



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 AM UTC

PDB ID : 6SKA / pdb_00006ska
Title : Teneurin 2 in complex with Latrophilin 1 Lec-Olf domains
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Deposited on : 2019-08-15
Resolution : 3.86 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

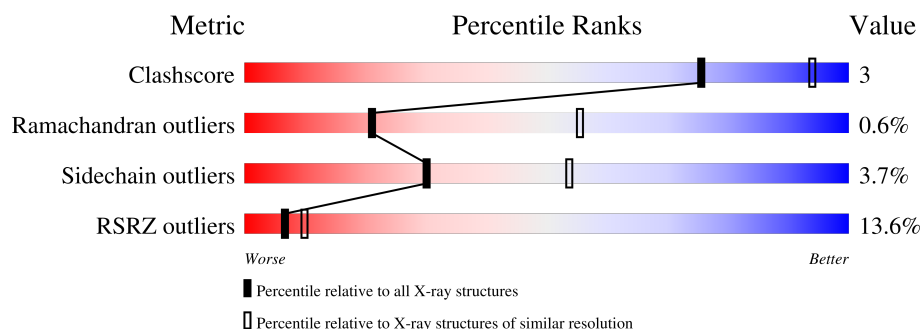
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 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))
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1836	
2	D	347	
3	B	8	
4	C	2	
4	E	2	
4	F	2	
4	G	2	

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Mol	Chain	Length	Quality of chain
4	H	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17628 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 Teneurin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1836	Total	C	N	O	S	0	1	0
			14513	9168	2508	2774	63			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9DER5
A	?	-	THR	deletion	UNP Q9DER5
A	?	-	GLU	deletion	UNP Q9DER5
A	?	-	GLU	deletion	UNP Q9DER5
A	?	-	ASN	deletion	UNP Q9DER5
A	?	-	SER	deletion	UNP Q9DER5
A	?	-	ILE	deletion	UNP Q9DER5

- Molecule 2 is a protein called Adhesion G protein-coupled receptor L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	347	Total	C	N	O	S	0	0	0
			2810	1775	479	539	17			

There are 11 discrepancies between the modelled and reference sequences:

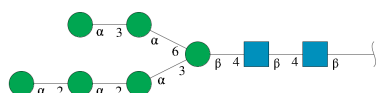
Chain	Residue	Modelled	Actual	Comment	Reference
D	132	VAL	ILE	conflict	UNP Q80TR1
D	?	-	VAL	deletion	UNP Q80TR1
D	?	-	TYR	deletion	UNP Q80TR1
D	?	-	VAL	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	ASP	deletion	UNP Q80TR1
D	?	-	SER	deletion	UNP Q80TR1
D	?	-	GLU	deletion	UNP Q80TR1

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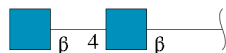
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP Q80TR1
D	?	-	ALA	deletion	UNP Q80TR1

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-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
3	B	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	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			
4	H	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
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

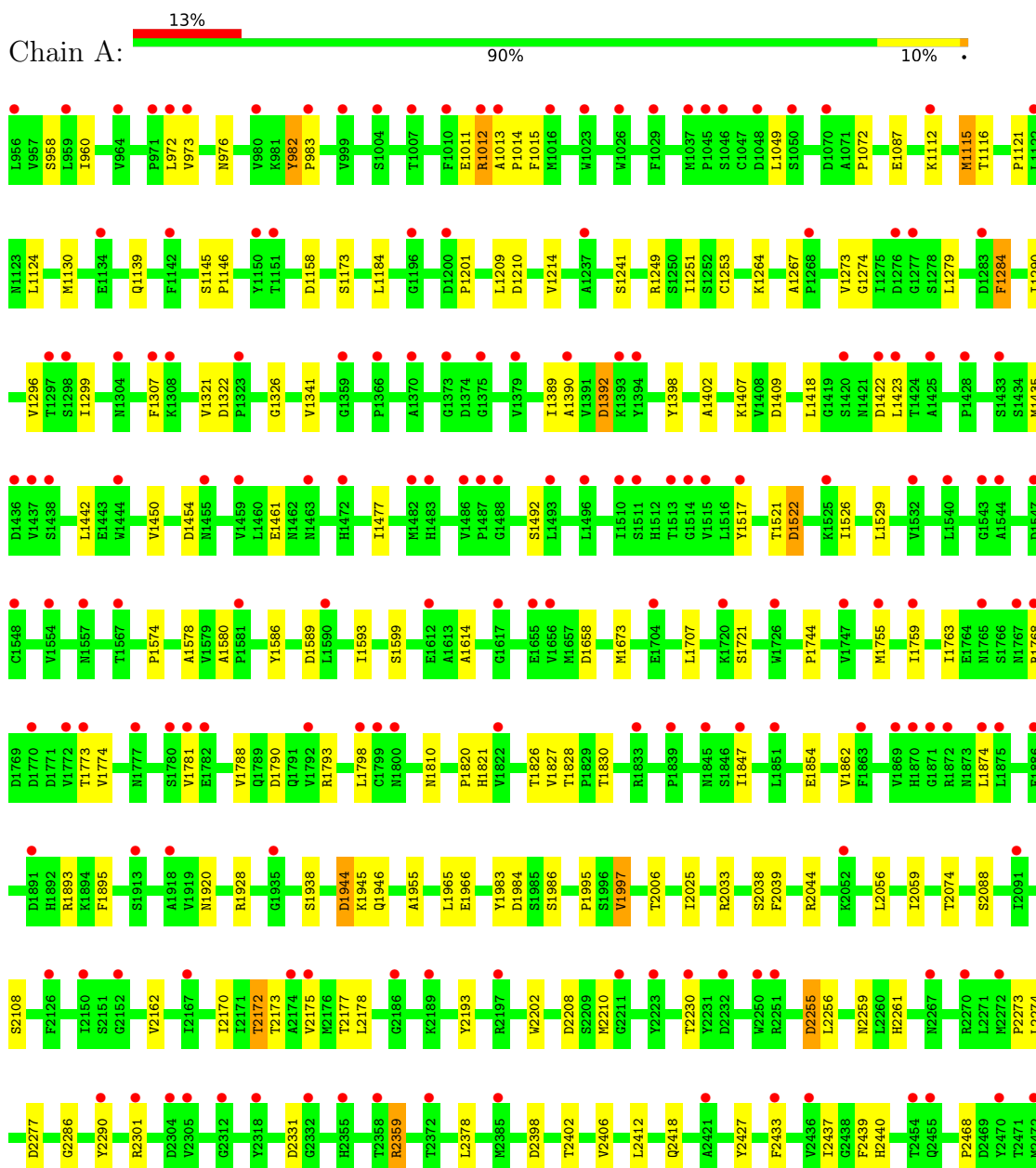
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

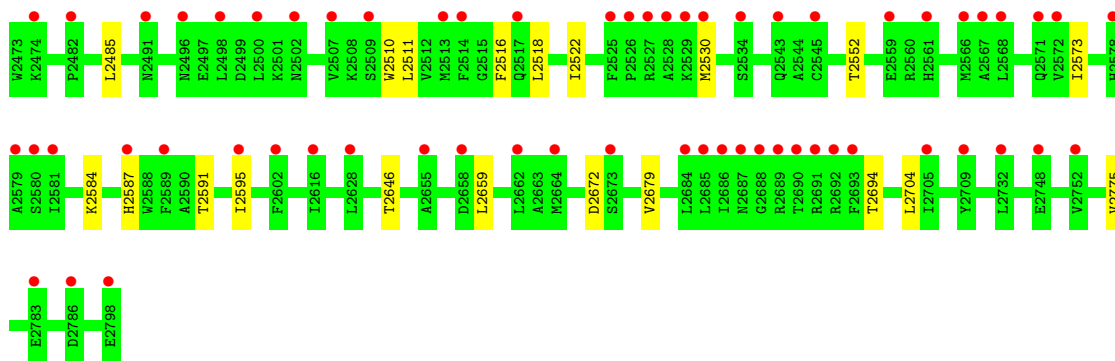
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

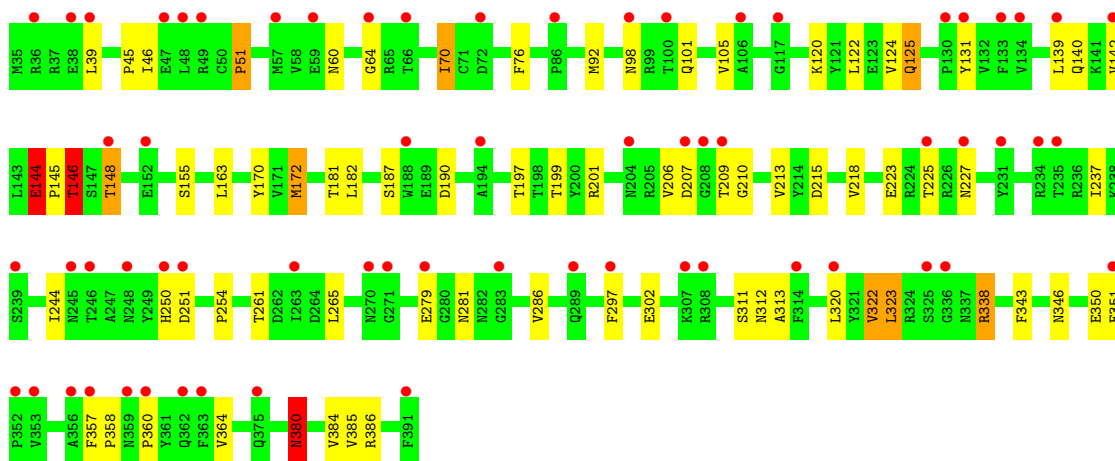
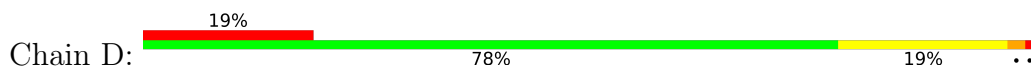
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Teneurin-2

