:183:PRO:HD3	2:B:211:LEU:HD11	1.97	0.47
2:B:409:ALA:HB2	2:B:457:LEU:HB3	1.94	0.47
2:B:346:ARG:O	2:B:351:THR:HA	2.14	0.47
1:A:320:VAL:H	1:A:321:GLY:HA2	1.80	0.47
1:A:589:PHE:HB3	1:A:594:LEU:HD13	1.97	0.47
2:B:331:ARG:HG2	2:B:335:ARG:HH12	1.80	0.46
1:A:32:TRP:CZ3	1:A:579:LYS:HD2	2.51	0.46
1:A:626:SER:O	1:A:636:PHE:HA	2.16	0.45
2:B:356:ILE:HG13	2:B:362:SER:HB3	1.99	0.45
2:B:492:LEU:HD13	2:B:529:PRO:HB3	1.98	0.45
1:A:114:VAL:O	1:A:125:VAL:HA	2.16	0.45
2:B:168:VAL:O	2:B:184:ILE:HA	2.16	0.45
2:B:331:ARG:O	2:B:335:ARG:HG2	2.17	0.45
1:A:444:ASP:O	1:A:472:PRO:HG3	2.17	0.45
1:A:587:TRP:CE2	1:A:609:LEU:HB2	2.52	0.45
2:B:230:PHE:HB2	2:B:249:SER:HB3	1.99	0.44
2:B:321:LEU:HD23	2:B:397:ILE:HD11	1.99	0.44
1:A:445:ARG:O	1:A:470:PHE:HA	2.17	0.44
2:B:249:SER:OG	2:B:261:TYR:CZ	2.69	0.44
1:A:251:PRO:HB2	1:A:279:LEU:HB3	1.99	0.44
1:A:279:LEU:HD12	1:A:279:LEU:HA	1.85	0.44
1:A:614:LEU:HB3	1:A:646:VAL:HG21	1.99	0.44
2:B:245:ARG:HB3	2:B:247:TYR:CE2	2.52	0.44
1:A:561:TYR:CD1	1:A:641:LYS:HB3	2.52	0.44
2:B:531:LEU:CB	2:B:532:GLY:HA2	2.43	0.44
1:A:192:SER:O	1:A:193:SER:HB3	2.18	0.44
2:B:350:GLY:HA2	2:B:351:THR:CB	2.48	0.43
2:B:343:ARG:HE	2:B:347:ALA:HA	1.83	0.43
2:B:77:ARG:NH1	2:B:146:ASN:O	2.51	0.43
1:A:284:PRO:C	1:A:286:SER:H	2.24	0.43
1:A:442:SER:HB2	1:A:473:VAL:HB	2.00	0.43
2:B:262:VAL:HG23	2:B:386:MET:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HA	5:A:3000:NAG:H82	2.00	0.42
2:B:279:ALA:HA	2:B:294:PHE:O	2.19	0.42
2:B:148:PRO:C	2:B:150:VAL:N	2.73	0.42
2:B:97:PRO:HD2	2:B:113:SER:HB2	2.02	0.42
1:A:113:ARG:HB2	1:A:156:CYS:SG	2.59	0.41
1:A:133:PRO:HB3	1:A:156:CYS:HB3	2.01	0.41
1:A:209:PRO:HA	1:A:236:THR:O	2.21	0.41
1:A:250:ILE:HG12	1:A:278:ARG:HG2	2.02	0.41
2:B:525:TRP:CE2	2:B:527:PHE:HB2	2.56	0.41
2:B:185:THR:HG22	2:B:205:LYS:HB3	2.02	0.41
2:B:229:TYR:HA	2:B:249:SER:O	2.21	0.41
1:A:110:ASN:OD1	1:A:127:GLY:HA3	2.20	0.40
2:B:440:HIS:ND1	2:B:440:HIS:C	2.79	0.40
2:B:438:ASP:C	2:B:440:HIS:H	2.29	0.40
1:A:74:ASN:HB3	1:A:80:GLU:HB2	2.03	0.40
1:A:629:ARG:HD2	1:A:629:ARG:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	608/663 (92%)	565 (93%)	42 (7%)	1 (0%)	43	76
2	B	486/528 (92%)	449 (92%)	30 (6%)	7 (1%)	9	36
All	All	1094/1191 (92%)	1014 (93%)	72 (7%)	8 (1%)	18	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	351	THR
2	B	149	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	529	PRO
2	B	148	PRO
2	B	347	ALA
1	A	616	GLU
2	B	456	ASP
2	B	439	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	539/582 (93%)	505 (94%)	34 (6%)	16	48
2	B	399/425 (94%)	373 (94%)	26 (6%)	15	47
All	All	938/1007 (93%)	878 (94%)	60 (6%)	16	48

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	37	VAL
1	A	55	LEU
1	A	59	LYS
1	A	89	VAL
1	A	90	SER
1	A	94	LYS
1	A	107	GLU
1	A	118	LEU
1	A	165	THR
1	A	175	SER
1	A	191	ASN
1	A	195	SER
1	A	203	ILE
1	A	210	SER
1	A	245	VAL
1	A	248	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	VAL
1	A	301	SER
1	A	313	PHE
1	A	320	VAL
1	A	350	GLN
1	A	417	ASP
1	A	418	VAL
1	A	422	GLN
1	A	431	LEU
1	A	435	VAL
1	A	453	SER
1	A	478	LEU
1	A	487	VAL
1	A	539	SER
1	A	549	ASP
1	A	579	LYS
1	A	644	LEU
2	B	63	GLN
2	B	92	GLN
2	B	104	SER
2	B	114	VAL
2	B	118	VAL
2	B	132	LEU
2	B	135	GLU
2	B	151	SER
2	B	195	GLN
2	B	205	LYS
2	B	220	SER
2	B	256	GLN
2	B	331	ARG
2	B	344	GLU
2	B	346	ARG
2	B	348	GLU
2	B	360	VAL
2	B	362	SER
2	B	370	ASP
2	B	412	MET
2	B	433	LEU
2	B	440	HIS
2	B	449	GLN
2	B	472	SER
2	B	504	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	512	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	74	ASN
1	A	105	GLN
1	A	132	GLN
1	A	207	ASN
1	A	429	GLN
1	A	474	GLN
1	A	506	HIS
1	A	568	HIS
2	B	99	GLN
2	B	158	GLN
2	B	366	GLN
2	B	416	HIS
2	B	427	GLN
2	B	449	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 ⓘ

