



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:34 AM BST

PDB ID : 6AHY
Title : Wnt signaling complex
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Deposited on : 2018-08-21
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

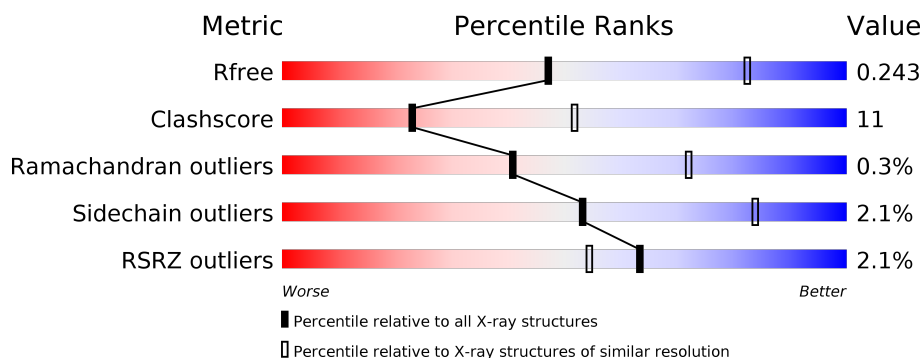
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.




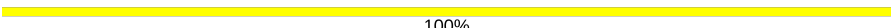
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	141	<div> <div></div> <div>72%13%15%</div> </div>
1	C	141	<div> <div></div> <div>64%21%13%</div> </div>
1	E	141	<div> <div>9%</div> <div>50%28%21%</div> </div>
2	B	319	<div> <div></div> <div>76%21%</div> </div>
2	D	319	<div> <div>2%</div> <div>69%26%</div> </div>
2	F	319	<div> <div></div> <div>70%16%14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 50%50%
3	H	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9947 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 Frizzled-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	0	0
			969	616	161	177	15			
1	C	122	Total	C	N	O	S	0	0	0
			991	631	164	181	15			
1	E	112	Total	C	N	O	S	0	0	0
			864	553	136	162	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	SER	-	expression tag	UNP Q61091
A	161	ARG	-	expression tag	UNP Q61091
A	162	PRO	-	expression tag	UNP Q61091
A	163	ALA	-	expression tag	UNP Q61091
A	164	PRO	-	expression tag	UNP Q61091
A	165	GLU	-	expression tag	UNP Q61091
A	166	LEU	-	expression tag	UNP Q61091
A	167	LEU	-	expression tag	UNP Q61091
A	168	GLY	-	expression tag	UNP Q61091
C	160	SER	-	expression tag	UNP Q61091
C	161	ARG	-	expression tag	UNP Q61091
C	162	PRO	-	expression tag	UNP Q61091
C	163	ALA	-	expression tag	UNP Q61091
C	164	PRO	-	expression tag	UNP Q61091
C	165	GLU	-	expression tag	UNP Q61091
C	166	LEU	-	expression tag	UNP Q61091
C	167	LEU	-	expression tag	UNP Q61091
C	168	GLY	-	expression tag	UNP Q61091
E	160	SER	-	expression tag	UNP Q61091
E	161	ARG	-	expression tag	UNP Q61091
E	162	PRO	-	expression tag	UNP Q61091
E	163	ALA	-	expression tag	UNP Q61091
E	164	PRO	-	expression tag	UNP Q61091

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Chain	Residue	Modelled	Actual	Comment	Reference
E	165	GLU	-	expression tag	UNP Q61091
E	166	LEU	-	expression tag	UNP Q61091
E	167	LEU	-	expression tag	UNP Q61091
E	168	GLY	-	expression tag	UNP Q61091

- Molecule 2 is a protein called Proto-oncogene Wnt-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	313	Total	C	N	O	S	0	0	0
			2460	1524	452	456	28			
2	D	309	Total	C	N	O	S	0	0	0
			2431	1502	448	453	28			
2	F	275	Total	C	N	O	S	0	0	0
			2066	1283	369	393	21			

There are 15 discrepancies between the modelled and reference sequences:

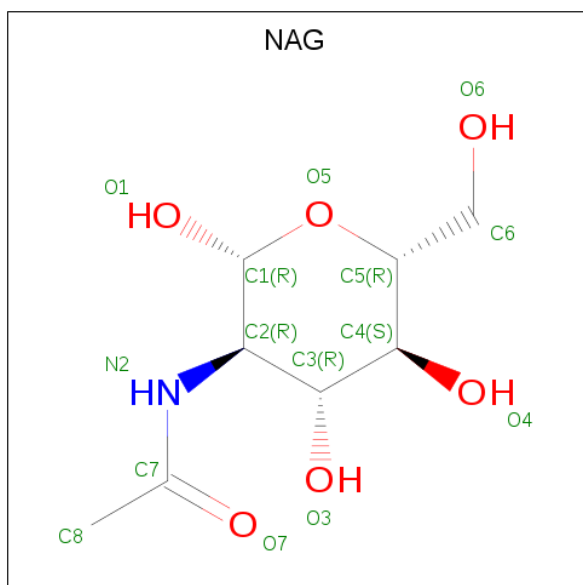
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	GLY	-	expression tag	UNP P56703
B	38	MLY	-	expression tag	UNP P56703
B	39	ASP	-	expression tag	UNP P56703
B	40	GLY	-	expression tag	UNP P56703
B	41	SER	-	expression tag	UNP P56703
D	37	GLY	-	expression tag	UNP P56703
D	38	MLY	-	expression tag	UNP P56703
D	39	ASP	-	expression tag	UNP P56703
D	40	GLY	-	expression tag	UNP P56703
D	41	SER	-	expression tag	UNP P56703
F	37	GLY	-	expression tag	UNP P56703
F	38	MLY	-	expression tag	UNP P56703
F	39	ASP	-	expression tag	UNP P56703
F	40	GLY	-	expression tag	UNP P56703
F	41	SER	-	expression tag	UNP P56703

- Molecule 3 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
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

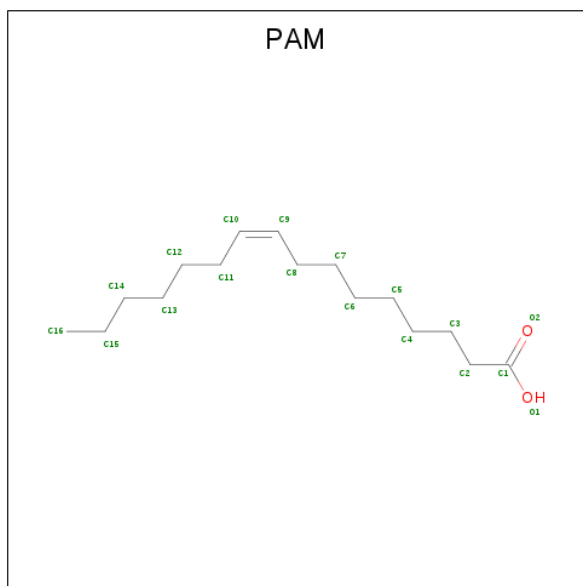


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PALMITOLEIC ACID (three-letter code: PAM) (formula: $C_{16}H_{30}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			17	16	1		
6	D	1	Total	C	O	0	0
			8	7	1		

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.

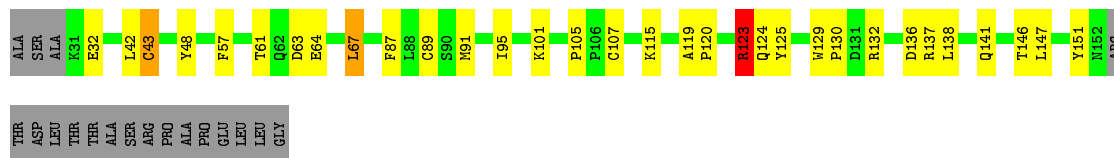
- Molecule 1: Frizzled-8

Chain A: 



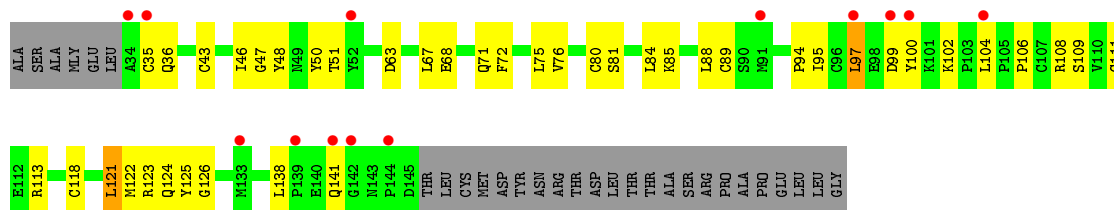
- Molecule 1: Frizzled-8

Chain C: 




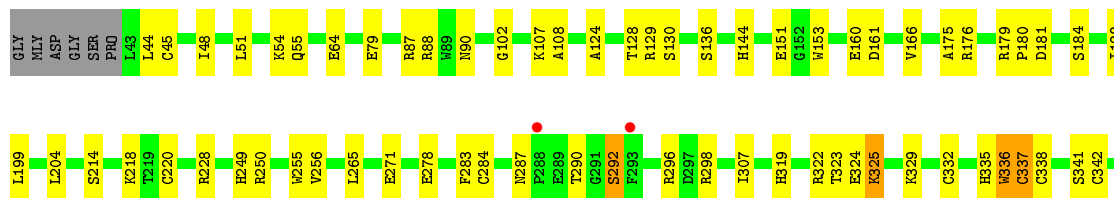
- Molecule 1: Frizzled-8

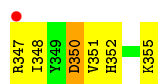
Chain E: 



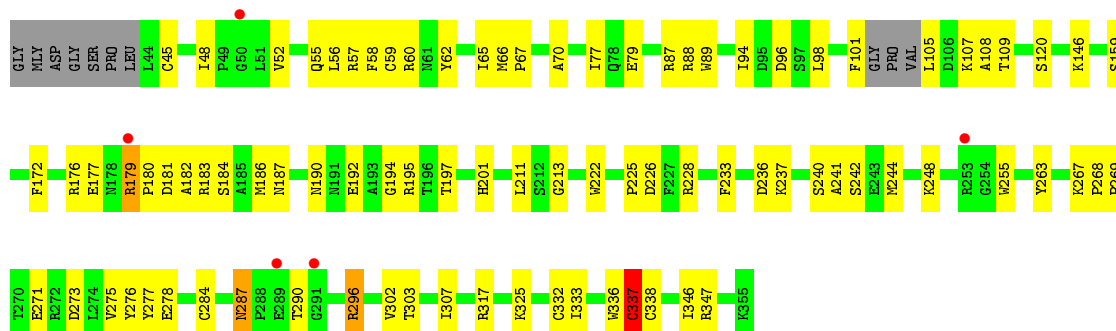
- Molecule 2: Proto-oncogene Wnt-3

Chain B: 