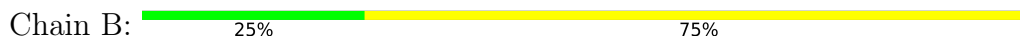




• Molecule 2: Adhesion G protein-coupled receptor L1



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



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.26Å 96.26Å 809.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.09 – 3.86 52.09 – 3.86	Depositor EDS
% Data completeness (in resolution range)	91.0 (52.09-3.86) 91.0 (52.09-3.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.89Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	(Not available) , (Not available) 0.285 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	104.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	17628	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, MAN, CA

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	0.69	0/14825	1.14	30/20101 (0.1%)
2	D	0.72	1/2886 (0.0%)	1.11	1/3935 (0.0%)
All	All	0.70	1/17711 (0.0%)	1.13	31/24036 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	140	GLN	CA-C	5.45	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2331	ASP	CA-CB-CG	6.19	118.79	112.60
2	D	380	ASN	CA-CB-CG	6.18	118.78	112.60
1	A	1984	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	1658	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	2208	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	2398	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	1589	ASP	CA-C-N	5.80	128.37	120.54
1	A	1589	ASP	C-N-CA	5.80	128.37	120.54
1	A	1522	ASP	N-CA-C	-5.79	106.38	113.50
1	A	2277	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	1209	LEU	CA-C-N	5.65	129.30	120.82
1	A	1209	LEU	C-N-CA	5.65	129.30	120.82
1	A	1920	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	1158	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	2672	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	1210	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	1392	ASP	CA-C-N	5.44	127.57	120.28
1	A	1392	ASP	C-N-CA	5.44	127.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1945	LYS	N-CA-C	-5.38	105.97	112.54
1	A	2255	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	2595	ILE	N-CA-C	-5.32	105.53	110.53
1	A	1422	ASP	CA-C-N	5.28	128.09	120.38
1	A	1422	ASP	C-N-CA	5.28	128.09	120.38
1	A	1322	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	2775	VAL	N-CA-C	-5.20	106.01	110.74
1	A	1409	ASP	CA-C-N	5.09	127.11	120.28
1	A	1409	ASP	C-N-CA	5.09	127.11	120.28
1	A	1983	TYR	CA-C-N	5.07	131.60	122.02
1	A	1983	TYR	C-N-CA	5.07	131.60	122.02
1	A	2172	THR	CA-C-N	5.02	130.44	121.75
1	A	2172	THR	C-N-CA	5.02	130.44	121.75

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	14513	0	14252	75	0
2	D	2810	0	2639	30	0
3	B	94	0	79	0	0
4	C	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	70	0	65	0	0
6	D	1	0	0	0	0
All	All	17628	0	17160	103	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 (103) 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:D:364:VAL:HA	2:D:380:ASN:HB2	1.58	0.85
1:A:1821:HIS:HD2	1:A:1830:THR:HG21	1.44	0.81
1:A:982:TYR:HB3	1:A:983:PRO:HD3	1.63	0.78
1:A:982:TYR:HB3	1:A:983:PRO:CD	2.17	0.74
1:A:2468:PRO:HB3	1:A:2485:LEU:HB3	1.76	0.67
1:A:1821:HIS:CD2	1:A:1830:THR:HG21	2.28	0.66
1:A:2172:THR:HG21	2:D:51:PRO:HA	1.79	0.65
1:A:1201:PRO:HB3	1:A:1214:VAL:HB	1.81	0.63
1:A:1130:MET:HB2	1:A:1173:SER:HB2	1.81	0.62
1:A:1521:THR:HB	1:A:1574:PRO:HD2	1.83	0.59
2:D:148:THR:HB	2:D:384:VAL:HG23	1.84	0.59
2:D:251:ASP:HA	2:D:254:PRO:HG3	1.85	0.58
1:A:1955:ALA:HB3	1:A:2210:MET:HE3	1.85	0.58
1:A:972:LEU:HD22	1:A:1012:ARG:HE	1.69	0.57
1:A:1895:PHE:HE1	1:A:2511:LEU:HA	1.68	0.57
1:A:1744:PRO:HB2	1:A:2006:THR:HG21	1.86	0.57
2:D:338:ARG:HA	2:D:357:PHE:HB3	1.86	0.56
2:D:172:MET:HE1	2:D:206:VAL:HG11	1.88	0.56
1:A:1130:MET:HG2	1:A:1139:GLN:HG2	1.88	0.55
1:A:1773:THR:HG23	1:A:1788:VAL:HB	1.88	0.55
1:A:2406:VAL:HG11	1:A:2433:PHE:HE2	1.71	0.55
1:A:2359:ARG:HH12	1:A:2530:MET:HE3	1.72	0.55
1:A:2418:GLN:HB2	1:A:2427:TYR:HB3	1.89	0.55
1:A:2173:THR:HG22	1:A:2175:VAL:H	1.72	0.54
2:D:170:TYR:HB3	2:D:182:LEU:HD11	1.90	0.54
2:D:311:SER:HB2	2:D:323:LEU:HB3	1.89	0.54
2:D:163:LEU:HD13	2:D:215:ASP:H	1.73	0.54
1:A:2511:LEU:HD13	1:A:2518:LEU:HD11	1.91	0.53
1:A:1274:GLY:HA2	1:A:1321:VAL:HG11	1.91	0.53
1:A:1390:ALA:HB1	1:A:1450:VAL:HG23	1.89	0.52
1:A:1279:LEU:HD23	1:A:1290:ILE:HD12	1.92	0.52
1:A:1995:PRO:HB2	1:A:2256:LEU:HB3	1.92	0.52
2:D:144:GLU:H	2:D:145:PRO:HD3	1.75	0.51
2:D:187:SER:H	2:D:190:ASP:HB2	1.76	0.51
1:A:2056:LEU:HD21	1:A:2059:ILE:HD11	1.93	0.51
1:A:1273:VAL:HG23	1:A:1578:ALA:HB1	1.92	0.50
1:A:2290:TYR:CZ	1:A:2301:ARG:HG3	2.47	0.50
1:A:1290:ILE:HG12	1:A:1296:VAL:HG22	1.94	0.50
2:D:45:PRO:HB3	2:D:105:VAL:HG22	1.94	0.49
1:A:1827:VAL:HG13	1:A:1828:THR:HG23	1.93	0.49
1:A:1013:ALA:HB3	1:A:1014:PRO:HD3	1.95	0.49
1:A:1299:ILE:HD12	1:A:1341:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ASN:HB3	2:D:125:GLN:HB2	1.95	0.49
2:D:207:ASP:HB2	2:D:223:GLU:HA	1.95	0.49
2:D:343:PHE:HD1	2:D:350:GLU:HB3	1.76	0.49
1:A:1820:PRO:HB3	1:A:1826:THR:HA	1.95	0.48
1:A:2261:HIS:HA	1:A:2274:LEU:HB2	1.95	0.48
2:D:142:VAL:HB	2:D:358:PRO:HD3	1.95	0.48
1:A:2039:PHE:HB2	1:A:2044:ARG:HB2	1.93	0.48
1:A:1854:GLU:HB2	1:A:1862:VAL:HB	1.94	0.48
1:A:2584:LYS:HB3	1:A:2587:HIS:HB2	1.95	0.48
1:A:1895:PHE:HZ	1:A:2510:TRP:HB3	1.78	0.47
2:D:313:ALA:HB2	2:D:322:VAL:HG13	1.97	0.47
1:A:2402:THR:HG23	1:A:2439:PHE:HA	1.96	0.47
2:D:244:ILE:HD12	2:D:297:PHE:HZ	1.80	0.47
1:A:1522:ASP:HB2	1:A:1526:ILE:HB	1.96	0.46
2:D:92:MET:HE2	2:D:124:VAL:HG21	1.97	0.46
1:A:1755:MET:HG3	1:A:1759:ILE:HG12	1.97	0.46
1:A:1580:ALA:HB2	1:A:1586:TYR:CE2	2.51	0.46
1:A:1517:TYR:HB3	1:A:1529:LEU:HD11	1.98	0.46
2:D:213:VAL:HG22	2:D:218:VAL:HG22	1.97	0.46
1:A:982:TYR:CB	1:A:983:PRO:CD	2.91	0.46
1:A:1145:SER:C	1:A:1146:PRO:N	2.74	0.46
1:A:1893:ARG:HB2	2:D:70:ILE:HD12	1.97	0.46
1:A:2178:LEU:HD13	1:A:2193:TYR:CD2	2.51	0.46
2:D:281:ASN:HD22	2:D:286:VAL:HG22	1.81	0.46
2:D:181:THR:HG22	2:D:201:ARG:HA	1.99	0.45
1:A:1788:VAL:HG22	1:A:1793:ARG:HG2	1.97	0.45
1:A:1121:PRO:HG2	1:A:1124:LEU:HB2	1.98	0.45
2:D:146:THR:HB	2:D:386:ARG:HB2	1.98	0.45
1:A:1249:ARG:HB3	1:A:1264:LYS:HB3	2.00	0.44
1:A:2646:THR:HG22	1:A:2704:LEU:HD22	1.98	0.44
1:A:1012:ARG:HD2	1:A:1015:PHE:HD2	1.82	0.44
2:D:209:THR:H	2:D:261:THR:HG22	1.83	0.44
1:A:1267:ALA:HB3	1:A:1284:PHE:HB2	2.00	0.44
1:A:1442:LEU:HG	1:A:1461:GLU:HG3	2.00	0.43
1:A:2659:LEU:HD21	1:A:2679:VAL:HG11	1.99	0.43
1:A:1072:PRO:HB2	1:A:1087:GLU:HG2	2.00	0.43
1:A:1251:ILE:HB	1:A:1307:PHE:HD2	1.83	0.43
1:A:2088:SER:HB3	1:A:2108:SER:HB3	2.00	0.42
2:D:244:ILE:HD12	2:D:297:PHE:CZ	2.54	0.42
1:A:1115:MET:H	1:A:1115:MET:HG2	1.73	0.42
1:A:1707:LEU:HB3	1:A:1721:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:ILE:HB	1:A:2038:SER:HB2	2.01	0.42
1:A:976:ASN:HB3	1:A:1011:GLU:HB2	2.01	0.42
1:A:2518:LEU:HB3	1:A:2522:ILE:HD12	2.01	0.42
1:A:2406:VAL:HG11	1:A:2433:PHE:CE2	2.54	0.42
2:D:46:ILE:HG21	2:D:122:LEU:HD23	2.02	0.42
2:D:64:GLY:HA2	2:D:120:LYS:HG2	2.01	0.42
1:A:1614:ALA:HB3	1:A:1828:THR:HG21	2.02	0.42
1:A:2511:LEU:O	1:A:2516:PHE:HB2	2.20	0.42
1:A:1944:ASP:HB3	1:A:1946:GLN:H	1.85	0.41
1:A:1398:TYR:CE1	1:A:1407:LYS:HG2	2.56	0.41
1:A:1938:SER:H	1:A:2210:MET:HE1	1.86	0.41
1:A:1049:LEU:HD12	1:A:1184:LEU:HD23	2.03	0.41
2:D:313:ALA:HB1	2:D:320:LEU:HD11	2.03	0.41
1:A:2255:ASP:HB3	1:A:2259:ASN:H	1.86	0.41
2:D:144:GLU:N	2:D:145:PRO:CD	2.84	0.41
1:A:2162:VAL:HG11	1:A:2378:LEU:HD11	2.03	0.40
1:A:1768:ARG:HH22	1:A:2033:ARG:HD2	1.85	0.40
1:A:1810:ASN:HA	1:A:2074:THR:HB	2.03	0.40
1:A:2172:THR:HG22	1:A:2177:THR:HG22	2.02	0.40
1:A:2273:PRO:HD2	1:A:2286:GLY:HA2	2.03	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	1829/1836 (100%)	1758 (96%)	63 (3%)	8 (0%)	30	64
2	D	343/347 (99%)	310 (90%)	27 (8%)	6 (2%)	7	35
All	All	2172/2183 (100%)	2068 (95%)	90 (4%)	14 (1%)	21	55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	TYR
2	D	360	PRO
1	A	1284	PHE
2	D	210	GLY
1	A	1966	GLU
1	A	1402	ALA
2	D	250	HIS
1	A	1492	SER
1	A	1790	ASP
1	A	1997	VAL
2	D	146	THR
2	D	144	GLU
1	A	1326	GLY
2	D	51	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	1601/1600 (100%)	1560 (97%)	41 (3%)	40	61
2	D	306/306 (100%)	277 (90%)	29 (10%)	8	29
All	All	1907/1906 (100%)	1837 (96%)	70 (4%)	30	54