15 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	NAG	C	1	1,3	14,14,15	0.58	0	17,19,21	1.09	1 (5%)
3	NAG	C	2	3	14,14,15	0.78	0	17,19,21	1.17	2 (11%)
3	BMA	C	3	3	11,11,12	0.75	0	15,15,17	0.61	0
4	NAG	D	1	1,4	14,14,15	0.56	0	17,19,21	1.31	3 (17%)
4	NAG	D	2	4	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.45	0	17,19,21	1.25	3 (17%)
3	NAG	E	2	3	14,14,15	0.73	0	17,19,21	1.02	2 (11%)
3	BMA	E	3	3	11,11,12	0.58	0	15,15,17	0.72	0
4	NAG	F	1	1,4	14,14,15	0.47	0	17,19,21	1.10	1 (5%)
4	NAG	F	2	4	14,14,15	0.60	0	17,19,21	0.99	1 (5%)
4	NAG	G	1	1,4	14,14,15	1.02	1 (7%)	17,19,21	0.99	0
4	NAG	G	2	4	14,14,15	0.67	0	17,19,21	1.09	1 (5%)
3	NAG	H	1	3,2	14,14,15	0.47	0	17,19,21	1.20	3 (17%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	1.18	2 (11%)
3	BMA	H	3	3	11,11,12	0.60	0	15,15,17	0.80	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C1-C2	2.27	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	-2.91	106.75	111.02
3	H	2	NAG	C4-C3-C2	-2.79	106.93	111.02
3	E	1	NAG	C4-C3-C2	-2.75	106.99	111.02
4	D	1	NAG	C4-C3-C2	-2.66	107.11	111.02
4	D	1	NAG	C2-N2-C7	-2.54	119.49	122.90
4	D	1	NAG	C8-C7-N2	2.50	120.26	116.12
3	E	1	NAG	C8-C7-N2	2.43	120.15	116.12
3	H	2	NAG	C8-C7-N2	2.43	120.14	116.12
4	F	2	NAG	C4-C3-C2	-2.42	107.48	111.02
4	G	2	NAG	C4-C3-C2	-2.37	107.54	111.02
3	E	2	NAG	C4-C3-C2	-2.35	107.57	111.02
3	E	1	NAG	C2-N2-C7	-2.32	119.79	122.90
3	H	1	NAG	C8-C7-N2	2.28	119.91	116.12
3	H	1	NAG	C4-C3-C2	-2.26	107.71	111.02
4	D	2	NAG	C4-C3-C2	-2.25	107.72	111.02
3	H	1	NAG	C6-C5-C4	-2.22	107.56	113.02
3	C	2	NAG	C8-C7-N2	2.22	119.80	116.12
3	E	2	NAG	C8-C7-N2	2.22	119.80	116.12
4	F	1	NAG	C3-C4-C5	-2.21	106.23	110.23
3	C	2	NAG	C4-C3-C2	-2.10	107.94	111.02
4	D	2	NAG	C8-C7-N2	2.05	119.51	116.12

