



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:05 AM UTC

PDB ID : 6AHY / pdb_00006ahy
Title : Wnt signaling complex
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Deposited on : 2018-08-21
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

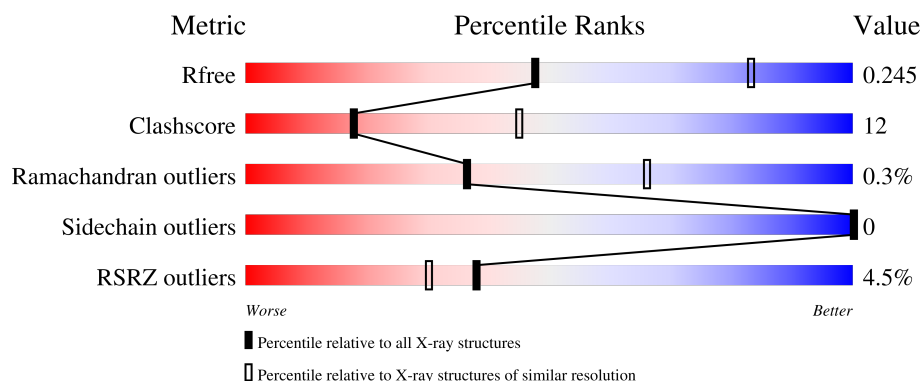
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



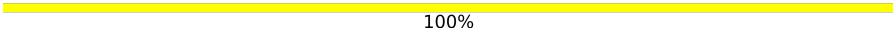
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 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	141	0% 68% 17% 15%
1	C	141	2% 65% 21% 13%
1	E	141	11% 47% 33% 21%
2	B	319	3% 77% 20%
2	D	319	4% 69% 27%

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Mol	Chain	Length	Quality of chain
2	F	319	
3	G	2	
3	H	2	

2 Entry composition [i](#)

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:

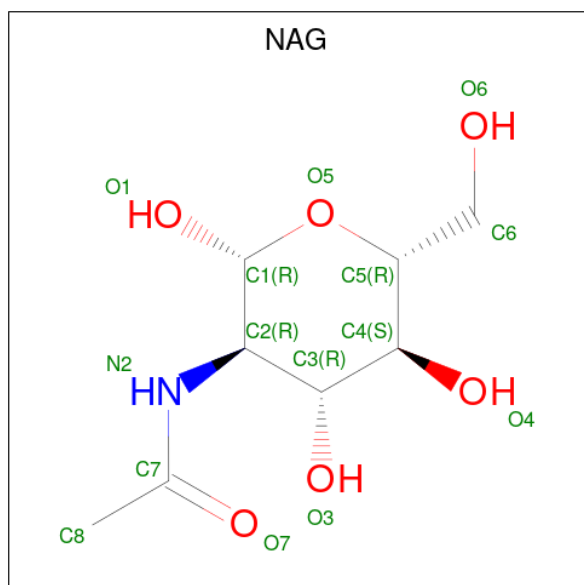
Chain	Residue	Modelled	Actual	Comment	Reference
B	37	GLY	-	expression tag	UNP P56703
B	38	MLY	-	expression tag	UNP P56703
B	39	ASP	-	expression tag	UNP P56703
B	40	GLY	-	expression tag	UNP P56703
B	41	SER	-	expression tag	UNP P56703
D	37	GLY	-	expression tag	UNP P56703
D	38	MLY	-	expression tag	UNP P56703
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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