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	958	SER
1	A	960	ILE
1	A	973	VAL
1	A	1012	ARG
1	A	1112	LYS
1	A	1115	MET
1	A	1116	THR
1	A	1241	SER
1	A	1253	CYS
1	A	1389	ILE

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Mol	Chain	Res	Type
1	A	1392	ASP
1	A	1418	LEU
1	A	1423	LEU
1	A	1435	MET
1	A	1454	ASP
1	A	1477	ILE
1	A	1593	ILE
1	A	1599	SER
1	A	1673	MET
1	A	1763	ILE
1	A	1774	VAL
1	A	1781	VAL
1	A	1798	LEU
1	A	1847	ILE
1	A	1874	LEU
1	A	1928	ARG
1	A	1944	ASP
1	A	1965	LEU
1	A	1986	SER
1	A	1997	VAL
1	A	2170	ILE
1	A	2202	TRP
1	A	2230	THR
1	A	2359	ARG
1	A	2412	LEU
1	A	2437	ILE
1	A	2440	HIS
1	A	2552	THR
1	A	2573	ILE
1	A	2591	THR
1	A	2694	THR
2	D	39	LEU
2	D	70	ILE
2	D	76	PHE
2	D	98	ASN
2	D	101	GLN
2	D	125	GLN
2	D	131	TYR
2	D	139	LEU
2	D	144	GLU
2	D	146	THR
2	D	148	THR

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Mol	Chain	Res	Type
2	D	155	SER
2	D	172	MET
2	D	197	THR
2	D	199	THR
2	D	225	THR
2	D	227	ASN
2	D	237	ILE
2	D	265	LEU
2	D	279	GLU
2	D	302	GLU
2	D	312	ASN
2	D	322	VAL
2	D	323	LEU
2	D	338	ARG
2	D	346	ASN
2	D	351	GLU
2	D	380	ASN
2	D	385	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1027	ASN
1	A	1203	ASN
1	A	1285	ASN
1	A	1353	ASN
1	A	1473	GLN
1	A	1631	GLN
1	A	1683	GLN
1	A	1701	GLN
1	A	1789	GLN
1	A	1892	HIS
1	A	2124	ASN
1	A	2185	HIS
1	A	2418	GLN
1	A	2502	ASN
1	A	2549	GLN
1	A	2562	ASN
1	A	2741	GLN
2	D	60	ASN
2	D	153	HIS
2	D	154	GLN

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Mol	Chain	Res	Type
2	D	245	ASN
2	D	270	ASN
2	D	281	ASN
2	D	282	ASN
2	D	346	ASN
2	D	348	ASN
2	D	375	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 ⓘ

18 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	B	1	1,3	14,14,15	0.43	0	17,19,21	0.69	1 (5%)
3	NAG	B	2	3	14,14,15	0.42	0	17,19,21	0.54	0
3	BMA	B	3	3	11,11,12	0.50	0	15,15,17	0.51	0
3	MAN	B	4	3	11,11,12	0.52	0	15,15,17	0.95	2 (13%)
3	MAN	B	5	3	11,11,12	0.58	0	15,15,17	0.87	1 (6%)
3	MAN	B	6	3	11,11,12	0.56	0	15,15,17	0.87	1 (6%)
3	MAN	B	7	3	11,11,12	0.56	0	15,15,17	0.88	1 (6%)
3	MAN	B	8	3	11,11,12	0.56	0	15,15,17	0.94	1 (6%)
4	NAG	C	1	1,4	14,14,15	0.44	0	17,19,21	0.70	0
4	NAG	C	2	4	14,14,15	0.45	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1	1,4	14,14,15	0.43	0	17,19,21	0.66	0
4	NAG	E	2	4	14,14,15	0.44	0	17,19,21	0.59	0
4	NAG	F	1	1,4	14,14,15	0.43	0	17,19,21	0.68	1 (5%)
4	NAG	F	2	4	14,14,15	0.45	0	17,19,21	0.60	0
4	NAG	G	1	1,4	14,14,15	0.44	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.44	0	17,19,21	0.55	0
4	NAG	H	1	1,4	14,14,15	0.44	0	17,19,21	0.71	1 (5%)
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.53	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	B	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	2/2/19/22	0/1/1/1
3	MAN	B	5	3	-	1/2/19/22	0/1/1/1
3	MAN	B	6	3	-	0/2/19/22	0/1/1/1
3	MAN	B	7	3	-	0/2/19/22	0/1/1/1
3	MAN	B	8	3	-	0/2/19/22	0/1/1/1
4	NAG	C	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	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	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	5	MAN	C1-O5-C5	2.73	115.85	112.19
3	B	8	MAN	C1-O5-C5	2.61	115.68	112.19
3	B	7	MAN	C1-O5-C5	2.39	115.39	112.19
3	B	4	MAN	C1-C2-C3	2.28	112.96	109.64
3	B	6	MAN	C1-O5-C5	2.24	115.19	112.19
3	B	4	MAN	C1-O5-C5	2.18	115.11	112.19
3	B	1	NAG	C1-O5-C5	2.13	115.04	112.19
4	F	1	NAG	C1-O5-C5	2.12	115.02	112.19
4	H	1	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
3	B	4	MAN	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	B	4	MAN	O5-C5-C6-O6