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

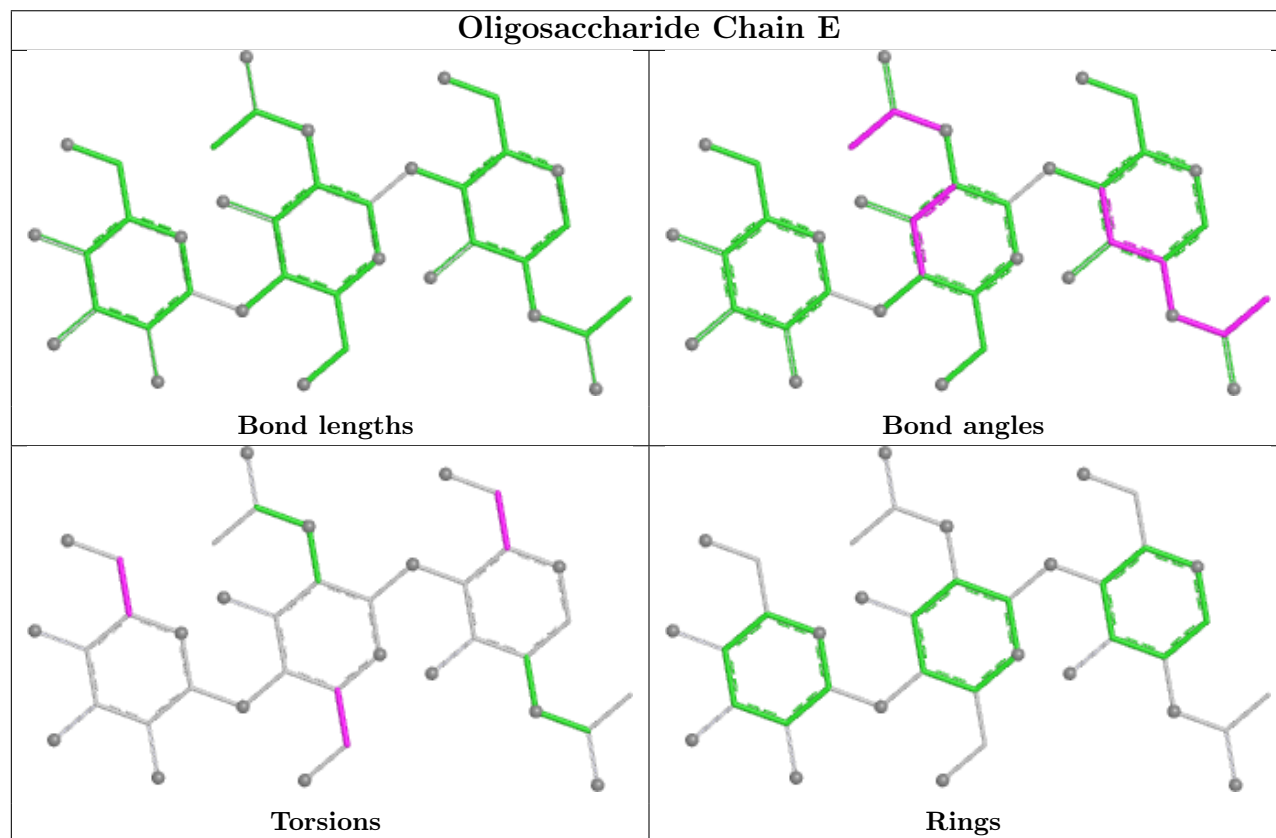
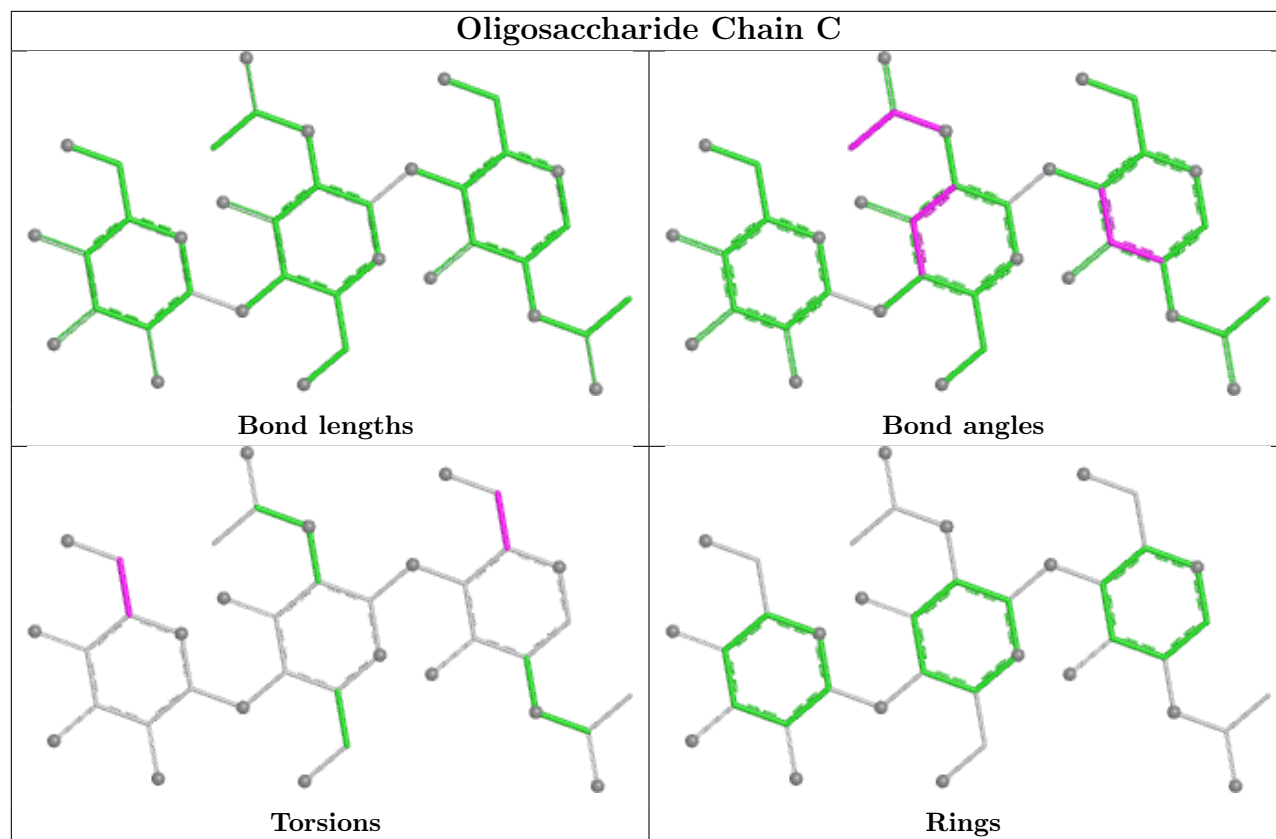
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C1-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7