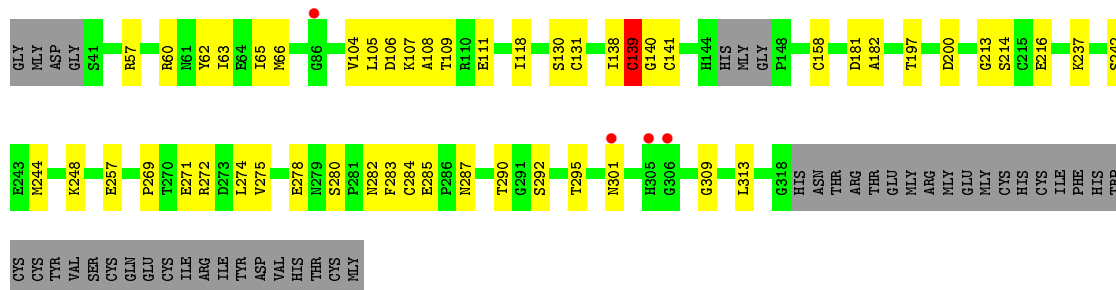




• Molecule 2: Proto-oncogene Wnt-3



• Molecule 2: Proto-oncogene Wnt-3



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.07Å 141.61Å 260.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.16 – 2.80 44.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.16-2.80) 99.9 (44.16-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.205 , 0.244 0.205 , 0.243	Depositor DCC
R_{free} test set	2717 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: CL, MLY, PAM, NAG

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	0.32	0/951	0.56	0/1299
1	C	0.53	3/961 (0.3%)	0.88	5/1314 (0.4%)
1	E	0.44	0/851	0.78	3/1169 (0.3%)
2	B	0.39	0/2352	0.57	1/3196 (0.0%)
2	D	0.39	0/2324	0.60	0/3155
2	F	0.43	2/1989 (0.1%)	0.55	1/2708 (0.0%)
All	All	0.41	5/9428 (0.1%)	0.63	10/12841 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	CYS	CB-SG	-7.42	1.69	1.82
2	F	139	CYS	CB-SG	-6.76	1.70	1.82
1	C	123	ARG	CB-CG	-6.10	1.36	1.52
2	F	141	CYS	CB-SG	-6.07	1.72	1.82
1	C	89	CYS	CB-SG	-5.60	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	CYS	CA-CB-SG	-12.72	91.11	114.00
1	C	89	CYS	CA-CB-SG	-12.54	91.42	114.00
1	C	123	ARG	CG-CD-NE	-11.84	86.95	111.80
1	E	89	CYS	CA-CB-SG	-11.25	93.75	114.00
1	C	123	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	C	123	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	E	43	CYS	CA-CB-SG	-7.60	100.31	114.00
2	F	158	CYS	CA-CB-SG	6.16	125.09	114.00
2	B	284	CYS	C-N-CA	5.43	135.26	121.70
1	E	97	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	TRP	Peptide
2	D	337	CYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	901	15	0
1	C	991	0	930	18	0
1	E	864	0	767	39	2
2	B	2460	0	2279	48	1
2	D	2431	0	2232	65	0
2	F	2066	0	1872	37	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	B	1	0	0	0	0
6	B	17	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	8	0	10	1	0
All	All	9947	0	9148	217	2

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 11.