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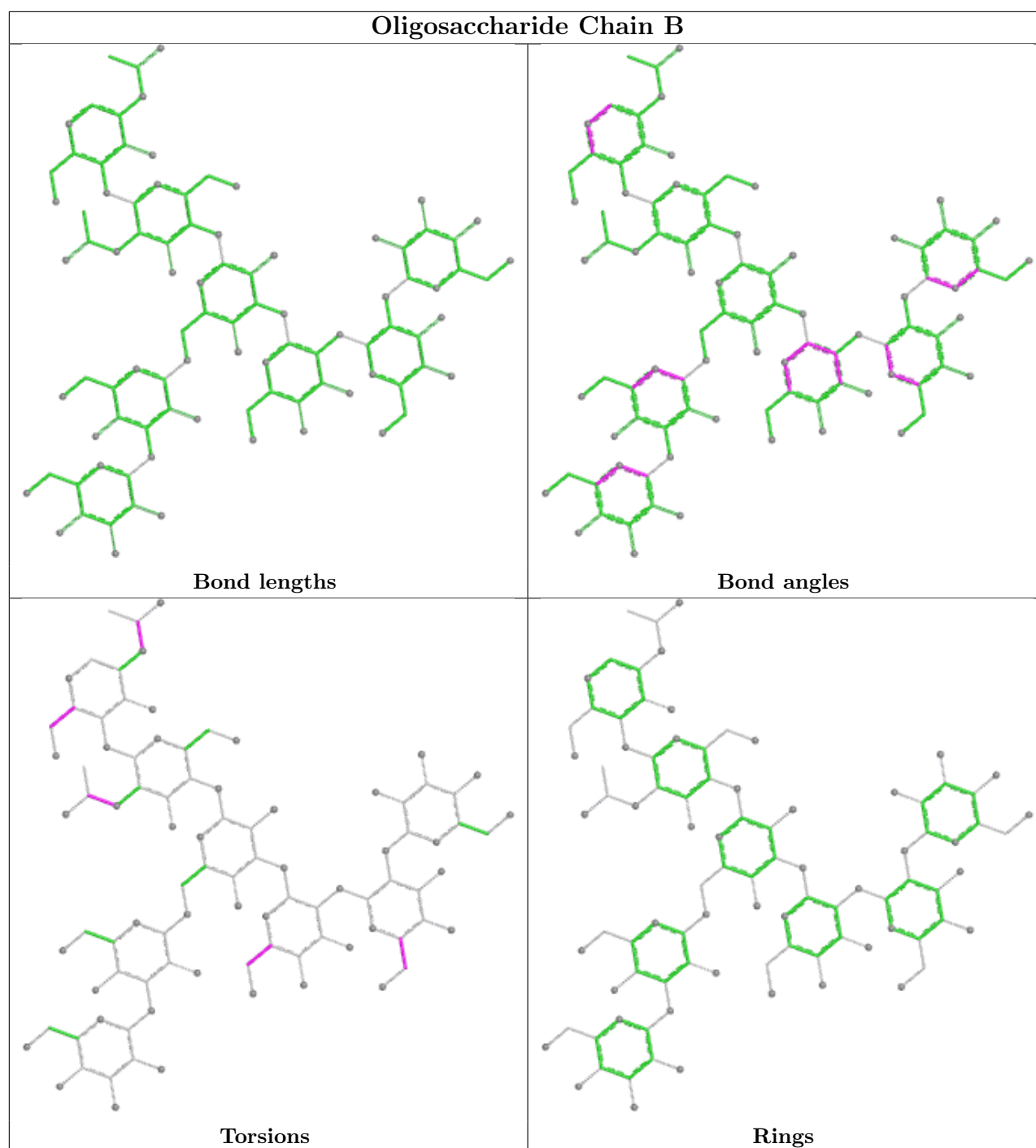
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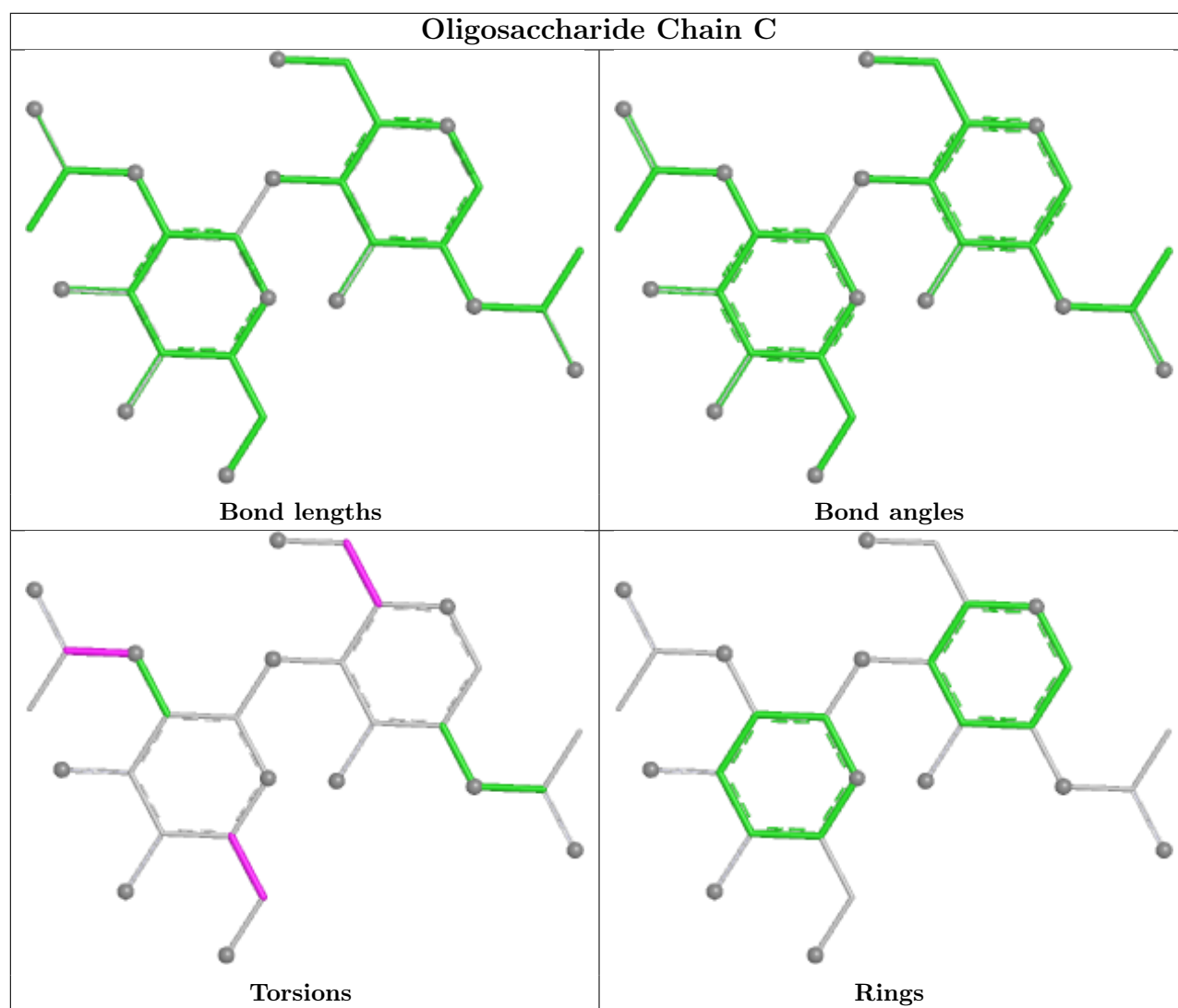
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
3	B	5	MAN	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

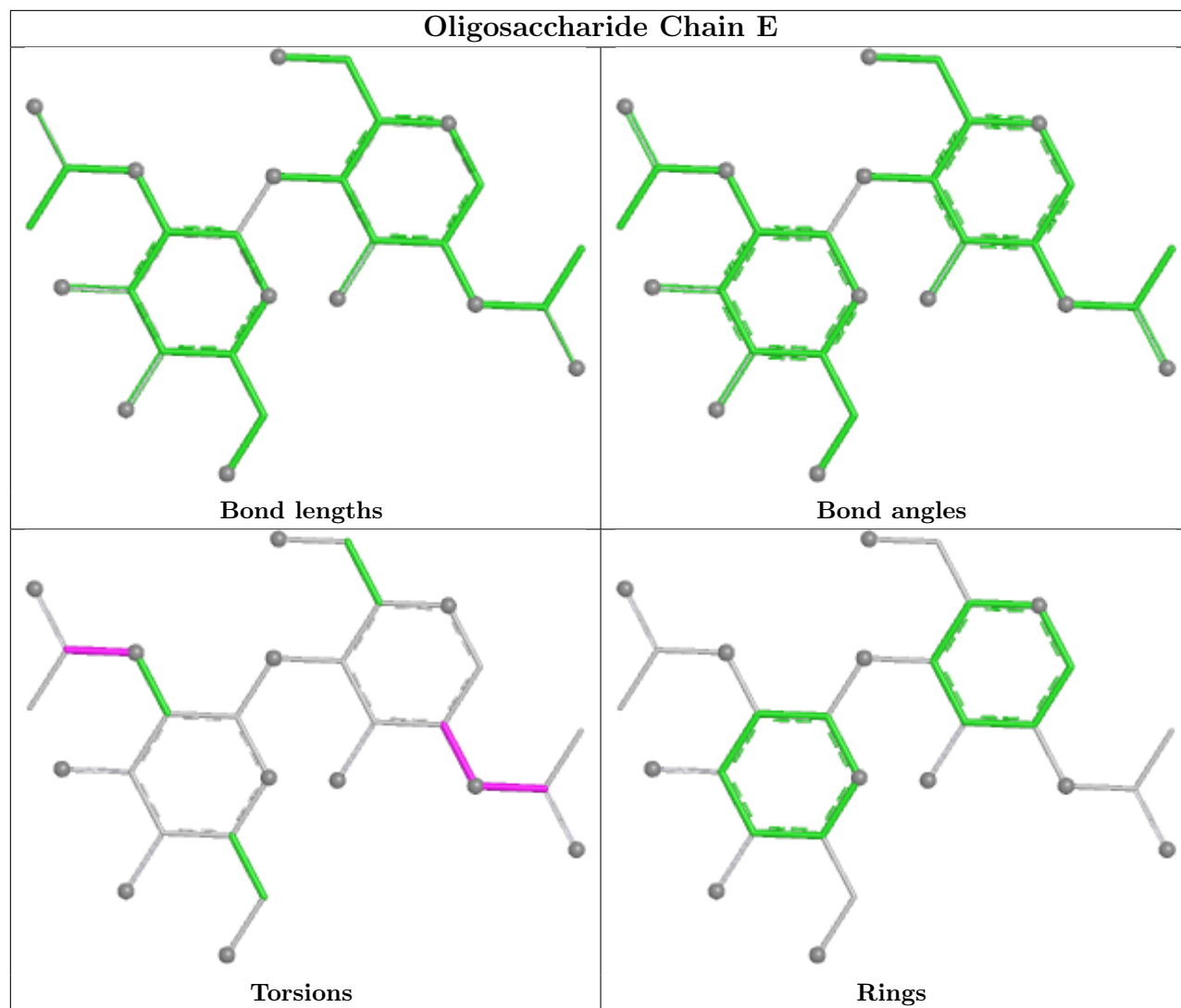
There are no ring outliers.