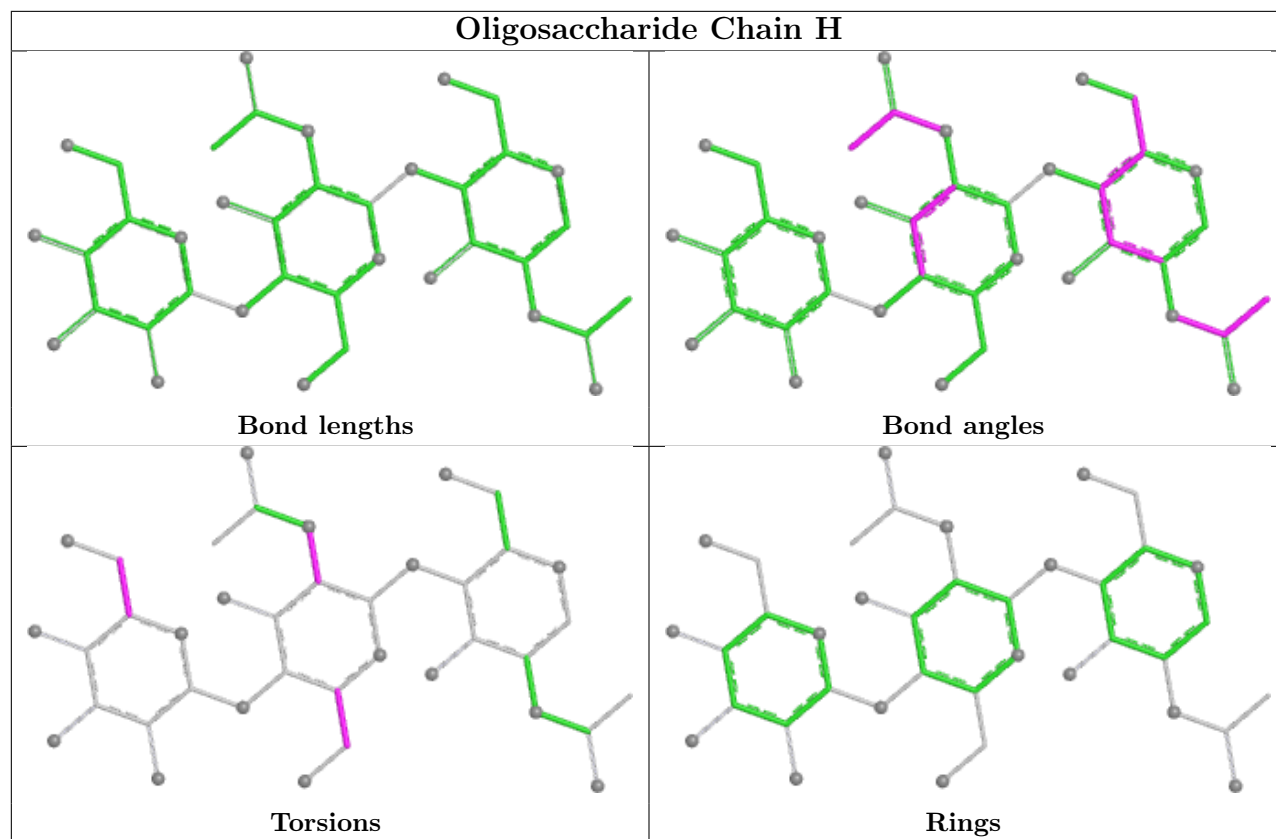
There are no ring outliers.

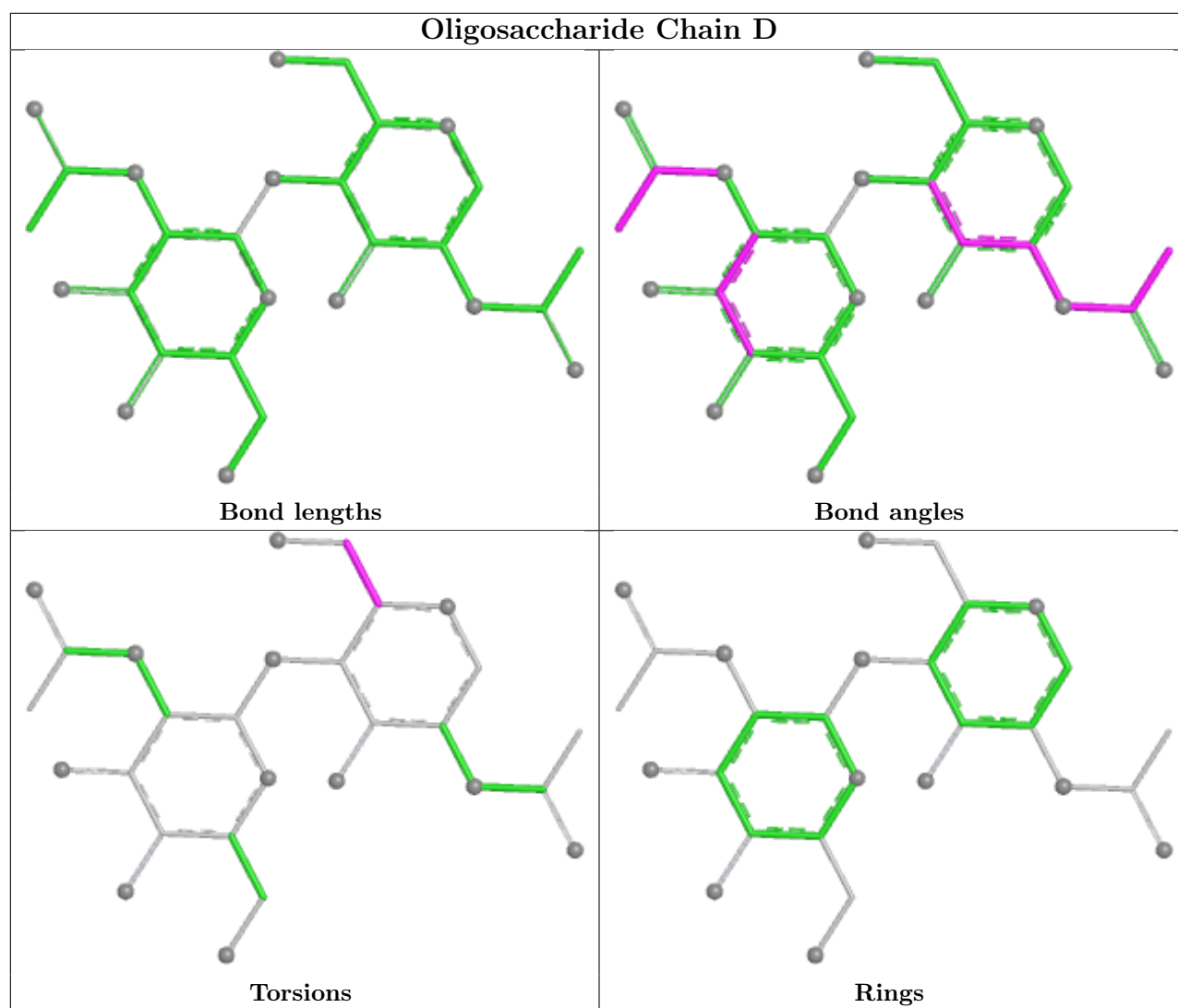
3 monomers are involved in 3 short contacts:

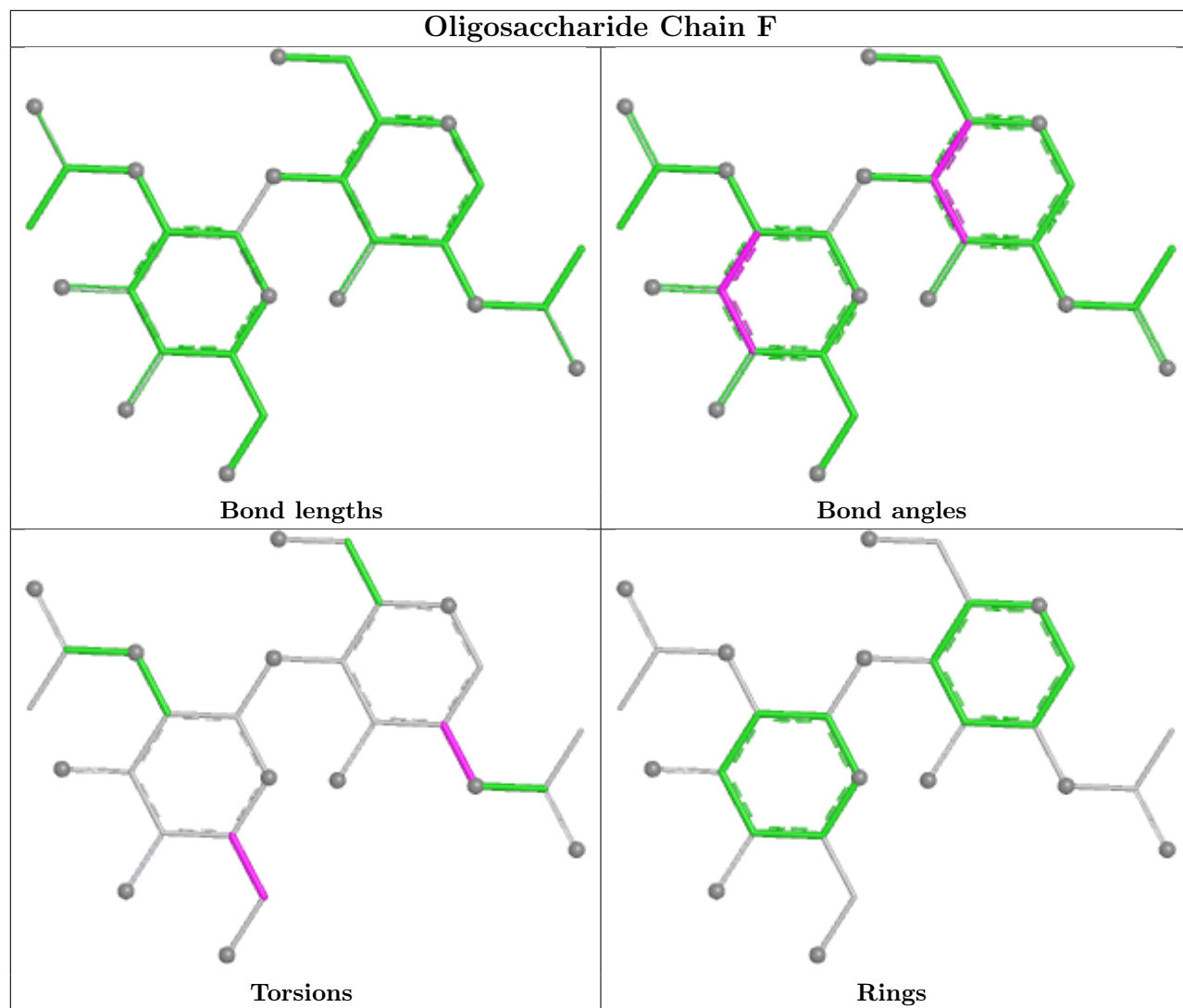
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
3	C	1	NAG	1	0
3	H	1	NAG	1	0