All (217) 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:E:46:ILE:HD12	1:E:47:GLY:N	1.84	0.93
2:F:109:THR:HG22	2:F:111:GLU:H	1.36	0.87
2:B:90:ASN:HD22	3:G:1:NAG:H83	1.42	0.83
2:D:88:ARG:NH1	2:D:284:CYS:SG	2.53	0.82
1:E:75:LEU:HD23	1:E:84:LEU:HD21	1.64	0.80
1:E:46:ILE:CD1	1:E:48:TYR:H	1.95	0.79
1:E:99:ASP:OD1	1:E:100:TYR:N	2.16	0.78
2:F:216:GLU:N	2:F:216:GLU:OE2	2.16	0.78
2:F:287:ASN:HB3	2:F:290:THR:HG22	1.66	0.77
1:E:75:LEU:CD2	1:E:84:LEU:HD21	2.15	0.77
2:B:87:ARG:O	2:B:298:ARG:NH1	2.15	0.76
2:D:79:GLU:OE2	2:D:228:ARG:NH2	2.19	0.75
2:B:153:TRP:HB3	2:B:218:MLY:HB2	1.68	0.75
2:D:183:ARG:HD3	2:D:277:TYR:OH	1.87	0.74
1:E:46:ILE:HD12	1:E:48:TYR:H	1.53	0.73
1:A:75:LEU:HD13	6:B:405:PAM:H72	1.72	0.71
1:C:123:ARG:HG2	1:C:123:ARG:NH1	2.05	0.71
2:D:228:ARG:HH21	2:D:228:ARG:HG3	1.56	0.70
1:E:76:VAL:HG11	1:E:85:MLY:HB3	1.75	0.68
1:E:46:ILE:HD12	1:E:46:ILE:C	2.14	0.66
1:E:121:LEU:O	1:E:124:GLN:HB3	1.96	0.65
1:E:102:MLY:HD2	1:E:104:LEU:HD23	1.78	0.65
2:D:179:ARG:HD2	2:D:181:ASP:HB2	1.79	0.65
1:E:108:ARG:O	1:E:111:CYS:SG	2.56	0.64
2:F:237:MLY:HB2	2:F:274:LEU:HD13	1.79	0.64
1:A:80:CYS:HB2	1:A:117:GLY:O	1.98	0.64
2:F:109:THR:HG22	2:F:111:GLU:N	2.12	0.63
2:F:138:ILE:HD12	2:F:139:CYS:HB2	1.79	0.63
2:B:325:MLY:HB2	2:B:348:ILE:HD12	1.80	0.63
2:D:56:LEU:HD23	2:D:60:ARG:HH11	1.64	0.63
2:D:52:VAL:O	2:D:55:GLN:HG2	1.98	0.63
1:C:61:THR:HG23	1:C:64:GLU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:PRO:HB2	2:B:256:VAL:HA	1.83	0.61
2:B:54:MLY:HD2	2:B:175:ALA:HA	1.84	0.60
2:D:105:LEU:HB2	2:D:107:MLY:NZ	2.17	0.60
1:A:78:ILE:HG13	6:B:405:PAM:H10	1.84	0.60
2:B:144:HIS:HB3	2:F:60:ARG:HD3	1.81	0.60
2:B:323:THR:HG22	2:B:350:ASP:OD2	2.02	0.60
2:B:249:HIS:O	2:B:256:VAL:HG22	2.02	0.59
2:D:52:VAL:HG12	2:D:55:GLN:OE1	2.02	0.59
2:F:108:ALA:HB3	2:F:278:GLU:HG3	1.82	0.59
2:F:200:ASP:OD1	2:F:272:ARG:NH1	2.36	0.59
2:B:151:GLU:HA	2:B:151:GLU:OE2	2.01	0.59
2:D:177:GLU:OE2	2:D:187:ASN:HB2	2.01	0.59
2:F:287:ASN:HB3	2:F:290:THR:CG2	2.33	0.59
1:C:63:ASP:O	1:C:67:LEU:HD12	2.02	0.59
2:B:271:GLU:CD	2:B:271:GLU:H	2.07	0.58
2:D:237:MLY:O	2:D:241:ALA:N	2.36	0.58
2:B:336:TRP:CD2	2:B:337:CYS:HB2	2.39	0.57
2:D:101:PHE:O	2:D:176:ARG:HD3	2.03	0.57
2:D:194:GLY:O	2:D:197:THR:HG22	2.04	0.57
2:D:179:ARG:HH11	2:D:180:PRO:HG2	1.69	0.57
2:B:79:GLU:OE2	2:B:228:ARG:HD3	2.05	0.57
1:E:51:THR:OG1	1:E:94:PRO:O	2.08	0.56
2:B:79:GLU:OE1	2:B:228:ARG:NH2	2.38	0.56
2:D:159:SER:HB3	2:D:222:TRP:HB2	1.87	0.56
1:E:121:LEU:HD23	1:E:121:LEU:H	1.70	0.56
2:F:295:THR:HG21	2:F:313:LEU:O	2.04	0.56
2:D:108:ALA:HB3	2:D:278:GLU:HG3	1.85	0.56
1:A:100:TYR:CZ	1:A:102:MLY:HB3	2.41	0.56
1:C:57:PHE:CD1	1:C:132:ARG:HD3	2.41	0.56
2:D:77:ILE:HG12	2:D:96:ASP:HB3	1.87	0.56
2:B:296:ARG:NH1	2:B:296:ARG:HB3	2.21	0.56
2:B:329:MLY:HD3	2:B:342:CYS:HB3	1.87	0.55
2:F:301:ASN:H	2:F:309:GLY:HA2	1.72	0.55
1:E:97:LEU:HD23	1:E:99:ASP:OD2	2.06	0.55
1:C:146:THR:HG22	1:C:147:LEU:O	2.07	0.55
2:D:183:ARG:NH1	2:D:277:TYR:OH	2.36	0.54
2:B:129:ARG:NH1	2:B:160:GLU:OE1	2.40	0.54
2:B:324:GLU:OE2	2:B:324:GLU:HA	2.07	0.54
1:E:46:ILE:C	1:E:46:ILE:CD1	2.75	0.54
2:D:181:ASP:OD1	2:D:182:ALA:N	2.41	0.54
2:F:63:ILE:HA	2:F:66:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:HG21	2:B:51:LEU:HD13	1.89	0.53
2:D:58:PHE:CE2	2:D:172:PHE:HB2	2.42	0.53
1:E:63:ASP:O	1:E:67:LEU:HD12	2.08	0.53
2:F:200:ASP:OD2	2:F:272:ARG:HD3	2.09	0.53
1:E:109:SER:HB2	1:E:113:ARG:HH21	1.75	0.52
1:E:81:SER:O	1:E:84:LEU:HB3	2.09	0.52
2:B:48:ILE:HD12	2:B:51:LEU:HD13	1.92	0.52
1:E:95:ILE:HG22	1:E:97:LEU:CD1	2.40	0.52
2:B:307:ILE:H	2:B:307:ILE:HD12	1.75	0.52
2:D:57:ARG:NH1	2:D:60:ARG:HH22	2.08	0.52
2:D:52:VAL:N	2:D:55:GLN:OE1	2.35	0.52
1:E:35:CYS:HB3	1:E:50:TYR:HB3	1.90	0.52
1:E:84:LEU:HD22	1:E:118:CYS:SG	2.50	0.51
2:B:102:GLY:O	2:B:176:ARG:HD3	2.10	0.51
1:E:75:LEU:HD21	1:E:84:LEU:HD21	1.93	0.51
1:E:68:GLU:OE2	2:F:213:GLY:HA2	2.11	0.51
1:C:136:ASP:OD1	1:C:137:ARG:N	2.44	0.51
1:E:84:LEU:HD12	1:E:88:LEU:HD13	1.93	0.51
1:A:100:TYR:CE1	1:A:102:MLY:HB3	2.46	0.51
2:B:204:LEU:HD22	2:B:220:CYS:HB3	1.94	0.50
2:D:179:ARG:NH1	2:D:180:PRO:HG2	2.26	0.50
2:F:197:THR:HA	2:F:200:ASP:HB2	1.93	0.50
2:F:248:MLY:HG3	2:F:257:GLU:HG2	1.92	0.50
1:C:87:PHE:CZ	1:C:91:MET:HE1	2.46	0.50
2:B:108:ALA:HB3	2:B:278:GLU:HG3	1.93	0.50
1:C:124:GLN:C	1:C:125:TYR:HD1	2.15	0.50
2:D:192:GLU:HG3	2:D:195:ARG:NH2	2.27	0.50
1:A:91:MET:HG3	1:A:133:MET:HE3	1.94	0.50
1:A:147:LEU:HD12	1:A:147:LEU:H	1.77	0.49
2:B:347:ARG:C	2:B:348:ILE:HD13	2.32	0.49
2:B:179:ARG:C	2:B:181:ASP:H	2.16	0.49
2:B:265:LEU:HD23	2:B:265:LEU:H	1.76	0.49
2:B:290:THR:HG22	2:B:290:THR:O	2.13	0.49
2:B:51:LEU:HD12	2:B:55:GLN:OE1	2.12	0.49
2:D:66:MET:N	2:D:67:PRO:HD2	2.27	0.49
2:D:211:LEU:HD21	6:D:404:PAM:H21	1.95	0.49
1:C:32:GLU:HG2	1:C:101:MLY:HB2	1.95	0.49
1:E:68:GLU:O	1:E:71:GLN:HG2	2.12	0.49
1:E:48:TYR:CZ	1:E:95:ILE:HG13	2.47	0.49
1:E:46:ILE:HD11	1:E:48:TYR:H	1.74	0.48
2:D:89:TRP:HZ2	2:D:94:ILE:HD11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:ARG:NH2	2:D:228:ARG:HG3	2.27	0.48
2:D:87:ARG:HD2	2:D:307:ILE:HD13	1.94	0.48
2:D:107:MLY:O	2:D:109:THR:N	2.43	0.48
2:B:319:HIS:ND1	2:B:352:HIS:HB3	2.29	0.48
2:D:59:CYS:HA	2:D:66:MET:HE1	1.96	0.47
1:E:95:ILE:HG22	1:E:97:LEU:HD12	1.96	0.47
2:D:287:ASN:HB3	2:D:290:THR:OG1	2.14	0.47
2:F:109:THR:HG23	2:F:280:SER:OG	2.14	0.47
2:D:267:MLY:HD2	2:D:267:MLY:HA	1.43	0.47
2:D:332:CYS:O	2:D:333:ILE:HD13	2.14	0.47
2:D:56:LEU:CD2	2:D:60:ARG:HH11	2.27	0.47
2:B:322:ARG:CZ	2:B:351:VAL:HG21	2.45	0.47
2:B:44:LEU:HD12	2:B:45:CYS:H	1.79	0.47
1:E:122:MET:O	1:E:126:GLY:N	2.48	0.47
2:D:271:GLU:CD	2:D:271:GLU:H	2.18	0.47
2:D:179:ARG:HD3	2:D:180:PRO:N	2.29	0.46
2:D:48:ILE:HG21	2:D:98:LEU:HB2	1.98	0.46
2:D:267:MLY:HD2	2:D:268:PRO:HD2	1.97	0.46
1:C:105:PRO:HB2	1:C:138:LEU:HD12	1.98	0.46
1:E:72:PHE:O	1:E:76:VAL:HG23	2.15	0.46
2:D:267:MLY:HA	2:D:268:PRO:HD2	1.71	0.46
2:D:186:MET:HG2	2:D:190:ASN:ND2	2.32	0.45
2:F:283:PHE:HD1	2:F:292:SER:HB2	1.81	0.45
2:D:240:SER:O	2:D:273:ASP:OD2	2.35	0.45
2:B:166:VAL:HG21	2:B:199:LEU:HG	1.99	0.45
1:E:46:ILE:CD1	1:E:48:TYR:CD1	3.00	0.45
2:D:62:TYR:O	2:D:65:ILE:HG22	2.17	0.45
1:C:107:CYS:SG	1:C:141:GLN:HG2	2.57	0.44
1:C:132:ARG:HE	2:D:213:GLY:HA3	1.82	0.44
1:E:68:GLU:HA	1:E:71:GLN:OE1	2.16	0.44
2:F:107:MLY:HB2	2:F:278:GLU:OE2	2.17	0.44
1:A:108:ARG:HD3	1:A:140:GLU:OE2	2.18	0.44
2:B:64:GLU:OE1	2:B:136:SER:OG	2.22	0.44
2:D:79:GLU:CD	2:D:228:ARG:HH22	2.20	0.44
2:D:325:MLY:CD	2:D:346:ILE:HD11	2.47	0.44
1:A:147:LEU:HD21	2:B:332:CYS:O	2.17	0.44
2:D:107:MLY:O	2:D:109:THR:HG23	2.18	0.44
1:A:42:LEU:O	1:A:42:LEU:HD13	2.17	0.44
2:B:335:HIS:O	2:B:337:CYS:N	2.51	0.44
2:F:242:SER:OG	2:F:269:PRO:HB3	2.17	0.44
1:A:39:THR:N	1:A:62:GLN:OE1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:THR:HG22	2:B:160:GLU:HB3	2.00	0.44
2:B:181:ASP:HB3	2:B:184:SER:H	1.82	0.44
2:B:296:ARG:HG3	2:B:355:MLY:O	2.18	0.44
2:D:57:ARG:HA	2:D:60:ARG:NH1	2.32	0.44
2:D:302:VAL:HG23	2:D:303:THR:HG23	1.98	0.43
2:B:124:ALA:HB3	2:B:198:ILE:HG13	2.01	0.43
2:D:181:ASP:HB3	2:D:184:SER:H	1.82	0.43
2:F:284:CYS:HB3	2:F:285:GLU:OE2	2.18	0.43
1:C:119:ALA:N	1:C:120:PRO:HD2	2.34	0.43
2:B:161:ASP:OD1	2:F:60:ARG:NH2	2.52	0.43
2:B:296:ARG:HG3	2:B:355:MLY:C	2.48	0.43
2:D:48:ILE:HD12	2:D:48:ILE:H	1.83	0.43
2:F:214:SER:HB2	2:F:216:GLU:OE2	2.18	0.43
2:F:181:ASP:HA	2:F:257:GLU:HB2	2.01	0.43
2:F:104:VAL:HG23	2:F:106:ASP:H	1.83	0.43
2:B:296:ARG:HB3	2:B:296:ARG:CZ	2.49	0.43
1:C:48:TYR:CG	1:C:95:ILE:HD12	2.54	0.43
2:D:186:MET:HG2	2:D:190:ASN:HD21	1.83	0.43
1:C:123:ARG:HB3	1:C:124:GLN:HG3	2.01	0.42
2:F:214:SER:CB	2:F:216:GLU:OE2	2.67	0.42
2:F:271:GLU:OE1	2:F:271:GLU:N	2.37	0.42
2:B:250:ARG:HB2	2:B:255:TRP:CD1	2.55	0.42
2:D:201:HIS:HB3	2:D:225:PRO:HG3	2.02	0.42
2:B:337:CYS:HA	2:B:338:CYS:HA	1.36	0.42
2:D:336:TRP:HA	2:D:337:CYS:HA	1.41	0.42
2:B:287:ASN:HB3	2:B:292:SER:H	1.85	0.42
2:D:186:MET:SD	2:D:276:TYR:HA	2.59	0.42
2:F:105:LEU:HA	2:F:105:LEU:HD23	1.90	0.42
1:E:84:LEU:HD12	1:E:88:LEU:CD1	2.49	0.42
1:A:150:ASP:OD1	1:A:151:TYR:N	2.53	0.42
2:F:244:MET:HG3	2:F:275:VAL:HB	2.02	0.42
1:A:145:ASP:OD1	1:A:145:ASP:N	2.53	0.41
2:D:45:CYS:HA	2:D:48:ILE:CD1	2.49	0.41
2:D:89:TRP:CZ2	2:D:94:ILE:HD11	2.55	0.41
2:D:296:ARG:HB3	2:D:317:ARG:HH22	1.84	0.41
1:E:106:PRO:HG2	1:E:138:LEU:HD12	2.02	0.41
2:D:233:PHE:O	2:D:236:ASP:HB3	2.20	0.41
1:A:72:PHE:CE2	6:B:405:PAM:H22	2.55	0.41
2:D:70:ALA:HB2	2:D:98:LEU:HD21	2.02	0.41
1:E:76:VAL:CG1	1:E:85:MLY:HB3	2.48	0.41
1:E:95:ILE:N	1:E:95:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:104:VAL:HG21	2:F:106:ASP:HB2	2.03	0.41
2:B:88:ARG:HB3	2:B:283:PHE:HB2	2.02	0.41
2:D:242:SER:CB	2:D:269:PRO:HG3	2.51	0.41
1:E:46:ILE:HD13	1:E:48:TYR:CD1	2.55	0.41
1:E:36:GLN:HG2	1:E:51:THR:O	2.21	0.41
2:F:118:ILE:HD12	2:F:118:ILE:HA	1.88	0.41
2:D:248:MLY:HD2	2:D:255:TRP:CE3	2.56	0.41
2:F:138:ILE:CD1	2:F:139:CYS:HB2	2.50	0.41
2:F:282:ASN:OD1	2:F:284:CYS:HB2	2.21	0.41
1:C:42:LEU:C	1:C:43:CYS:SG	2.99	0.41
2:D:263:TYR:N	2:D:263:TYR:CD1	2.89	0.41
2:F:62:TYR:HB3	2:F:65:ILE:HD11	2.03	0.41
2:D:146:MLY:HE3	2:D:146:MLY:HB3	1.89	0.40
2:B:44:LEU:HD12	2:B:44:LEU:HA	1.84	0.40
1:A:62:GLN:HE21	1:A:62:GLN:HB2	1.64	0.40
1:C:129:TRP:HA	1:C:130:PRO:HD3	1.91	0.40
2:F:131:CYS:O	2:F:140:GLY:HA2	2.21	0.40
2:D:244:MET:HG3	2:D:275:VAL:HB	2.02	0.40
2:F:182:ALA:N	2:F:257:GLU:OE1	2.48	0.40
1:C:115:MLY:HB3	1:C:129:TRP:CE2	2.57	0.40
1:E:46:ILE:HD12	1:E:48:TYR:N	2.29	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ARG:NH2	1:E:123:ARG:O[1_455]	2.05	0.15
1:E:125:TYR:OH	1:E:125:TYR:OH[8_554]	2.13	0.07