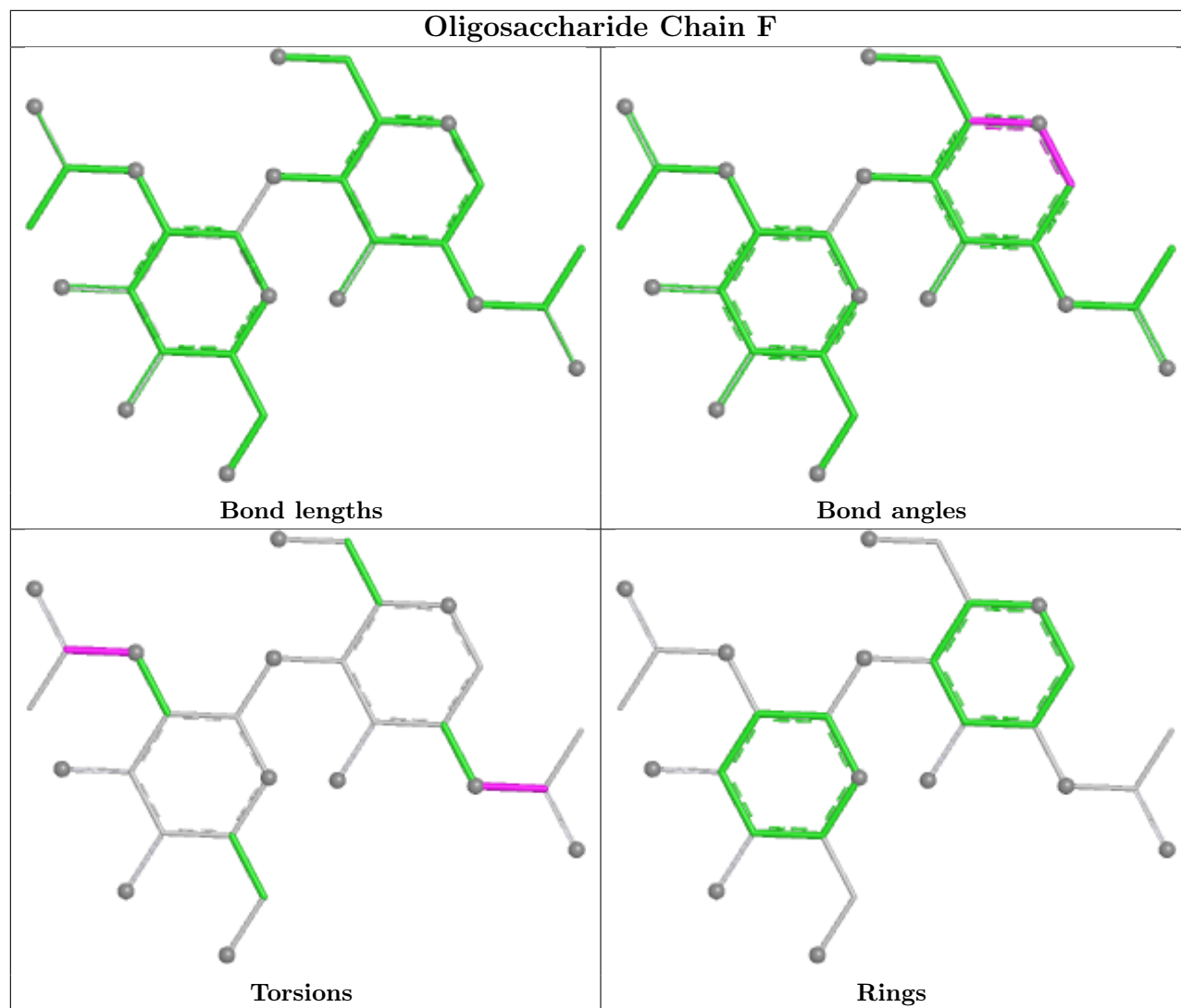
No monomer is involved in short contacts.

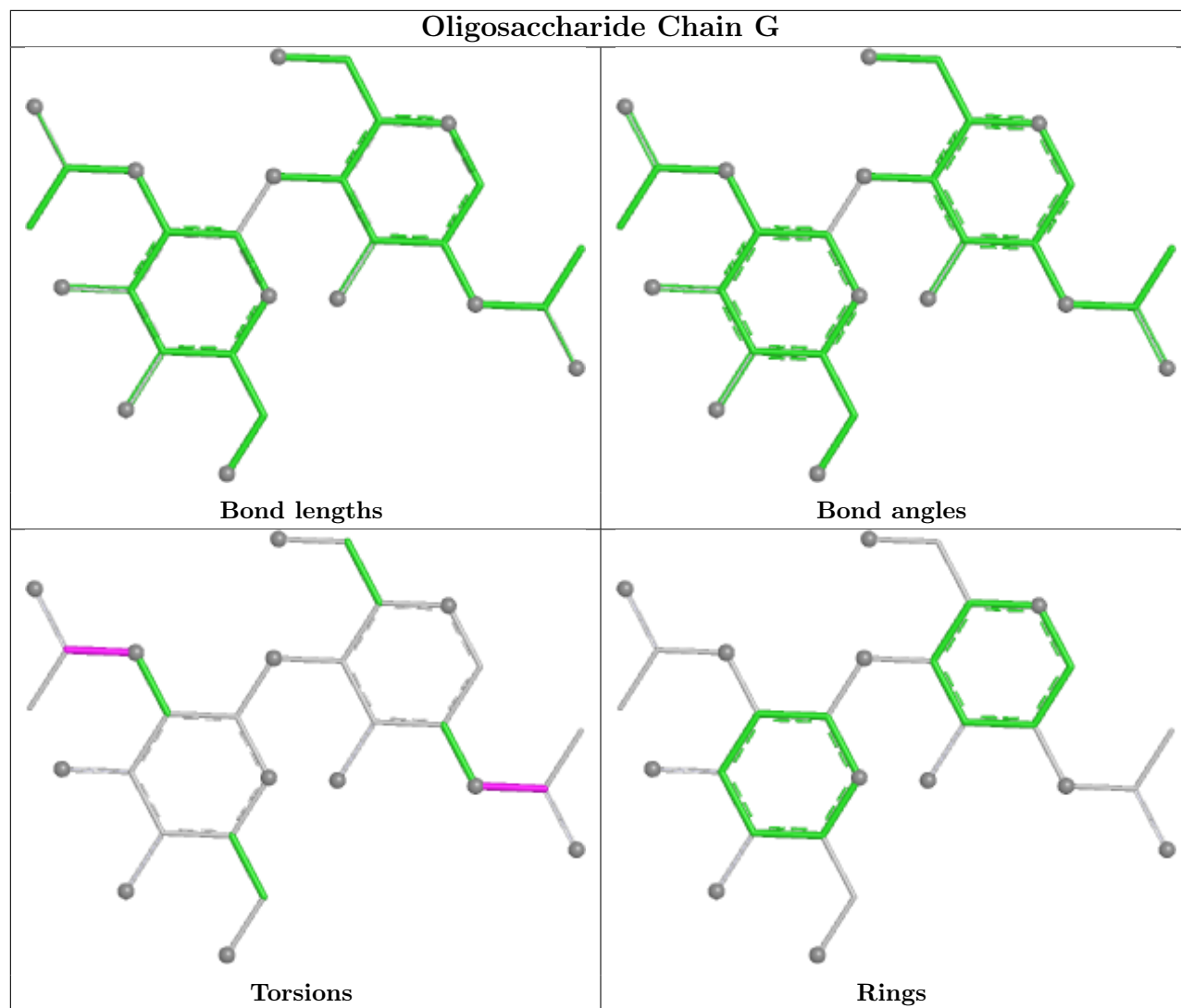
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