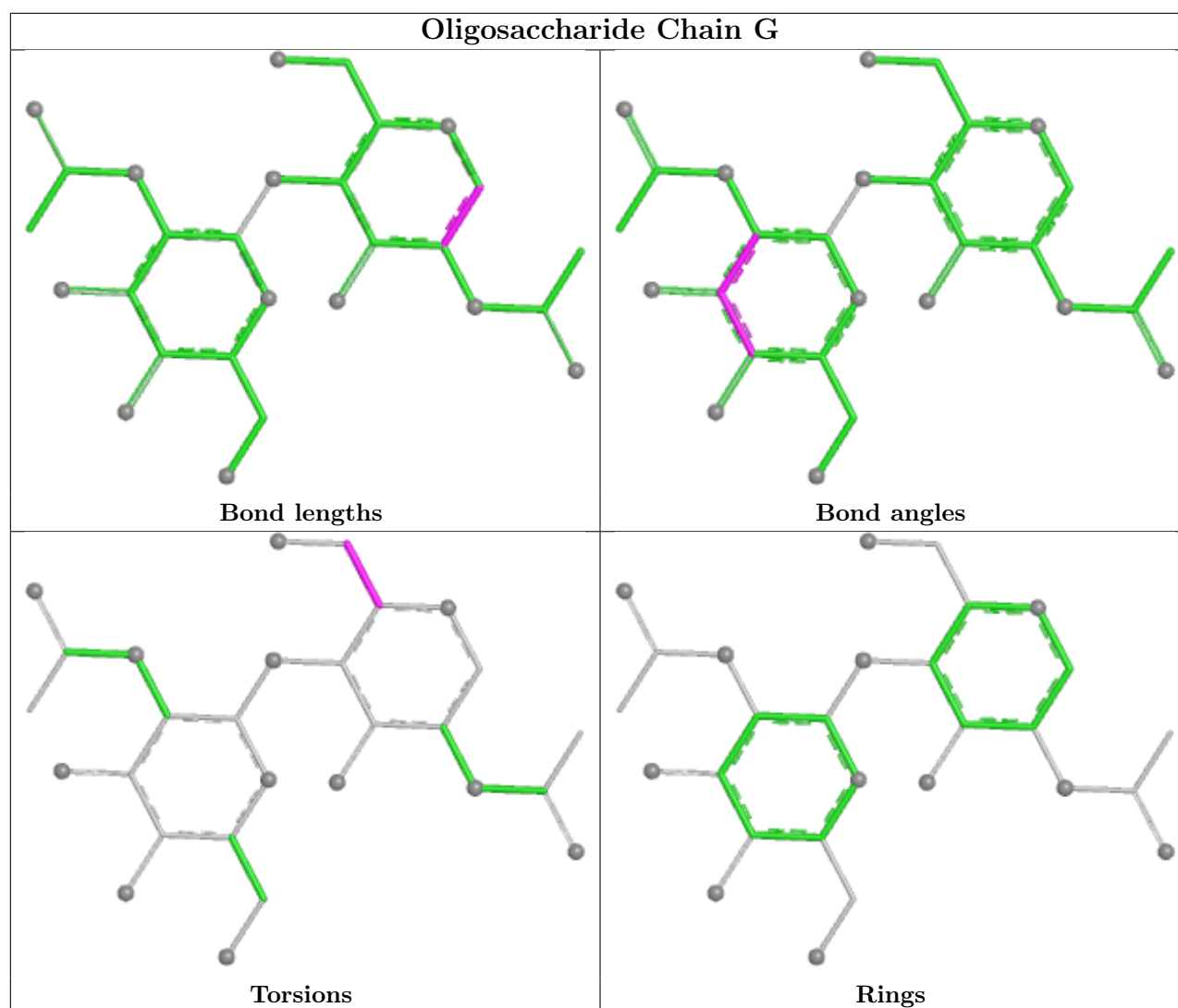
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	A	3000	1	14,14,15	0.56	0	17,19,21	1.20	3 (17%)

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	A	3000	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3000	NAG	C8-C7-N2	2.44	120.16	116.12
5	A	3000	NAG	C4-C3-C2	-2.25	107.72	111.02
5	A	3000	NAG	C2-N2-C7	-2.21	119.93	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3000	NAG	C4-C5-C6-O6
5	A	3000	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3000	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	614/663 (92%)	-0.04	6 (0%) 79 59	47, 78, 116, 144	0
2	B	496/528 (93%)	-0.22	10 (2%) 65 41	43, 61, 100, 129	0
All	All	1110/1191 (93%)	-0.12	16 (1%) 73 51	43, 70, 112, 144	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	648	VAL	5.4
2	B	23	LEU	4.7
2	B	531	LEU	4.1
2	B	532	GLY	3.7
2	B	178	GLY	3.4
2	B	284	SER	3.1
1	A	226	GLY	3.1
2	B	308	PRO	2.9
2	B	302	PRO	2.7
2	B	288	ALA	2.6
2	B	520	PRO	2.5
1	A	302	PRO	2.4
2	B	515	SER	2.2
1	A	422	GLN	2.1
1	A	630	VAL	2.1
1	A	617	GLY	2.1

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 ⓘ

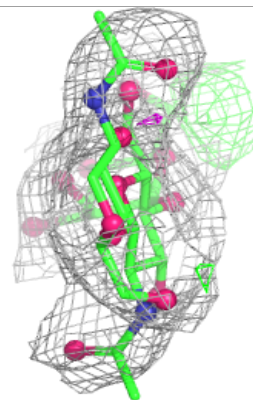
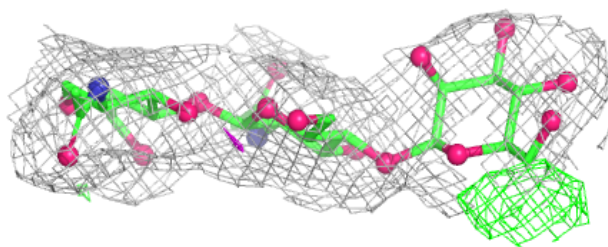
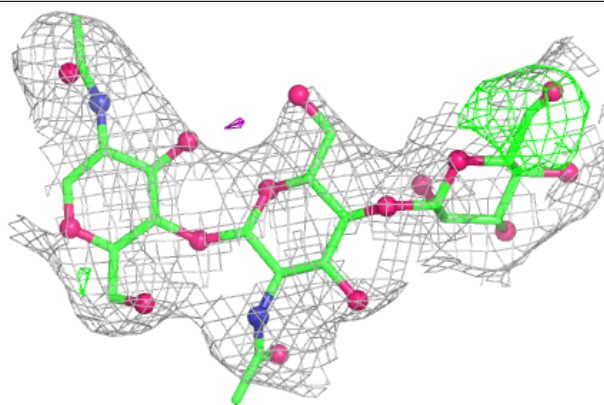
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BMA	C	3	11/12	0.09	0.15	123,128,131,132	0
3	BMA	H	3	11/12	0.38	0.13	125,128,131,131	0
3	BMA	E	3	11/12	0.41	0.12	151,153,158,159	0
4	NAG	G	2	14/15	0.62	0.14	126,133,139,141	0
4	NAG	D	2	14/15	0.70	0.13	124,130,140,141	0
4	NAG	F	2	14/15	0.72	0.15	112,119,121,123	0
3	NAG	C	2	14/15	0.75	0.11	107,116,121,125	0
3	NAG	E	2	14/15	0.76	0.12	138,143,149,150	0
4	NAG	G	1	14/15	0.80	0.17	111,124,129,132	0
3	NAG	H	2	14/15	0.82	0.11	94,110,118,124	0
3	NAG	E	1	14/15	0.84	0.12	112,118,126,134	0
4	NAG	F	1	14/15	0.85	0.11	88,93,101,109	0
4	NAG	D	1	14/15	0.89	0.12	114,118,122,125	0
3	NAG	C	1	14/15	0.94	0.07	65,82,91,103	0
3	NAG	H	1	14/15	0.95	0.06	61,78,89,99	0