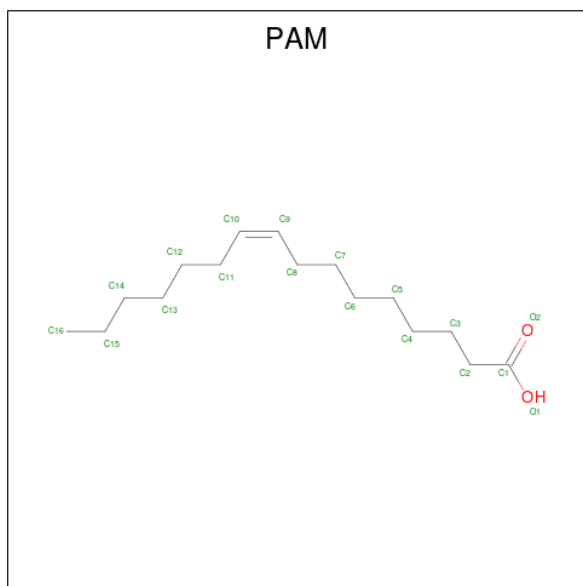


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

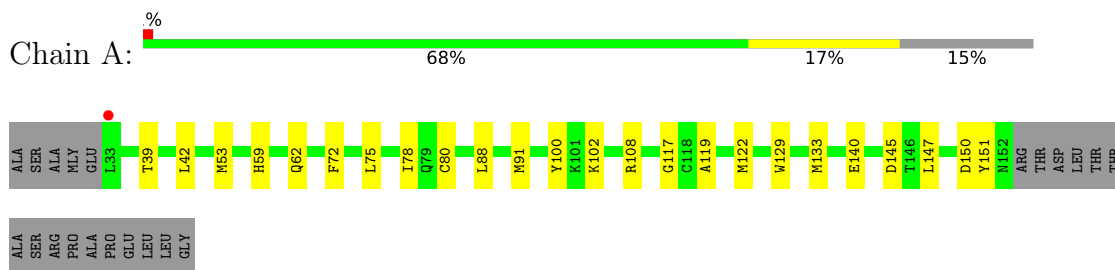


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			17	16	1		
6	D	1	Total	C	O	0	0
			8	7	1		

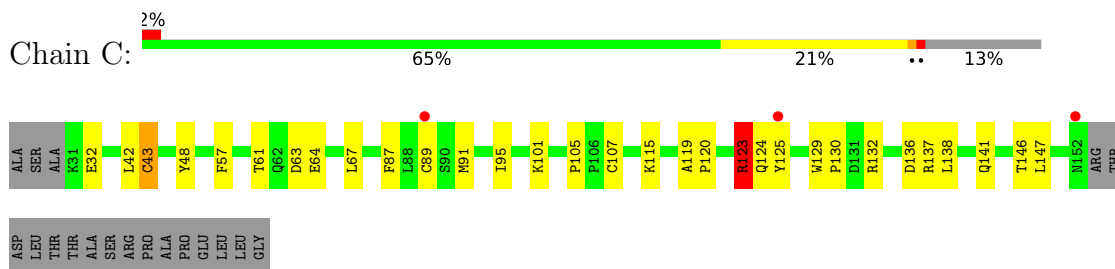
3 Residue-property plots

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.