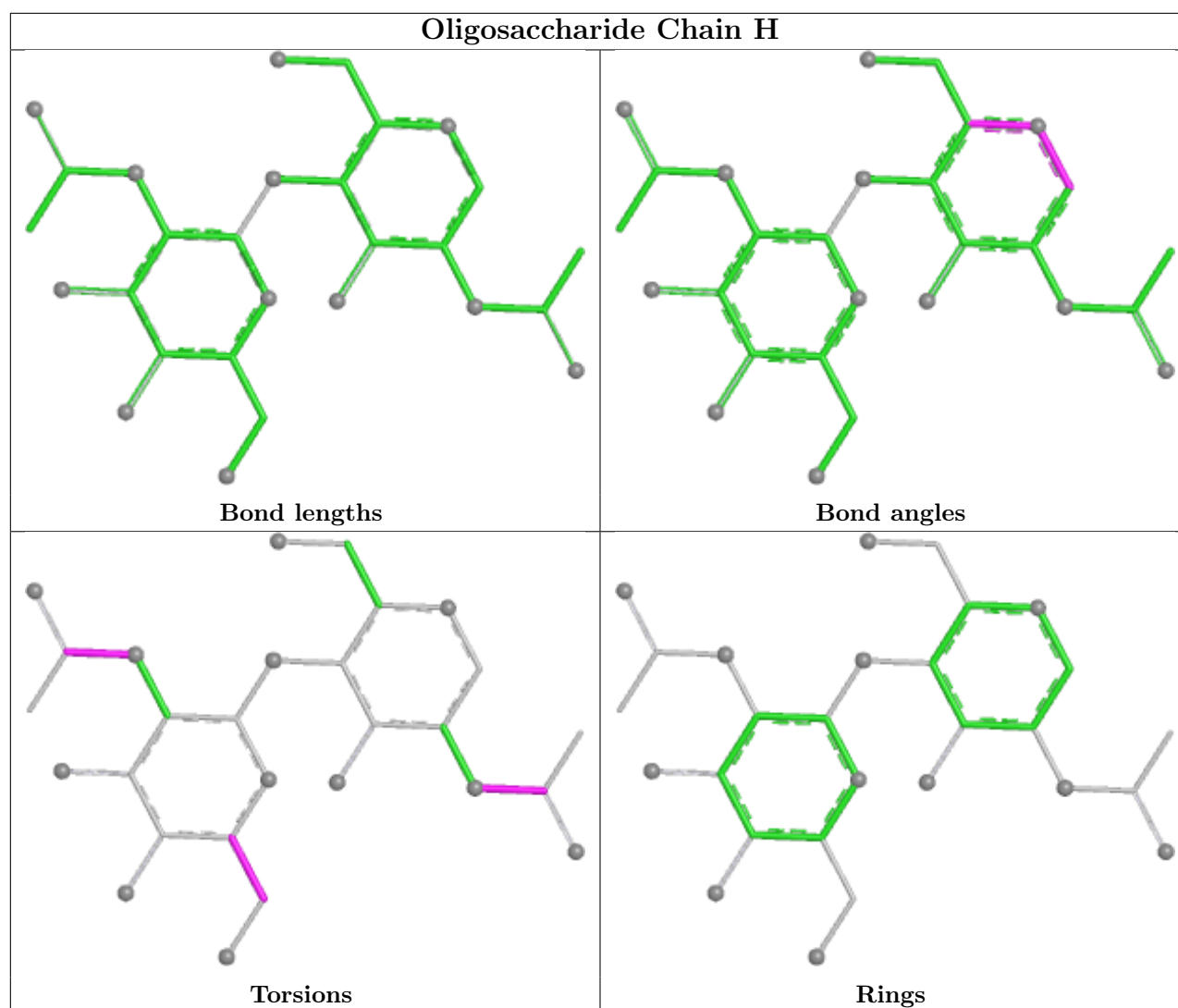












5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	3022	1	14,14,15	0.44	0	17,19,21	0.69	0
5	NAG	A	3019	1	14,14,15	0.46	0	17,19,21	0.64	0
5	NAG	A	3000	1	14,14,15	0.44	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	3014	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
5	NAG	A	3011	1	14,14,15	0.44	0	17,19,21	0.65	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	A	3022	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3019	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3000	1	-	2/6/23/26	0/1/1/1
5	NAG	A	3014	1	-	4/6/23/26	0/1/1/1
5	NAG	A	3011	1	-	5/6/23/26	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(°)
5	A	3014	NAG	C1-C2-N2	3.27	115.59	110.43
5	A	3014	NAG	C2-N2-C7	3.26	127.27	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3000	NAG	C8-C7-N2-C2
5	A	3000	NAG	O7-C7-N2-C2
5	A	3011	NAG	C8-C7-N2-C2
5	A	3011	NAG	O7-C7-N2-C2
5	A	3014	NAG	C1-C2-N2-C7
5	A	3014	NAG	C8-C7-N2-C2
5	A	3014	NAG	O7-C7-N2-C2
5	A	3019	NAG	C8-C7-N2-C2
5	A	3019	NAG	O7-C7-N2-C2
5	A	3011	NAG	O5-C5-C6-O6
5	A	3022	NAG	C8-C7-N2-C2
5	A	3022	NAG	O7-C7-N2-C2
5	A	3022	NAG	O5-C5-C6-O6
5	A	3014	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	3011	NAG	C4-C5-C6-O6
5	A	3022	NAG	C4-C5-C6-O6
5	A	3011	NAG	C1-C2-N2-C7

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1037:MET	C	1045:PRO	N	15.82
1	D	325:SER	C	336:GLY	N	7.27
1	A	1891:ASP	C	1892:HIS	N	3.08
1	A	1145:SER	C	1146:PRO	N	2.74

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	1836/1836 (100%)	1.07	232 (12%)	8 11	45, 123, 188, 241	1 (0%)
2	D	347/347 (100%)	1.22	65 (18%)	3 6	70, 144, 230, 300	0
All	All	2183/2183 (100%)	1.09	297 (13%)	7 10	45, 126, 194, 300	1 (0%)

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	263	ILE	5.7
1	A	2568	LEU	5.7
1	A	2684	LEU	5.3
1	A	2530	MET	5.1
1	A	2571	GLN	5.0
1	A	1845	ASN	4.5
1	A	2658	ASP	4.5
1	A	2655	ALA	4.4
2	D	49	ARG	4.2
2	D	130	PRO	4.2
1	A	2587	HIS	4.2
2	D	98	ASN	4.2
2	D	308	ARG	4.1
1	A	2616	ILE	4.1
1	A	1425	ALA	4.0
1	A	2686	ILE	3.9
2	D	204	ASN	3.9
1	A	1045	PRO	3.9
1	A	2528	ALA	3.9
1	A	2526	PRO	3.9
1	A	2305	VAL	3.8
2	D	362	GLN	3.8
2	D	194	ALA	3.8
1	A	2690	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1444	TRP	3.7
1	A	2211	GLY	3.7
1	A	2685	LEU	3.7
2	D	59	GLU	3.6
1	A	2052	LYS	3.6
1	A	2525	PHE	3.6
1	A	2496	ASN	3.5
1	A	2688	GLY	3.5
2	D	271	GLY	3.5
2	D	359	ASN	3.5
2	D	325	SER	3.5
1	A	2301	ARG	3.5
1	A	2567	ALA	3.5
1	A	2581	ILE	3.5
1	A	2223	TYR	3.4
1	A	1196	GLY	3.4
2	D	246	THR	3.4
1	A	1486	VAL	3.4
1	A	2673	SER	3.4
1	A	973	VAL	3.4
1	A	2752	VAL	3.4
1	A	2578	HIS	3.4
1	A	2454	THR	3.4
2	D	227	ASN	3.4
1	A	2561	HIS	3.4
1	A	2513	MET	3.3
1	A	956	LEU	3.3
1	A	2798	GLU	3.3
1	A	2691	ARG	3.3
1	A	1773	THR	3.3
1	A	2689	ARG	3.2
1	A	2186	GLY	3.2
1	A	1581	PRO	3.2
1	A	1488	GLY	3.2
2	D	375	GLN	3.2
1	A	1016	MET	3.2
2	D	131	TYR	3.2
1	A	1782	GLU	3.2
2	D	188	TRP	3.2
2	D	208	GLY	3.2
2	D	356	ALA	3.1
2	D	245	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	980	VAL	3.1
1	A	1656	VAL	3.0
2	D	36	ARG	3.0
2	D	352	PRO	3.0
2	D	142	VAL	3.0
1	A	1359	GLY	3.0
1	A	1704	GLU	3.0
1	A	2559	GLU	3.0
1	A	1487	PRO	3.0
1	A	1720	LYS	3.0
1	A	2662	LEU	3.0
1	A	1013	ALA	3.0
1	A	2579	ALA	3.0
2	D	133	PHE	3.0
2	D	134	VAL	3.0
2	D	148	THR	3.0
1	A	2529	LYS	2.9
2	D	239	SER	2.9
1	A	1759	ILE	2.9
1	A	1525	LYS	2.9
2	D	314	PHE	2.9
1	A	1422	ASP	2.9
1	A	2491	ASN	2.9
1	A	1297	THR	2.9
1	A	1918	ALA	2.9
1	A	2566	MET	2.9
1	A	1437	VAL	2.8
1	A	1142	PHE	2.8
2	D	307	LYS	2.8
2	D	250	HIS	2.8
1	A	2436	VAL	2.8
1	A	1799	CYS	2.8
2	D	235	THR	2.8
1	A	1023	TRP	2.8
1	A	1755	MET	2.8
1	A	1875	LEU	2.8
1	A	1004	SER	2.8
1	A	2572	VAL	2.8
2	D	47	GLU	2.8
1	A	1767	ASN	2.8
1	A	1037	MET	2.8
1	A	1048	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1747	VAL	2.8
1	A	1781	VAL	2.7
1	A	2507	VAL	2.7
2	D	48	LEU	2.7
1	A	1514	GLY	2.7
1	A	2332	GLY	2.7
1	A	1655	GLU	2.7
1	A	1510	ILE	2.7
1	A	1050	SER	2.7
1	A	1122	LEU	2.7
1	A	2152	GLY	2.7
1	A	1112	LYS	2.7
2	D	57	MET	2.7
1	A	1792	VAL	2.7
1	A	2628	LEU	2.7
2	D	106	ALA	2.7
1	A	2732	LEU	2.7
1	A	2174	ALA	2.7
2	D	64	GLY	2.7
1	A	1007	THR	2.7
1	A	1800	ASN	2.7
1	A	2474	LYS	2.7
1	A	1590	LEU	2.7
1	A	964	VAL	2.6
1	A	2705	ILE	2.6
2	D	209	THR	2.6
1	A	1557	ASN	2.6
1	A	1436	ASP	2.6
1	A	2498	LEU	2.6
1	A	1822	VAL	2.6
1	A	2290	TYR	2.6
1	A	2150	ILE	2.6
1	A	2272	MET	2.6
1	A	1026	TRP	2.6
1	A	1308	LYS	2.6
1	A	983	PRO	2.6
1	A	1770	ASP	2.6
1	A	2267	ASN	2.6
1	A	2455	GLN	2.6
1	A	1863	PHE	2.6
1	A	2514	PHE	2.5
1	A	999	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1493	LEU	2.5
1	A	1617	GLY	2.5
1	A	2372	THR	2.5
1	A	1532	VAL	2.5
1	A	1874	LEU	2.5
2	D	152	GLU	2.5
1	A	1768	ARG	2.5
1	A	2358	THR	2.5
1	A	2312	GLY	2.5
1	A	1870	HIS	2.5
1	A	1886	GLU	2.5
2	D	279	GLU	2.5
1	A	2602	PHE	2.5
1	A	2421	ALA	2.5
2	D	207	ASP	2.5
1	A	1513	THR	2.5
1	A	2693	PHE	2.4
1	A	1370	ALA	2.4
2	D	231	TYR	2.4
1	A	1283	ASP	2.4
1	A	1482	MET	2.4
2	D	248	ASN	2.4
1	A	1548	CYS	2.4
2	D	391	PHE	2.4
2	D	100	THR	2.4
1	A	2318	TYR	2.4
1	A	2786	ASP	2.4
1	A	2534	SER	2.3
1	A	2580	SER	2.3
2	D	283	GLY	2.3
1	A	2091	ILE	2.3
1	A	2664	MET	2.3
1	A	2709	TYR	2.3
1	A	1547	ASP	2.3
1	A	2304	ASP	2.3
2	D	38	GLU	2.3
1	A	2126	PHE	2.3
1	A	971	PRO	2.3
1	A	1375	GLY	2.3
1	A	1871	GLY	2.3
1	A	2500	LEU	2.3
1	A	1567	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1012	ARG	2.3
1	A	1307	PHE	2.3
2	D	357	PHE	2.3
1	A	1277	GLY	2.3
1	A	1237	ALA	2.3
2	D	39	LEU	2.3
1	A	1298	SER	2.3
1	A	1379	VAL	2.3
1	A	2189	LYS	2.3
1	A	2692	ARG	2.3
1	A	1390	ALA	2.3
2	D	351	GLU	2.3
1	A	1780	SER	2.3
1	A	1323	PRO	2.3
1	A	1726	TRP	2.3
1	A	2595	ILE	2.3
1	A	2545	CYS	2.3
1	A	1913	SER	2.3
1	A	1515	VAL	2.3
2	D	336	GLY	2.3
1	A	1200	ASP	2.3
1	A	2502	ASN	2.2
1	A	1010	PHE	2.2
1	A	1612	GLU	2.2
1	A	2783	GLU	2.2
1	A	1543	GLY	2.2
2	D	353	VAL	2.2
1	A	2232	ASP	2.2
2	D	66	THR	2.2
2	D	139	LEU	2.2
1	A	1463	ASN	2.2
2	D	117	GLY	2.2
2	D	225	THR	2.2
1	A	1765	ASN	2.2
1	A	2543	GLN	2.2
1	A	2385	MET	2.2
1	A	1833	ARG	2.2
1	A	1268	PRO	2.2
2	D	86	PRO	2.2
2	D	363	PHE	2.2
1	A	1393	LYS	2.2
2	D	72	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2355	HIS	2.2
1	A	1433	SER	2.2
1	A	1438	SER	2.2
1	A	2509	SER	2.2
1	A	1872	ARG	2.2
1	A	2748	GLU	2.2
1	A	2687	ASN	2.2
1	A	2250	TRP	2.2
1	A	2517	GLN	2.2
1	A	2527	ARG	2.2
1	A	1150	TYR	2.2
1	A	2482	PRO	2.2
1	A	1046	SER	2.1
1	A	1420	SER	2.1
1	A	1472	HIS	2.1
1	A	1483	HIS	2.1
1	A	1373	GLY	2.1
1	A	1839	PRO	2.1
1	A	1851	LEU	2.1
1	A	1070	ASP	2.1
1	A	2470	TYR	2.1
1	A	1366	PRO	2.1
1	A	1151	THR	2.1
1	A	1304	ASN	2.1
2	D	234	ARG	2.1
1	A	2167	ILE	2.1
1	A	1554	VAL	2.1
1	A	959	LEU	2.1
1	A	1134	GLU	2.1
2	D	270	ASN	2.1
2	D	289	GLN	2.1
1	A	1276	ASP	2.1
1	A	1540	LEU	2.1
2	D	251	ASP	2.1
1	A	2270	ARG	2.1
1	A	1777	ASN	2.1
1	A	1869	VAL	2.1
1	A	2175	VAL	2.1
1	A	1496	LEU	2.1
1	A	1428	PRO	2.1
1	A	1891	ASP	2.1
1	A	1935	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1394	TYR	2.0
1	A	1517	TYR	2.0
1	A	2230	THR	2.0
1	A	1847	ILE	2.0
1	A	1544	ALA	2.0
1	A	2433	PHE	2.0
2	D	297	PHE	2.0
1	A	1798	LEU	2.0
1	A	1772	VAL	2.0
1	A	1455	ASN	2.0
1	A	2472	MET	2.0
1	A	2197	ARG	2.0
1	A	1029	PHE	2.0
1	A	2589	PHE	2.0
1	A	972	LEU	2.0
2	D	320	LEU	2.0
1	A	1459	VAL	2.0
1	A	2251	ARG	2.0
2	D	360	PRO	2.0
1	A	1423	LEU	2.0
1	A	1511	SER	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.