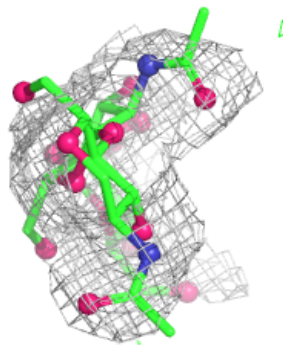
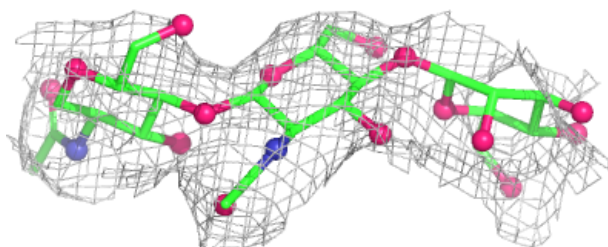
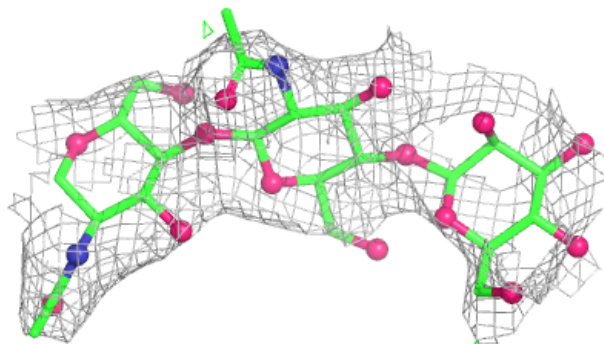
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

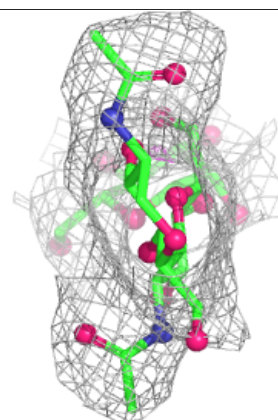
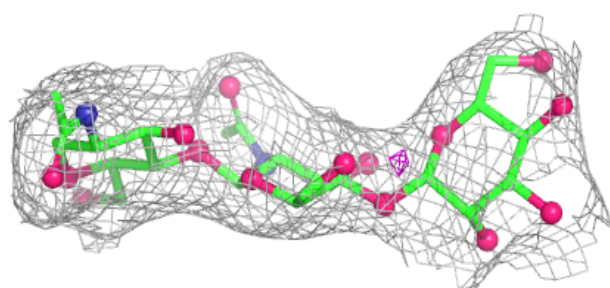
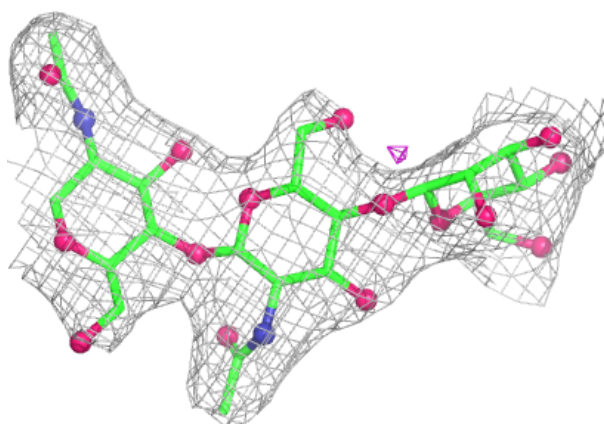
**Electron density around Chain E:**

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



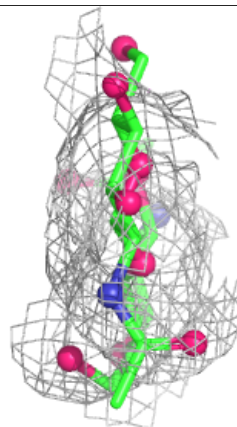
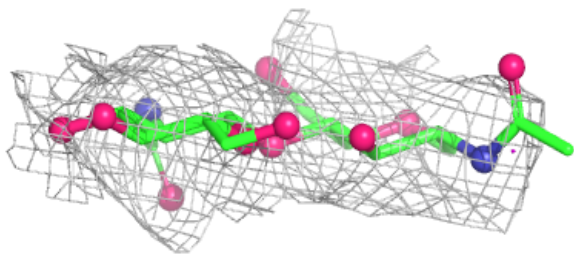
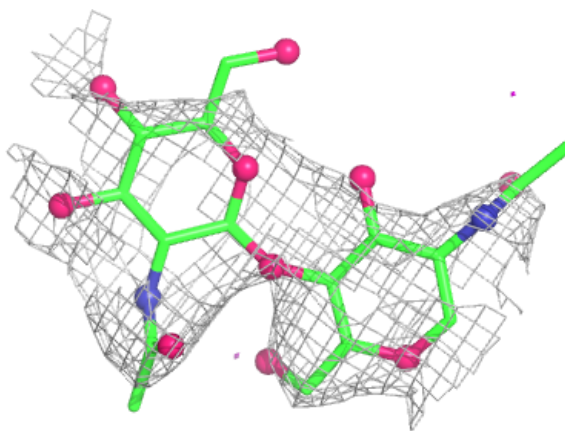
Electron density around Chain H:

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



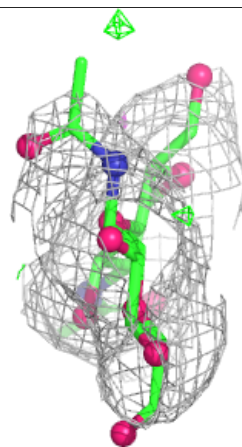
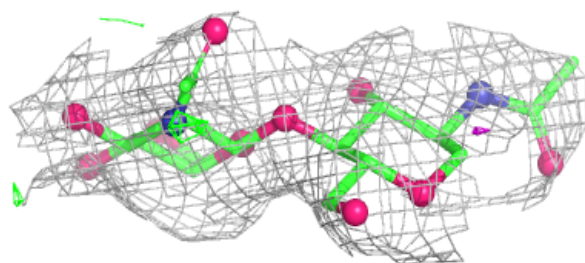
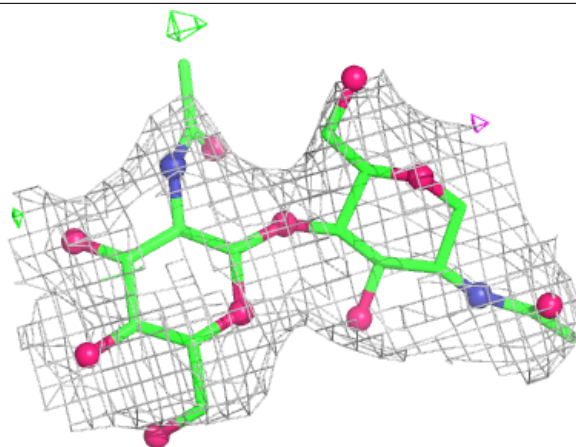
Electron density around Chain D:

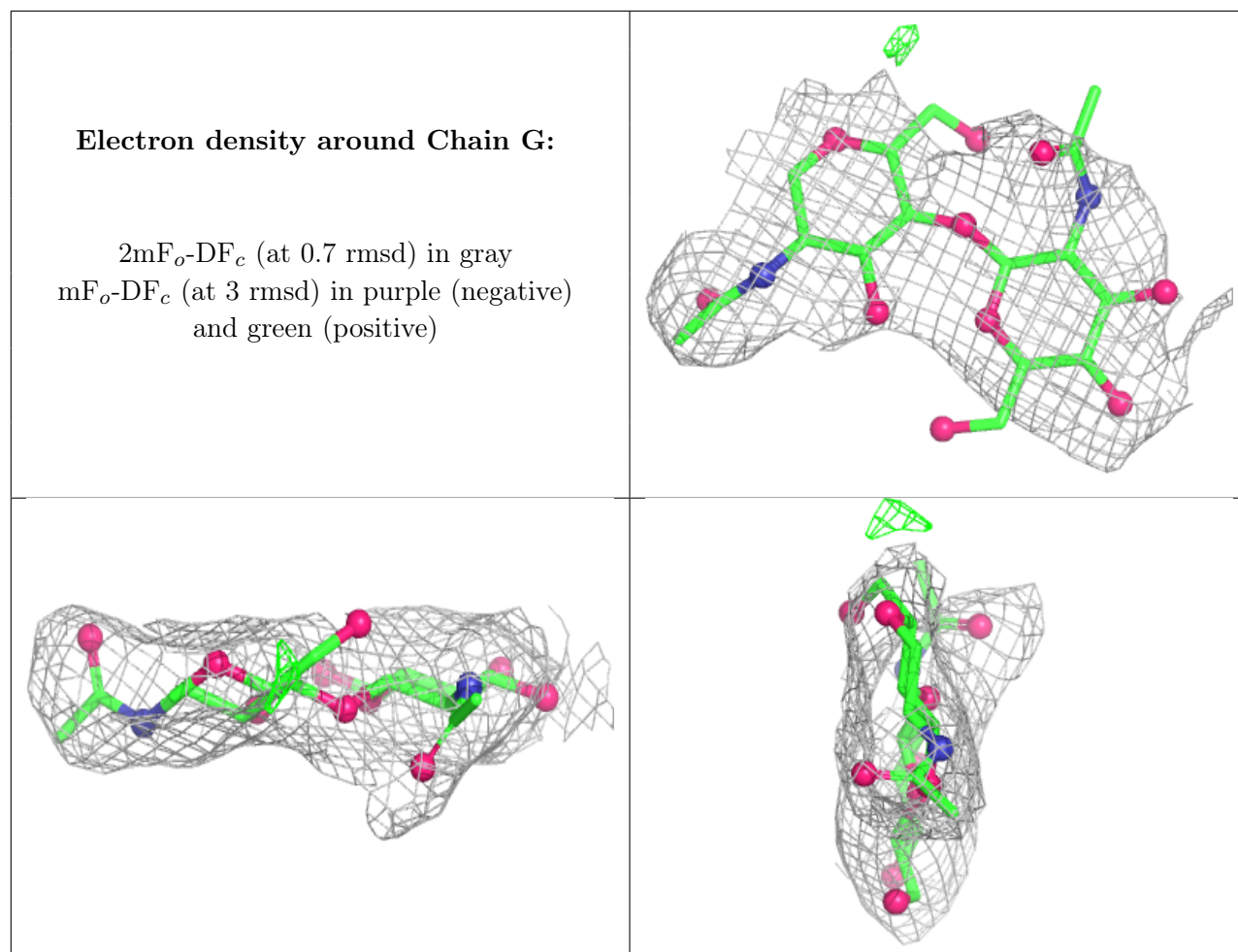
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o - DF_c$ (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
5	NAG	A	3000	14/15	0.65	0.15	131,133,141,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.