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	113/141 (80%)	111 (98%)	2 (2%)	0	100	100
1	C	115/141 (82%)	113 (98%)	1 (1%)	1 (1%)	17	46
1	E	105/141 (74%)	100 (95%)	5 (5%)	0	100	100
2	B	294/319 (92%)	275 (94%)	18 (6%)	1 (0%)	41	72
2	D	288/319 (90%)	277 (96%)	10 (4%)	1 (0%)	41	72
2	F	258/319 (81%)	247 (96%)	11 (4%)	0	100	100
All	All	1173/1380 (85%)	1123 (96%)	47 (4%)	3 (0%)	41	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	CYS
2	D	338	CYS
1	C	123	ARG

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	103/118 (87%)	103 (100%)	0	100	100
1	C	104/118 (88%)	101 (97%)	3 (3%)	42	76
1	E	89/118 (75%)	86 (97%)	3 (3%)	37	71
2	B	249/252 (99%)	244 (98%)	5 (2%)	55	84
2	D	246/252 (98%)	239 (97%)	7 (3%)	43	77
2	F	199/252 (79%)	196 (98%)	3 (2%)	65	89
All	All	990/1110 (89%)	969 (98%)	21 (2%)	53	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	130	SER
2	B	214	SER

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Mol	Chain	Res	Type
2	B	292	SER
2	B	341	SER
2	B	350	ASP
1	C	67	LEU
1	C	123	ARG
1	C	151	TYR
2	D	120	SER
2	D	179	ARG
2	D	226	ASP
2	D	287	ASN
2	D	296	ARG
2	D	337	CYS
2	D	347	ARG
1	E	80	CYS
1	E	121	LEU
1	E	141	GLN
2	F	57	ARG
2	F	130	SER
2	F	139	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
2	D	287	ASN
1	E	56	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

65 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLY	D	188	2	7,8,11	0.65	0	3,8,13	0.17	0
2	MLY	D	262	2	7,8,11	0.43	0	3,8,13	0.30	0
2	MLY	B	205	2	7,8,11	0.57	0	3,8,13	0.40	0
2	MLY	D	154	2	7,8,11	0.44	0	3,8,13	0.28	0
2	MLY	B	327	2	7,8,11	0.48	0	3,8,13	0.61	0
2	MLY	B	146	2	7,8,11	0.62	0	3,8,13	0.26	0
1	MLY	A	102	1	7,8,11	0.52	0	3,8,13	0.49	0
2	MLY	D	54	2	7,8,11	0.45	0	3,8,13	0.29	0
2	MLY	F	154	2	9,10,11	0.65	0	6,11,13	0.67	0
2	MLY	D	218	2	7,8,11	0.59	0	3,8,13	0.27	0
2	MLY	B	325	2	7,8,11	0.59	0	3,8,13	1.49	1 (33%)
2	MLY	B	235	2	7,8,11	0.56	0	3,8,13	0.27	0
2	MLY	F	267	2	7,8,11	0.49	0	3,8,13	0.67	0
1	MLY	A	115	1	7,8,11	0.50	0	3,8,13	0.44	0
2	MLY	B	262	2	9,10,11	0.48	0	6,11,13	1.00	0
2	MLY	D	107	2	7,8,11	0.53	0	3,8,13	0.59	0
2	MLY	D	355	2	5,9,11	0.29	0	4,10,13	0.35	0
1	MLY	C	44	1	7,8,11	0.78	0	3,8,13	0.66	0
2	MLY	D	205	2	7,8,11	0.49	0	3,8,13	0.49	0
2	MLY	D	237	2	7,8,11	0.50	0	3,8,13	0.23	0
1	MLY	E	115	1	3,4,11	0.63	0	2,4,13	0.81	0
1	MLY	E	44	1	7,8,11	0.60	0	3,8,13	0.40	0
2	MLY	D	248	2	7,8,11	0.45	0	3,8,13	0.46	0
1	MLY	C	102	1	9,10,11	0.56	0	6,11,13	0.75	0
1	MLY	C	85	1	9,10,11	0.57	0	6,11,13	0.82	0
2	MLY	B	248	2	7,8,11	0.47	0	3,8,13	0.44	0
1	MLY	A	85	1	9,10,11	0.60	0	6,11,13	0.78	0
2	MLY	F	107	2	7,8,11	0.53	0	3,8,13	0.27	0
2	MLY	D	207	2	7,8,11	0.66	0	3,8,13	0.52	0
2	MLY	F	188	2	9,10,11	0.59	0	6,11,13	0.88	0
2	MLY	B	329	2	7,8,11	0.43	0	3,8,13	0.52	0
2	MLY	B	188	2	7,8,11	0.54	0	3,8,13	0.24	0
2	MLY	F	54	2	9,10,11	0.75	0	6,11,13	0.74	0
2	MLY	B	74	2	7,8,11	0.55	0	3,8,13	0.39	0
2	MLY	B	355	2	9,10,11	0.52	0	6,11,13	0.87	0
2	MLY	B	54	2	7,8,11	0.53	0	3,8,13	0.46	0
2	MLY	B	237	2	7,8,11	0.54	0	3,8,13	0.24	0
2	MLY	B	218	2	7,8,11	0.37	0	3,8,13	0.81	0
2	MLY	B	267	2	7,8,11	0.54	0	3,8,13	0.37	0
2	MLY	F	218	2	7,8,11	0.60	0	3,8,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	44	1	7,8,11	0.53	0	3,8,13	0.26	0
2	MLY	F	235	2	7,8,11	0.60	0	3,8,13	0.27	0
1	MLY	E	101	1	7,8,11	0.52	0	3,8,13	0.34	0
2	MLY	F	207	2	7,8,11	0.70	0	3,8,13	0.84	0
1	MLY	E	85	1	7,8,11	0.46	0	3,8,13	0.32	0
2	MLY	D	235	2	7,8,11	0.55	0	3,8,13	0.23	0
2	MLY	D	74	2	9,10,11	0.73	0	6,11,13	0.89	0
2	MLY	F	248	2	9,10,11	0.55	0	6,11,13	0.62	0
2	MLY	D	146	2	7,8,11	0.45	0	3,8,13	0.44	0
2	MLY	D	329	2	7,8,11	0.49	0	3,8,13	0.28	0
1	MLY	A	101	1	7,8,11	0.45	0	3,8,13	0.40	0
1	MLY	C	115	1	7,8,11	0.57	0	3,8,13	0.38	0
2	MLY	F	205	2	7,8,11	0.55	0	3,8,13	0.35	0
2	MLY	F	237	2	7,8,11	0.45	0	3,8,13	0.37	0
2	MLY	B	154	2	7,8,11	0.53	0	3,8,13	0.30	0
2	MLY	B	107	2	9,10,11	0.64	0	6,11,13	1.28	1 (16%)
2	MLY	D	325	2	7,8,11	0.57	0	3,8,13	0.35	0
1	MLY	C	101	1	9,10,11	0.50	0	6,11,13	1.10	0
2	MLY	B	207	2	7,8,11	0.56	0	3,8,13	0.45	0
1	MLY	C	31	1	7,8,11	0.49	0	3,8,13	0.33	0
2	MLY	F	74	2	7,8,11	0.64	0	3,8,13	0.25	0
2	MLY	D	327	2	7,8,11	0.52	0	3,8,13	0.49	0
2	MLY	D	267	2	7,8,11	0.58	0	3,8,13	0.50	0
2	MLY	F	262	2	7,8,11	0.46	0	3,8,13	0.40	0
1	MLY	E	102	1	7,8,11	0.45	0	3,8,13	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
2	MLY	D	188	2	-	2/6/7/11	-
2	MLY	D	262	2	-	2/6/7/11	-
2	MLY	B	205	2	-	1/6/7/11	-
2	MLY	D	154	2	-	1/6/7/11	-
2	MLY	B	327	2	-	2/6/7/11	-
2	MLY	B	146	2	-	2/6/7/11	-
1	MLY	A	102	1	-	1/6/7/11	-
2	MLY	D	54	2	-	0/6/7/11	-
2	MLY	F	154	2	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	D	218	2	-	1/6/7/11	-
2	MLY	B	325	2	-	0/6/7/11	-
2	MLY	B	235	2	-	1/6/7/11	-
2	MLY	F	267	2	-	2/6/7/11	-
1	MLY	A	115	1	-	0/6/7/11	-
2	MLY	B	262	2	-	2/8/9/11	-
2	MLY	D	107	2	-	2/6/7/11	-
2	MLY	D	355	2	-	0/5/9/11	-
1	MLY	C	44	1	-	0/6/7/11	-
2	MLY	D	205	2	-	0/6/7/11	-
2	MLY	D	237	2	-	0/6/7/11	-
1	MLY	E	115	1	-	0/0/2/11	-
1	MLY	E	44	1	-	2/6/7/11	-
2	MLY	D	248	2	-	3/6/7/11	-
1	MLY	C	102	1	-	1/8/9/11	-
1	MLY	C	85	1	-	2/8/9/11	-
2	MLY	B	248	2	-	0/6/7/11	-
1	MLY	A	85	1	-	3/8/9/11	-
2	MLY	F	107	2	-	0/6/7/11	-
2	MLY	D	207	2	-	1/6/7/11	-
2	MLY	F	188	2	-	4/8/9/11	-
2	MLY	B	329	2	-	0/6/7/11	-
2	MLY	B	188	2	-	1/6/7/11	-
2	MLY	F	54	2	-	2/8/9/11	-
2	MLY	B	74	2	-	1/6/7/11	-
2	MLY	B	355	2	-	0/8/9/11	-
2	MLY	B	54	2	-	0/6/7/11	-
2	MLY	B	237	2	-	1/6/7/11	-
2	MLY	B	218	2	-	4/6/7/11	-
2	MLY	B	267	2	-	0/6/7/11	-
2	MLY	F	218	2	-	0/6/7/11	-
1	MLY	A	44	1	-	2/6/7/11	-
2	MLY	F	235	2	-	1/6/7/11	-
1	MLY	E	101	1	-	2/6/7/11	-
2	MLY	F	207	2	-	2/6/7/11	-
1	MLY	E	85	1	-	2/6/7/11	-
2	MLY	D	235	2	-	0/6/7/11	-
2	MLY	D	74	2	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	F	248	2	-	2/8/9/11	-
2	MLY	D	146	2	-	3/6/7/11	-
2	MLY	D	329	2	-	0/6/7/11	-
1	MLY	A	101	1	-	2/6/7/11	-
1	MLY	C	115	1	-	3/6/7/11	-
2	MLY	F	205	2	-	4/6/7/11	-
2	MLY	F	237	2	-	1/6/7/11	-
2	MLY	B	154	2	-	0/6/7/11	-
2	MLY	B	107	2	-	3/8/9/11	-
2	MLY	D	325	2	-	0/6/7/11	-
1	MLY	C	101	1	-	4/8/9/11	-
2	MLY	B	207	2	-	2/6/7/11	-
1	MLY	C	31	1	-	1/6/7/11	-
2	MLY	F	74	2	-	0/6/7/11	-
2	MLY	D	327	2	-	1/6/7/11	-
2	MLY	D	267	2	-	3/6/7/11	-
2	MLY	F	262	2	-	2/6/7/11	-
1	MLY	E	102	1	-	2/6/7/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	325	MLY	CD-CG-CB	-2.54	104.63	113.62
2	B	107	MLY	CD-CE-NZ	-2.33	107.49	113.79