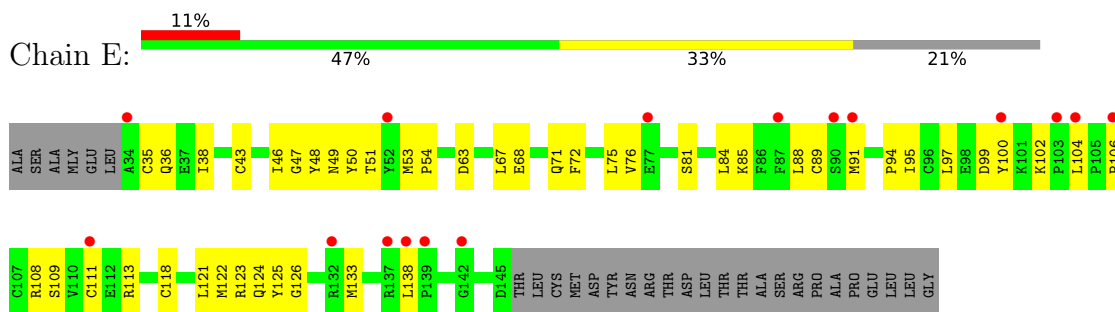
- Molecule 1: Frizzled-8



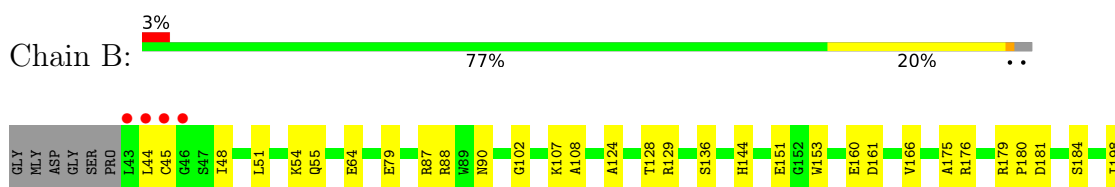
- Molecule 1: Frizzled-8

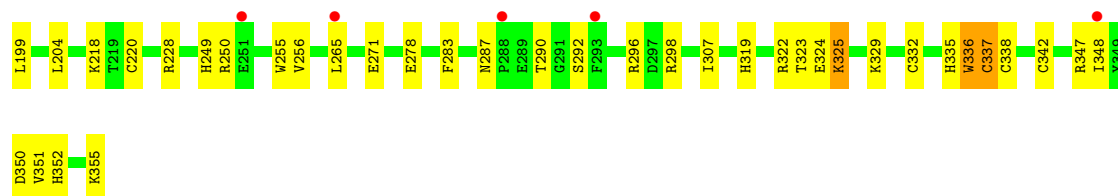


- Molecule 1: Frizzled-8

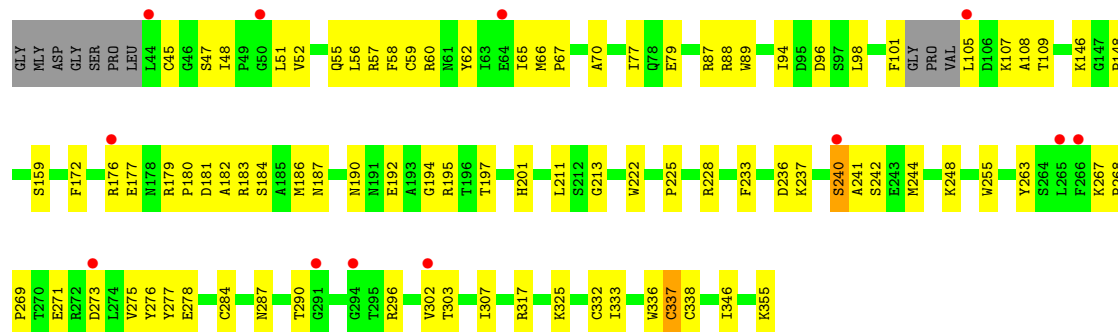


- Molecule 2: Proto-oncogene Wnt-3

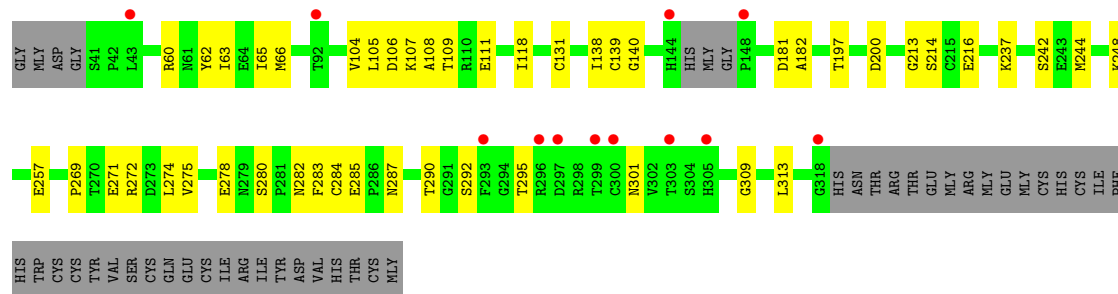




• Molecule 2: Proto-oncogene Wnt-3



• 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) 99.8 (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 , 0.245	Depositor DCC
R_{free} test set	2731 reflections (4.90%)	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 , 62.2	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PAM, CL, MLY