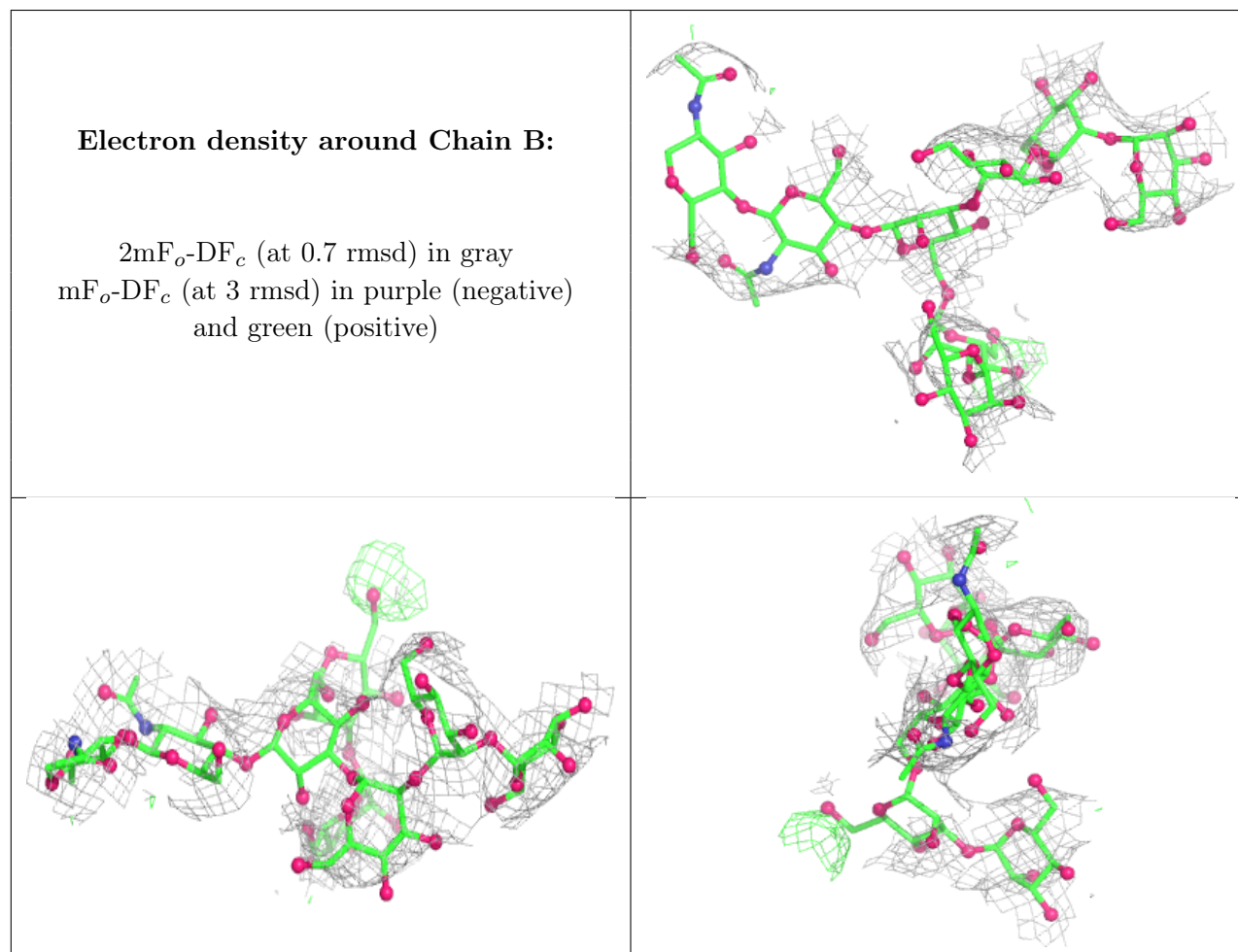
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	151,158,168,169	0
3	NAG	B	2	14/15	-	-	168,177,183,189	0
3	BMA	B	3	11/12	-	-	194,198,204,207	0
3	MAN	B	4	11/12	-	-	201,202,203,205	0
3	MAN	B	5	11/12	-	-	208,209,210,213	0
3	MAN	B	6	11/12	-	-	215,217,218,219	0
3	MAN	B	7	11/12	-	-	210,212,213,213	0