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	188	MLY	C-CA-CB-CG
2	B	205	MLY	C-CA-CB-CG
2	B	327	MLY	O-C-CA-CB
2	B	146	MLY	O-C-CA-CB
1	E	102	MLY	O-C-CA-CB
2	F	267	MLY	N-CA-CB-CG
2	F	267	MLY	C-CA-CB-CG
2	D	107	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	D	107	MLY	C-CA-CB-CG
2	D	207	MLY	O-C-CA-CB
2	F	188	MLY	C-CA-CB-CG
2	F	54	MLY	N-CA-CB-CG
2	F	54	MLY	C-CA-CB-CG
2	B	74	MLY	C-CA-CB-CG
2	B	237	MLY	O-C-CA-CB
2	B	218	MLY	N-CA-CB-CG
2	B	218	MLY	C-CA-CB-CG
2	B	218	MLY	O-C-CA-CB
2	F	235	MLY	O-C-CA-CB
1	E	101	MLY	O-C-CA-CB
2	F	207	MLY	N-CA-CB-CG
2	F	207	MLY	C-CA-CB-CG
2	D	74	MLY	C-CA-CB-CG
2	F	248	MLY	O-C-CA-CB
2	D	146	MLY	C-CA-CB-CG
2	D	146	MLY	O-C-CA-CB
1	A	101	MLY	O-C-CA-CB
1	C	115	MLY	C-CA-CB-CG
2	B	107	MLY	O-C-CA-CB
1	C	101	MLY	O-C-CA-CB
2	B	207	MLY	O-C-CA-CB
2	D	327	MLY	C-CA-CB-CG
2	B	262	MLY	CD-CE-NZ-CH2
1	A	85	MLY	CD-CE-NZ-CH1
1	A	85	MLY	CD-CE-NZ-CH2
2	B	107	MLY	CD-CE-NZ-CH1
2	B	107	MLY	CD-CE-NZ-CH2
1	C	101	MLY	CD-CE-NZ-CH1
1	C	101	MLY	CD-CE-NZ-CH2
1	E	102	MLY	CA-CB-CG-CD
2	F	237	MLY	CA-CB-CG-CD
2	D	267	MLY	CA-CB-CG-CD
1	C	102	MLY	CD-CE-NZ-CH2
2	D	146	MLY	CA-CB-CG-CD
1	A	101	MLY	CA-CB-CG-CD
2	B	207	MLY	CE-CD-CG-CB
2	D	218	MLY	CE-CD-CG-CB
1	E	44	MLY	CE-CD-CG-CB
1	A	85	MLY	CE-CD-CG-CB
1	A	44	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	F	188	MLY	CE-CD-CG-CB
2	B	146	MLY	CA-CB-CG-CD
1	C	85	MLY	CE-CD-CG-CB
2	D	248	MLY	CA-CB-CG-CD
1	E	85	MLY	C-CA-CB-CG
2	D	267	MLY	C-CA-CB-CG
2	F	154	MLY	CE-CD-CG-CB
2	F	205	MLY	CG-CD-CE-NZ
2	D	262	MLY	CE-CD-CG-CB
1	C	31	MLY	CA-CB-CG-CD
1	C	85	MLY	CD-CE-NZ-CH2
1	E	85	MLY	CE-CD-CG-CB
2	F	262	MLY	CE-CD-CG-CB
2	D	154	MLY	CE-CD-CG-CB
2	D	262	MLY	CG-CD-CE-NZ
2	F	248	MLY	CD-CE-NZ-CH2
2	B	218	MLY	CE-CD-CG-CB
2	D	267	MLY	CE-CD-CG-CB
1	C	115	MLY	N-CA-CB-CG
2	F	205	MLY	N-CA-CB-CG
1	E	44	MLY	C-CA-CB-CG
2	F	205	MLY	C-CA-CB-CG
1	A	102	MLY	CG-CD-CE-NZ
2	F	188	MLY	CG-CD-CE-NZ
2	D	248	MLY	CE-CD-CG-CB
2	D	74	MLY	CA-CB-CG-CD
2	B	327	MLY	CE-CD-CG-CB
2	B	262	MLY	CD-CE-NZ-CH1
2	F	205	MLY	CE-CD-CG-CB
1	C	101	MLY	CG-CD-CE-NZ
2	D	248	MLY	CG-CD-CE-NZ
1	A	44	MLY	CG-CD-CE-NZ
1	C	115	MLY	CE-CD-CG-CB
2	F	188	MLY	CA-CB-CG-CD
2	B	188	MLY	CG-CD-CE-NZ
2	F	262	MLY	CG-CD-CE-NZ
2	B	235	MLY	CE-CD-CG-CB
2	D	188	MLY	N-CA-CB-CG
1	E	101	MLY	N-CA-CB-CG

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	102	MLY	2	0
2	B	325	MLY	1	0
2	D	107	MLY	3	0
2	D	237	MLY	1	0
2	D	248	MLY	1	0
2	F	107	MLY	1	0
2	B	329	MLY	1	0
2	B	355	MLY	2	0
2	B	54	MLY	1	0
2	B	218	MLY	1	0
1	E	85	MLY	2	0
2	F	248	MLY	1	0
2	D	146	MLY	1	0
1	C	115	MLY	1	0
2	F	237	MLY	1	0
2	D	325	MLY	1	0
1	C	101	MLY	1	0
2	D	267	MLY	3	0
1	E	102	MLY	1	0

5.5 Carbohydrates

4 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	G	1	3,2	14,14,15	0.82	0	17,19,21	1.31	3 (17%)
3	NAG	G	2	3	14,14,15	0.93	0	17,19,21	2.26	4 (23%)
3	NAG	H	1	3,2	14,14,15	0.81	0	17,19,21	1.83	5 (29%)
3	NAG	H	2	3	14,14,15	1.03	1 (7%)	17,19,21	1.11	2 (11%)

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	G	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	5/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	C8-C7	2.33	1.55	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C2-N2-C7	6.84	132.64	122.90
3	H	1	NAG	C1-C2-N2	4.33	117.89	110.49
3	G	2	NAG	O5-C1-C2	-3.15	106.32	111.29
3	G	2	NAG	C8-C7-N2	3.07	121.30	116.10
3	H	1	NAG	C1-O5-C5	-2.90	108.26	112.19
3	G	2	NAG	C1-C2-N2	2.80	115.26	110.49
3	H	1	NAG	C2-N2-C7	2.78	126.86	122.90
3	H	1	NAG	O5-C5-C6	-2.73	102.93	107.20
3	G	1	NAG	C2-N2-C7	2.61	126.63	122.90
3	H	2	NAG	O5-C5-C6	-2.53	103.25	107.20
3	G	1	NAG	C1-O5-C5	2.38	115.42	112.19
3	H	2	NAG	C1-C2-N2	2.34	114.49	110.49
3	H	1	NAG	C3-C4-C5	2.15	114.07	110.24
3	G	1	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

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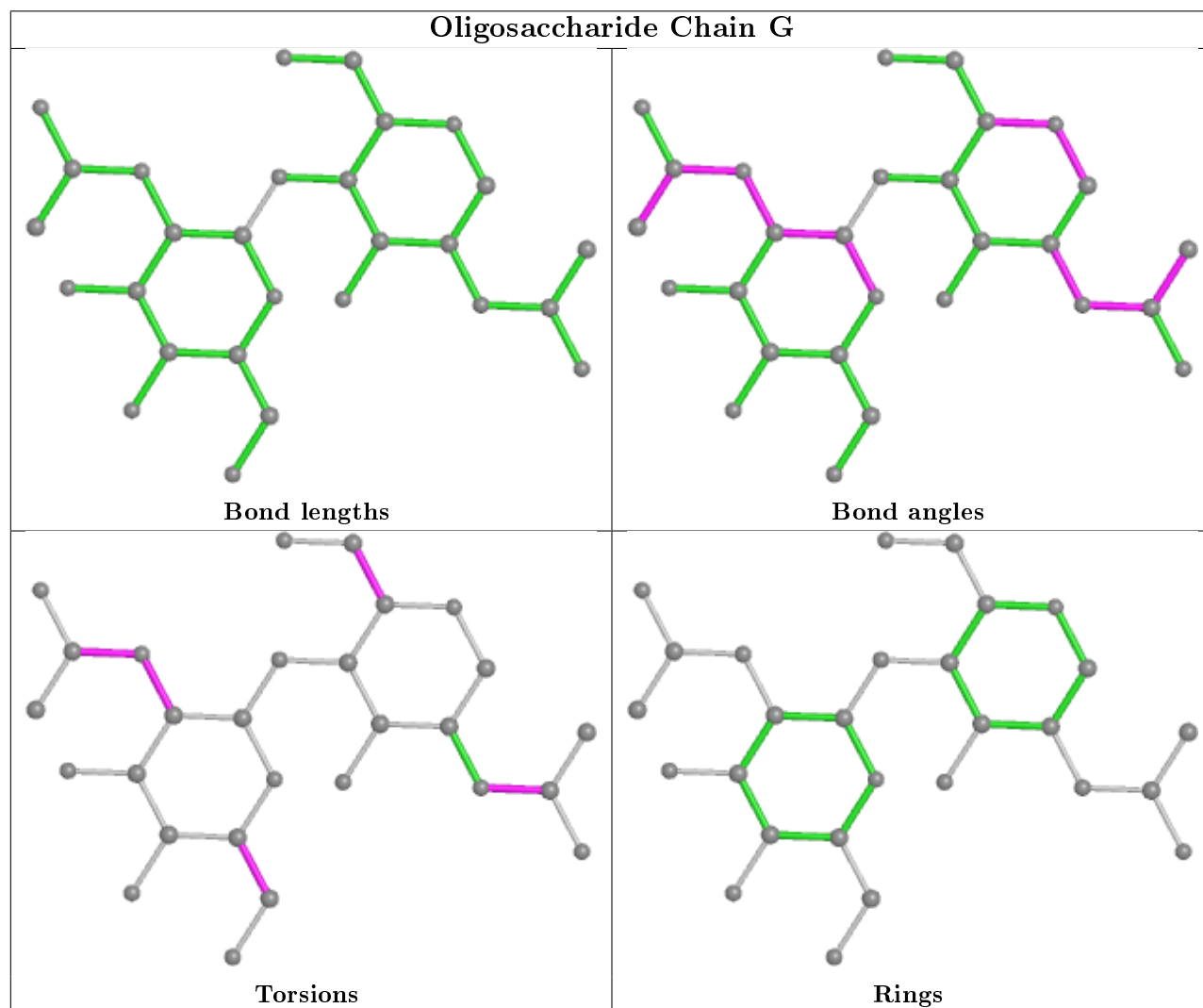
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7

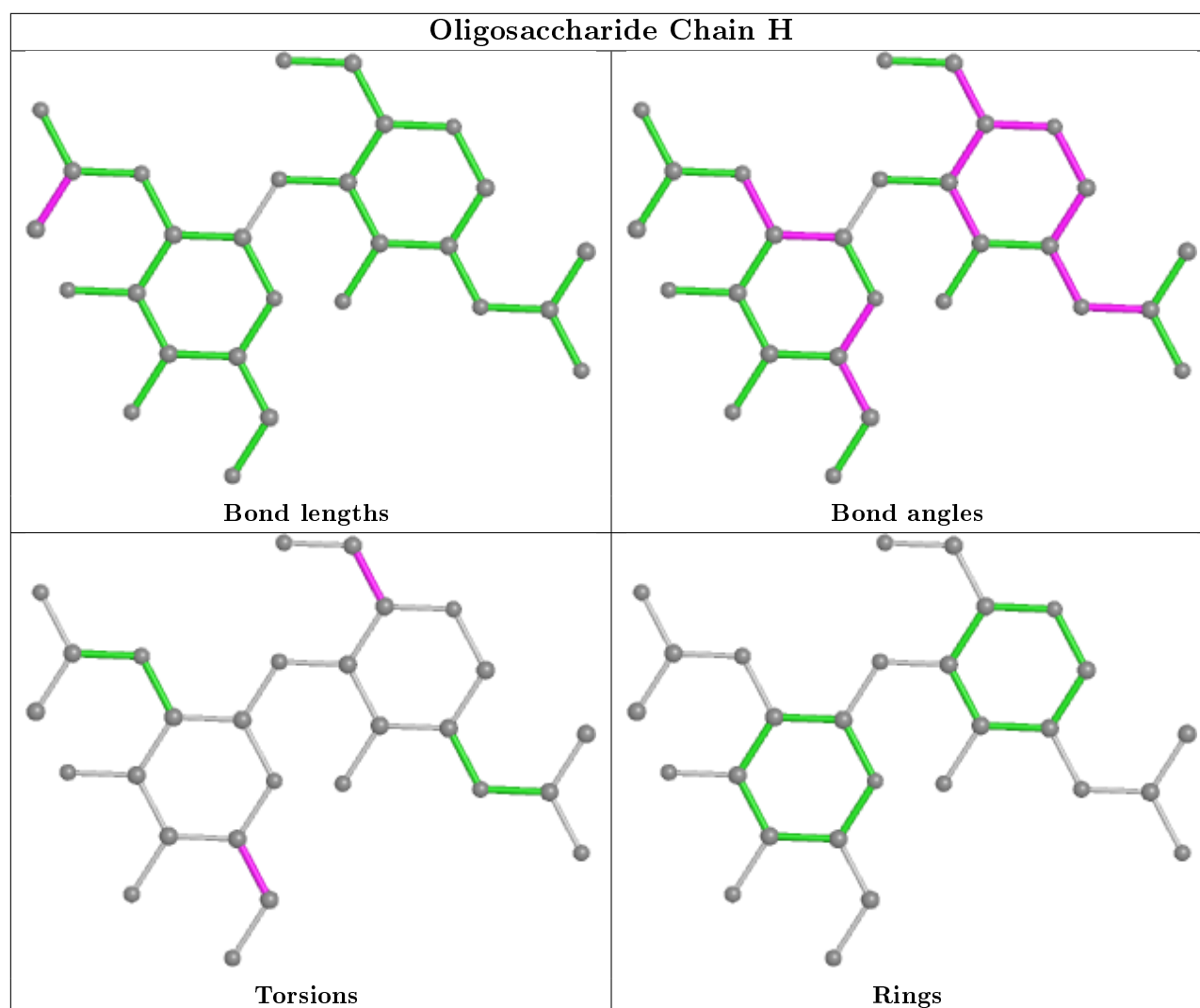
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	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 ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
6	PAM	D	404	2	7,7,17	0.58	0	6,6,17	0.90	0
4	NAG	F	500	2	14,14,15	0.84	0	17,19,21	1.38	3 (17%)
4	NAG	D	403	2	14,14,15	0.81	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	404	2	14,14,15	0.79	0	17,19,21	0.87	0
4	NAG	C	500	1	14,14,15	0.79	0	17,19,21	0.92	0
6	PAM	B	405	2	16,16,17	0.85	1 (6%)	15,15,17	0.80	0
4	NAG	E	500	1	14,14,15	0.81	0	17,19,21	0.87	0
4	NAG	A	500	1	14,14,15	0.82	0	17,19,21	0.92	1 (5%)

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
6	PAM	D	404	2	-	2/4/5/15	-
4	NAG	F	500	2	-	2/6/23/26	0/1/1/1
4	NAG	D	403	2	-	2/6/23/26	0/1/1/1
4	NAG	B	404	2	-	0/6/23/26	0/1/1/1
4	NAG	C	500	1	-	0/6/23/26	0/1/1/1
6	PAM	B	405	2	-	8/14/14/15	-
4	NAG	E	500	1	-	0/6/23/26	0/1/1/1
4	NAG	A	500	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	405	PAM	O1-C1	-3.15	1.25	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	500	NAG	C1-O5-C5	3.03	116.30	112.19
4	A	500	NAG	C4-C3-C2	-2.80	106.92	111.02
4	F	500	NAG	O5-C5-C6	-2.46	103.34	107.20
4	F	500	NAG	C6-C5-C4	-2.38	107.42	113.00

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	403	NAG	O5-C5-C6-O6
4	D	403	NAG	C4-C5-C6-O6