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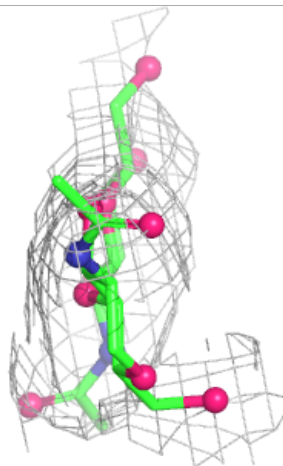
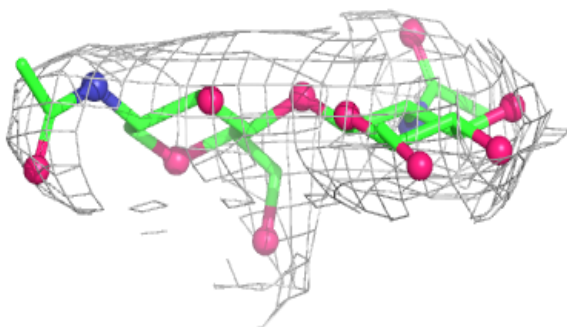
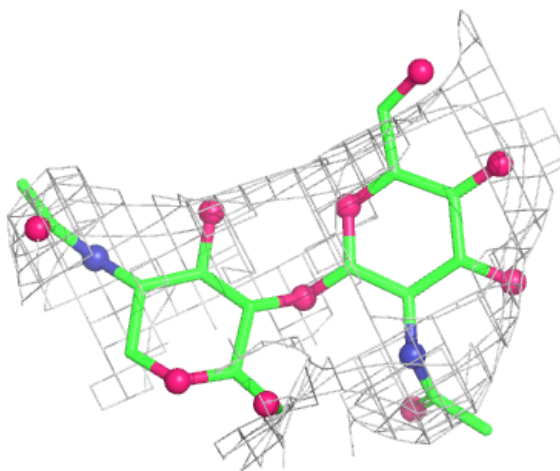
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	B	8	11/12	-	-	212,213,214,215	0
4	NAG	G	2	14/15	0.26	0.20	152,155,160,161	0
4	NAG	F	2	14/15	0.49	0.16	156,160,165,166	0
4	NAG	G	1	14/15	0.59	0.17	128,137,143,147	0
4	NAG	H	2	14/15	0.69	0.16	139,140,142,144	0
4	NAG	C	2	14/15	0.73	0.15	145,151,157,160	0
4	NAG	H	1	14/15	0.75	0.15	122,132,138,138	0
4	NAG	C	1	14/15	0.78	0.15	129,133,137,141	0
4	NAG	E	2	14/15	0.81	0.16	155,158,162,164	0
4	NAG	E	1	14/15	0.82	0.17	137,140,145,149	0
4	NAG	F	1	14/15	0.89	0.10	125,138,146,150	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.



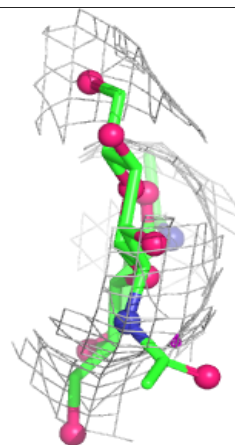
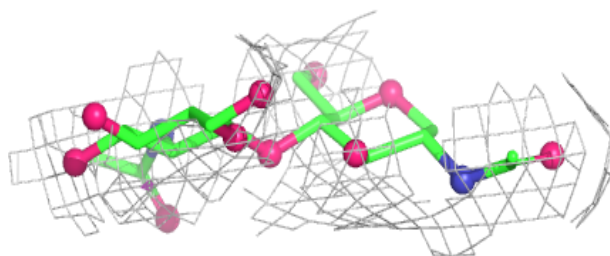
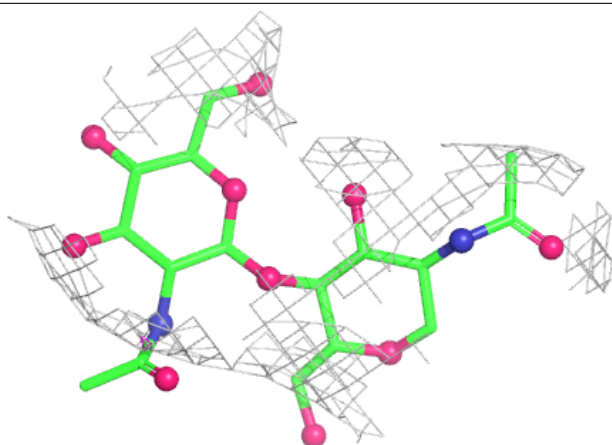
Electron density around Chain C:

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

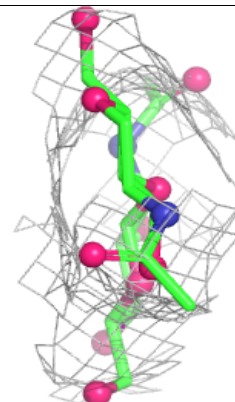
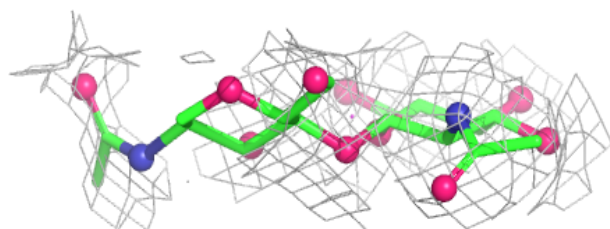
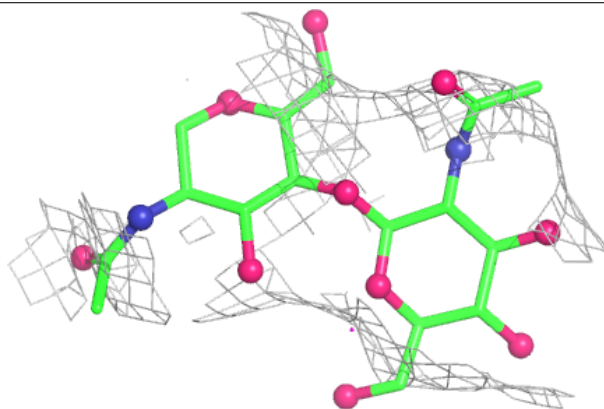


Electron density around Chain E:

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

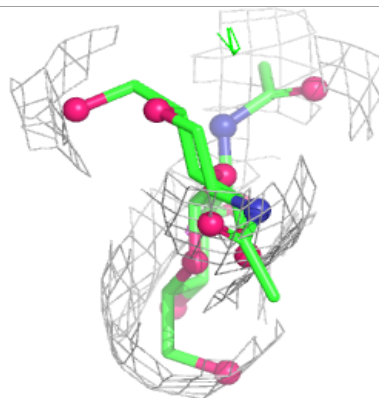
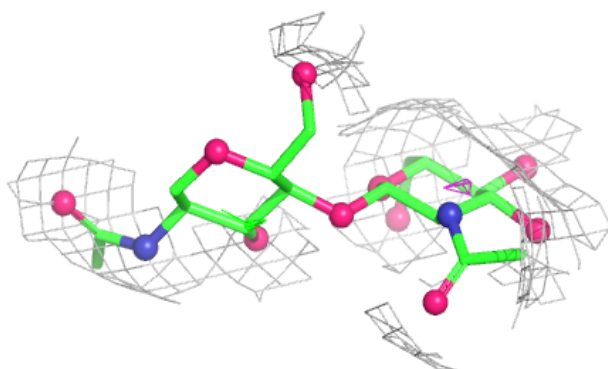
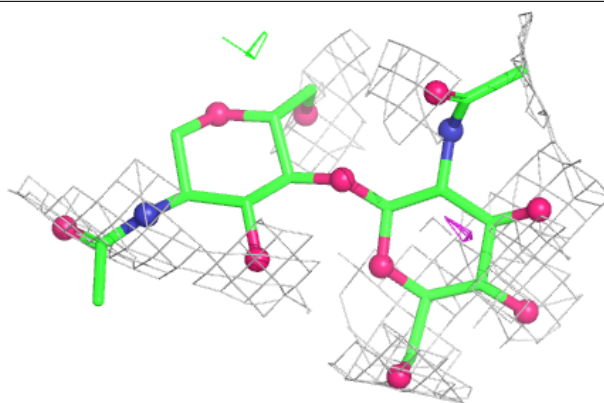
**Electron density around Chain F:**

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

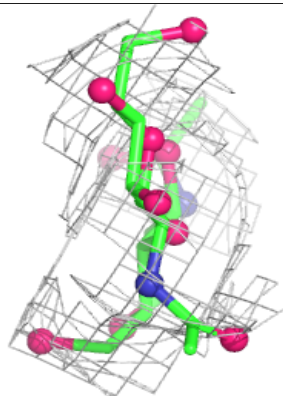
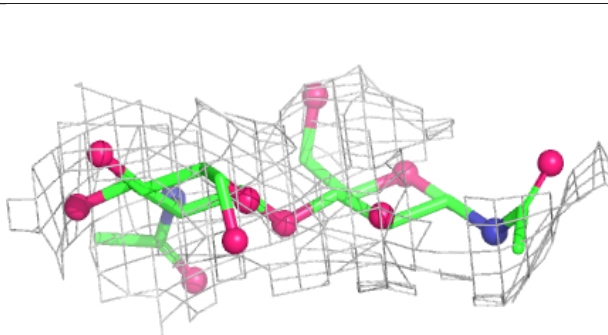
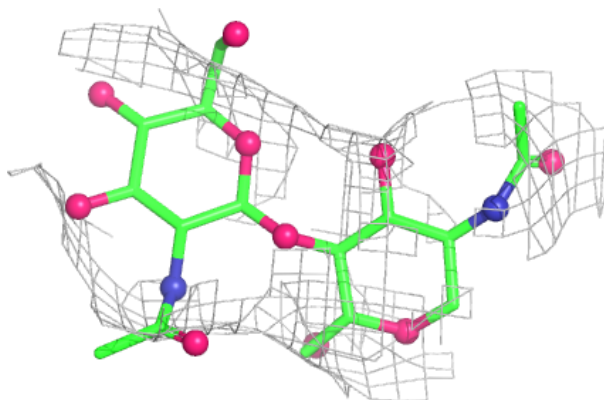


Electron density around Chain G:

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

**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)



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	3014	14/15	0.42	0.21	152,156,159,159	0
5	NAG	A	3019	14/15	0.43	0.18	215,217,218,219	0
5	NAG	A	3000	14/15	0.62	0.18	224,225,228,228	0
5	NAG	A	3022	14/15	0.63	0.14	187,190,194,194	0
5	NAG	A	3011	14/15	0.75	0.18	139,144,149,149	0
6	CA	D	1100	1/1	0.99	0.14	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.