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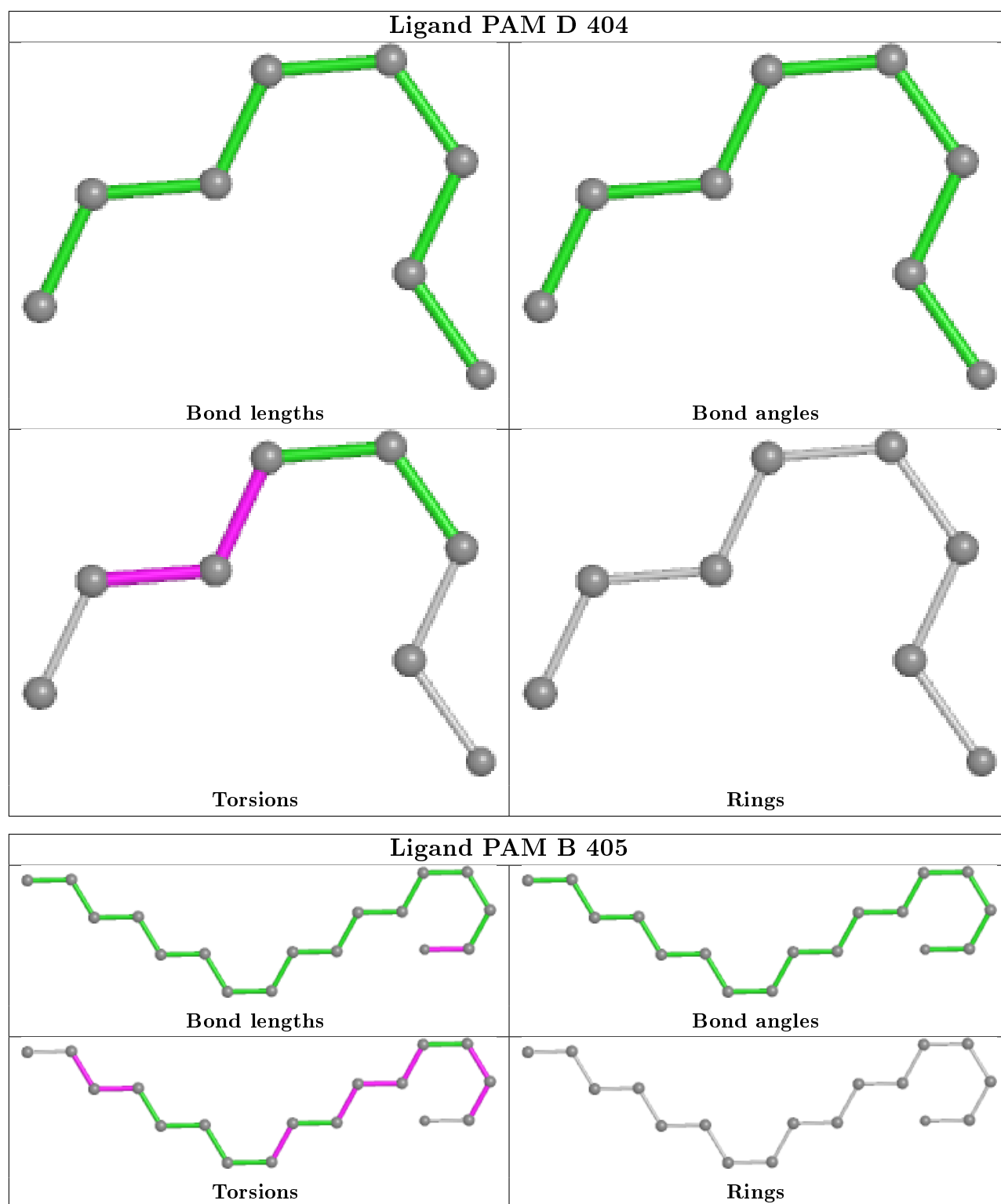
Mol	Chain	Res	Type	Atoms
6	B	405	PAM	C3-C4-C5-C6
6	D	404	PAM	C3-C4-C5-C6
6	B	405	PAM	C5-C6-C7-C8
4	A	500	NAG	C4-C5-C6-O6
4	F	500	NAG	C4-C5-C6-O6
6	B	405	PAM	C4-C5-C6-C7
6	D	404	PAM	C4-C5-C6-C7
6	B	405	PAM	C13-C14-C15-C16
4	F	500	NAG	O5-C5-C6-O6
6	B	405	PAM	C12-C13-C14-C15
6	B	405	PAM	C1-C2-C3-C4
4	A	500	NAG	O5-C5-C6-O6
6	B	405	PAM	O1-C1-C2-C3
6	B	405	PAM	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	404	PAM	1	0
6	B	405	PAM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	115/141 (81%)	-0.33	0	100 100	53, 76, 113, 131	0
1	C	116/141 (82%)	-0.16	0	100 100	52, 81, 132, 170	0
1	E	107/141 (75%)	0.56	13 (12%)	4 2	84, 147, 191, 204	0
2	B	295/319 (92%)	-0.12	3 (1%)	82 77	43, 77, 136, 200	0
2	D	291/319 (91%)	-0.14	5 (1%)	70 63	50, 89, 164, 192	0
2	F	262/319 (82%)	-0.13	4 (1%)	73 68	51, 79, 147, 184	0
All	All	1186/1380 (85%)	-0.09	25 (2%)	63 54	43, 84, 166, 204	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	GLY	8.2
1	E	34	ALA	7.2
2	B	288	PRO	4.1
1	E	104	LEU	4.1
1	E	144	PRO	4.0
1	E	52	TYR	3.8
1	E	100	TYR	3.7
1	E	35	CYS	3.5
1	E	141	GLN	3.3
2	F	306	GLY	3.3
1	E	91	MET	3.1
1	E	139	PRO	3.1
2	B	293	PHE	3.0
2	F	305	HIS	3.0
1	E	97	LEU	2.9
2	D	50	GLY	2.8
1	E	99	ASP	2.6
2	F	301	ASN	2.5
2	D	289	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	253	ARG	2.2
2	D	179	ARG	2.2
2	D	291	GLY	2.1
2	B	347	ARG	2.1
1	E	133	MET	2.0
2	F	86	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLY	D	267	9/12	0.70	0.32	151,155,162,162	0
1	MLY	E	85	9/12	0.76	0.35	111,125,135,135	0
2	MLY	D	248	9/12	0.76	0.19	139,148,154,155	0
2	MLY	B	146	9/12	0.81	0.26	126,132,139,140	0
1	MLY	C	31	9/12	0.84	0.34	130,137,140,149	0
2	MLY	D	146	9/12	0.84	0.23	80,105,122,123	0
1	MLY	E	102	9/12	0.85	0.29	148,150,161,171	0
2	MLY	D	355	10/12	0.86	0.20	98,105,128,131	0
2	MLY	D	54	9/12	0.88	0.26	108,117,137,138	0
2	MLY	B	327	9/12	0.90	0.27	110,116,124,126	0
2	MLY	D	262	9/12	0.90	0.19	107,110,131,133	0
2	MLY	D	107	9/12	0.91	0.16	133,146,161,165	0
2	MLY	F	218	9/12	0.91	0.22	88,98,113,114	0
2	MLY	B	325	9/12	0.91	0.36	130,139,157,158	0
2	MLY	D	237	9/12	0.92	0.20	70,77,90,93	0
1	MLY	A	102	9/12	0.92	0.13	79,85,91,91	0
2	MLY	B	267	9/12	0.93	0.18	74,83,111,114	0
2	MLY	B	329	9/12	0.93	0.24	93,101,104,105	0
1	MLY	E	101	9/12	0.93	0.33	123,132,146,168	0
2	MLY	B	355	11/12	0.93	0.25	98,102,107,108	0
1	MLY	A	44	9/12	0.94	0.22	63,81,99,100	0
2	MLY	B	207	9/12	0.94	0.13	52,54,85,86	0
2	MLY	D	325	9/12	0.94	0.14	60,66,82,84	0
2	MLY	F	248	11/12	0.94	0.20	52,59,98,106	0
2	MLY	F	154	11/12	0.94	0.19	93,98,108,109	0
2	MLY	F	207	9/12	0.95	0.19	68,76,92,105	0
2	MLY	D	188	9/12	0.95	0.18	69,80,85,90	0

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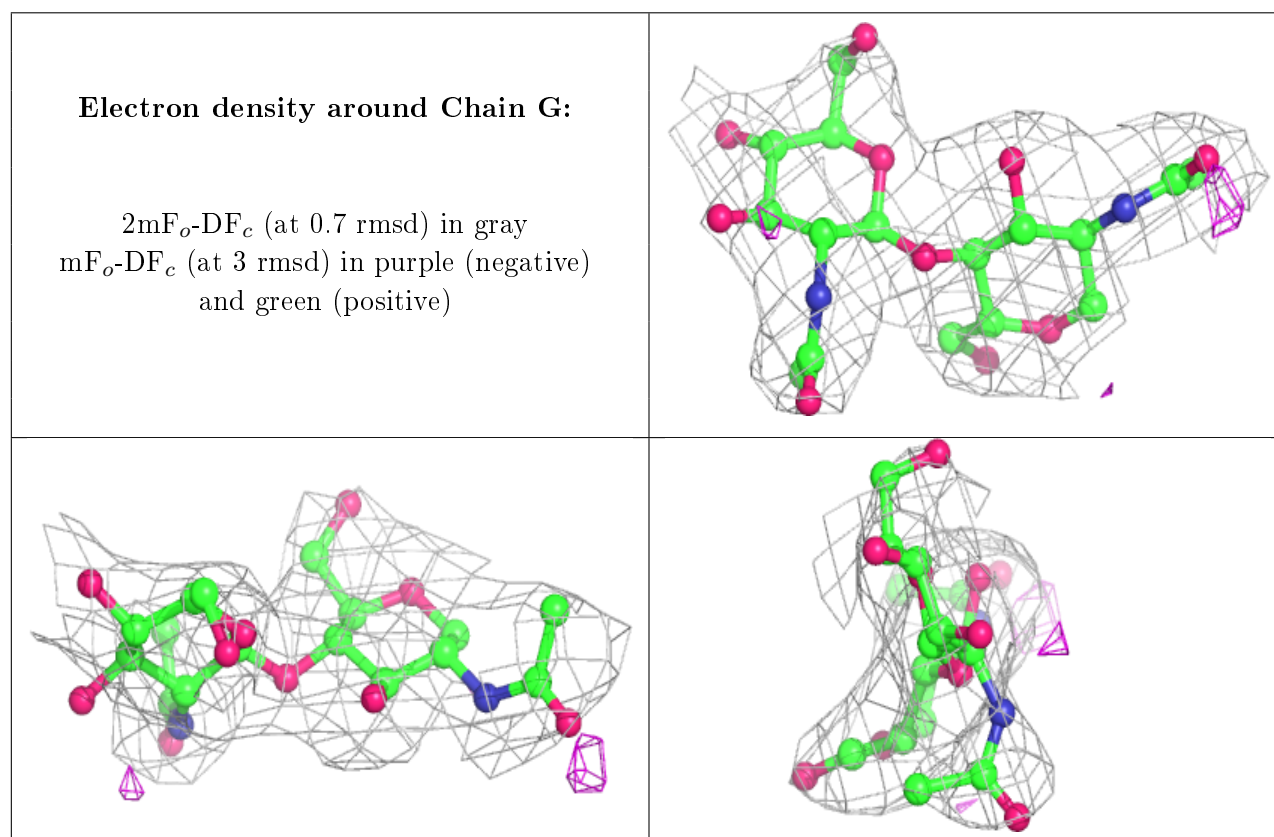
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MLY	F	54	11/12	0.95	0.22	61,76,111,117	0
1	MLY	E	44	9/12	0.95	0.17	93,100,111,122	0
2	MLY	D	329	9/12	0.95	0.12	74,77,91,95	0
2	MLY	F	205	9/12	0.95	0.18	66,84,97,104	0
2	MLY	B	218	9/12	0.95	0.14	59,67,73,76	0
2	MLY	F	267	9/12	0.95	0.16	71,82,85,87	0
1	MLY	C	102	11/12	0.95	0.22	91,98,108,110	0
1	MLY	A	85	11/12	0.95	0.19	46,62,75,79	0
2	MLY	F	107	9/12	0.95	0.19	64,78,86,100	0
2	MLY	D	205	9/12	0.96	0.18	45,72,90,95	0
2	MLY	D	207	9/12	0.96	0.15	51,61,72,74	0
2	MLY	F	188	11/12	0.96	0.25	54,62,91,96	0
2	MLY	D	74	11/12	0.96	0.29	52,73,106,106	0
2	MLY	B	205	9/12	0.96	0.14	47,52,77,79	0
2	MLY	B	188	9/12	0.96	0.21	56,69,96,98	0
1	MLY	E	115	5/12	0.96	0.11	152,157,163,165	0
1	MLY	A	101	9/12	0.96	0.14	68,80,100,101	0
1	MLY	C	115	9/12	0.96	0.19	70,85,92,98	0
1	MLY	A	115	9/12	0.96	0.16	55,62,69,78	0
2	MLY	B	154	9/12	0.96	0.21	65,73,95,99	0
2	MLY	B	107	11/12	0.96	0.24	65,83,108,120	0
2	MLY	B	54	9/12	0.96	0.22	60,72,84,89	0
2	MLY	B	262	11/12	0.96	0.12	73,79,102,105	0
2	MLY	D	218	9/12	0.96	0.17	65,70,76,77	0
2	MLY	D	327	9/12	0.96	0.22	78,85,101,101	0
2	MLY	B	248	9/12	0.96	0.21	90,103,117,118	0
2	MLY	F	262	9/12	0.96	0.13	62,67,74,80	0
2	MLY	D	154	9/12	0.96	0.18	64,73,98,100	0
2	MLY	F	235	9/12	0.97	0.17	70,79,92,95	0
1	MLY	C	101	11/12	0.97	0.11	73,82,94,97	0
2	MLY	B	237	9/12	0.97	0.18	53,56,67,70	0
1	MLY	C	44	9/12	0.97	0.15	59,74,85,87	0
2	MLY	F	74	9/12	0.97	0.15	60,64,84,92	0
2	MLY	B	74	9/12	0.97	0.17	44,61,94,101	0
2	MLY	D	235	9/12	0.97	0.15	65,77,89,93	0
1	MLY	C	85	11/12	0.97	0.18	56,65,82,85	0
2	MLY	B	235	9/12	0.97	0.20	56,63,71,82	0
2	MLY	F	237	9/12	0.98	0.18	64,67,85,88	0

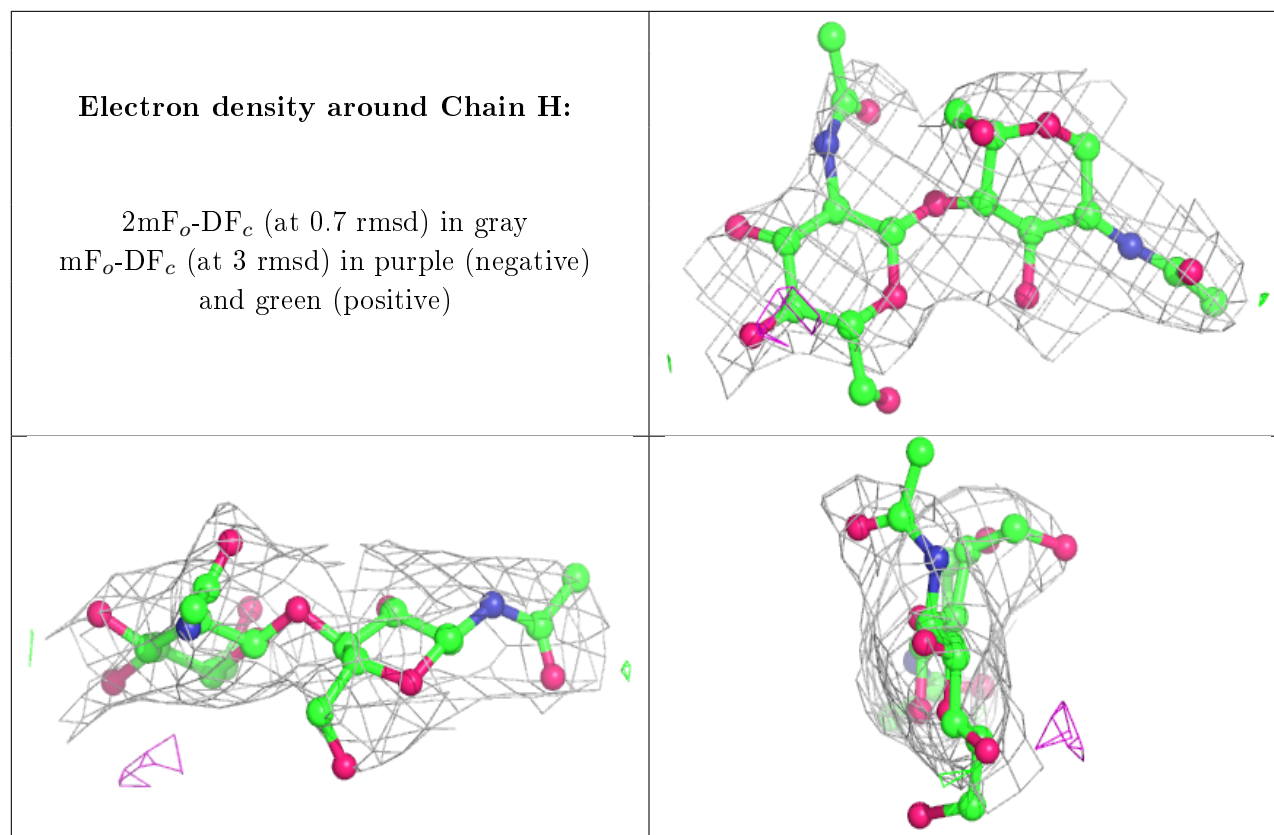
6.3 Carbohydrates ⓘ

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	NAG	G	2	14/15	0.82	0.30	119,125,128,129	0
3	NAG	H	2	14/15	0.86	0.29	102,108,112,113	14
3	NAG	H	1	14/15	0.94	0.16	53,71,99,102	0
3	NAG	G	1	14/15	0.95	0.15	59,69,94,97	0

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





6.4 Ligands ⓘ

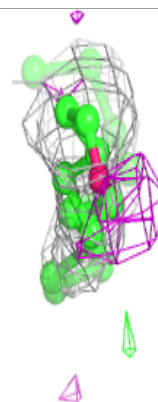
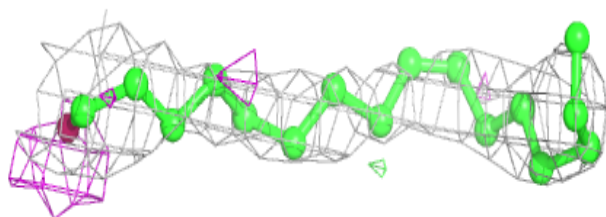
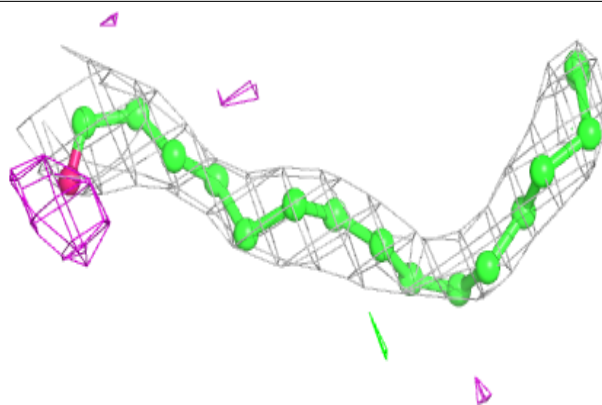
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	E	500	14/15	0.76	0.39	88,114,119,120	14
4	NAG	C	500	14/15	0.83	0.19	81,110,119,121	14
4	NAG	B	404	14/15	0.90	0.17	93,100,104,105	0
4	NAG	D	403	14/15	0.92	0.21	78,113,123,123	0
6	PAM	B	405	17/18	0.92	0.38	54,82,105,113	0
4	NAG	F	500	14/15	0.92	0.16	72,95,106,108	0
4	NAG	A	500	14/15	0.93	0.15	106,126,139,140	0
6	PAM	D	404	8/18	0.96	0.24	60,68,78,79	0
5	CL	B	401	1/1	0.98	0.22	31,31,31,31	1

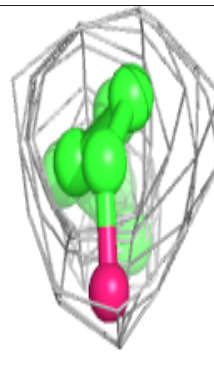
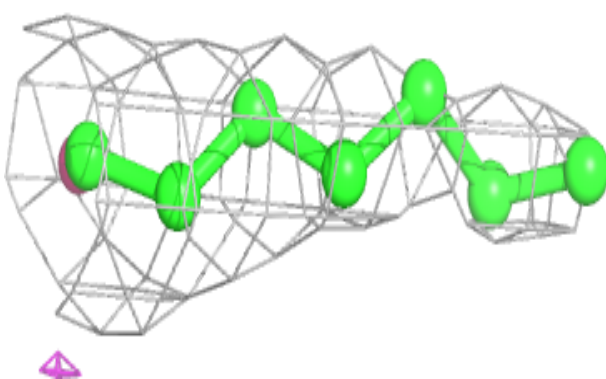
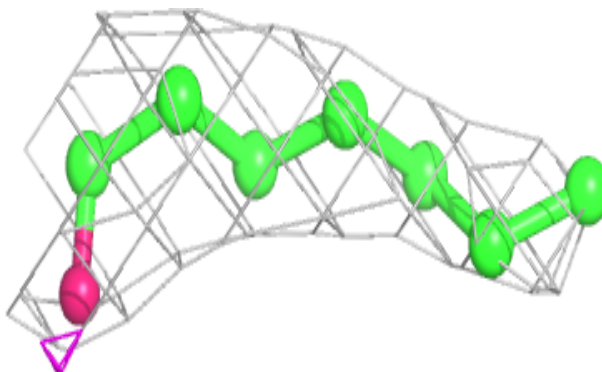
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAM B 405:

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

**Electron density around PAM D 404:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.