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	0.25	0/951	0.54	0/1299
1	C	0.39	1/961 (0.1%)	0.78	5/1314 (0.4%)
1	E	0.37	0/851	0.79	2/1169 (0.2%)
2	B	0.29	0/2352	0.57	0/3196
2	D	0.38	1/2324 (0.0%)	0.64	4/3155 (0.1%)
2	F	0.30	0/1989	0.52	0/2708
All	All	0.33	2/9428 (0.0%)	0.62	11/12841 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	148	PRO	CA-C	-9.27	1.46	1.52
1	C	123	ARG	CB-CG	-5.46	1.36	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ARG	CG-CD-NE	-11.39	86.95	112.00
1	C	43	CYS	CA-CB-SG	-10.13	91.11	114.40
1	C	89	CYS	CA-CB-SG	-9.99	91.42	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	148	PRO	O-C-N	-9.71	116.59	121.15
1	E	89	CYS	CA-CB-SG	-8.98	93.75	114.40

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	21	0
1	C	991	0	930	18	0
1	E	864	0	767	43	2
2	B	2460	0	2279	49	1
2	D	2431	0	2235	70	0
2	F	2066	0	1872	38	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
6	D	8	0	10	1	0
All	All	9947	0	9151	234	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 12.

The worst 5 of 234 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

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%)	14	41
1	E	105/141 (74%)	100 (95%)	5 (5%)	0	100	100
2	B	294/319 (92%)	275 (94%)	18 (6%)	1 (0%)	36	66
2	D	288/319 (90%)	277 (96%)	10 (4%)	1 (0%)	36	66
2	F	258/319 (81%)	247 (96%)	11 (4%)	0	100	100
All	All	1173/1380 (85%)	1123 (96%)	47 (4%)	3 (0%)	36	66

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 [i](#)

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%)	104 (100%)	0	100	100
1	E	89/118 (75%)	89 (100%)	0	100	100
2	B	249/252 (99%)	249 (100%)	0	100	100
2	D	246/252 (98%)	246 (100%)	0	100	100
2	F	199/252 (79%)	199 (100%)	0	100	100
All	All	990/1110 (89%)	990 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	331	HIS
2	D	145	HIS
1	E	56	GLN
2	B	82	HIS
1	A	152	ASN

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	355	2	8,9,11	0.84	1 (12%)	7,10,13	1.10	1 (14%)
2	MLY	D	207	2	7,8,11	0.67	0	3,8,13	0.49	0
2	MLY	D	237	2	7,8,11	0.49	0	3,8,13	0.22	0
2	MLY	D	146	2	7,8,11	0.46	0	3,8,13	0.40	0
1	MLY	C	44	1	7,8,11	0.80	0	3,8,13	0.62	0
1	MLY	C	31	1	7,8,11	0.49	0	3,8,13	0.30	0
2	MLY	B	74	2	7,8,11	0.56	0	3,8,13	0.36	0
2	MLY	B	54	2	7,8,11	0.54	0	3,8,13	0.42	0
2	MLY	D	325	2	7,8,11	0.57	0	3,8,13	0.33	0
2	MLY	D	248	2	7,8,11	0.45	0	3,8,13	0.43	0
1	MLY	E	85	1	7,8,11	0.47	0	3,8,13	0.29	0
2	MLY	B	218	2	7,8,11	0.38	0	3,8,13	0.76	0
1	MLY	C	101	1	9,10,11	0.50	0	6,11,13	1.11	0
2	MLY	D	154	2	7,8,11	0.45	0	3,8,13	0.26	0
2	MLY	D	74	2	9,10,11	0.74	0	6,11,13	0.89	0
1	MLY	E	101	1	7,8,11	0.54	0	3,8,13	0.31	0
1	MLY	E	44	1	7,8,11	0.61	0	3,8,13	0.37	0
2	MLY	B	188	2	7,8,11	0.54	0	3,8,13	0.22	0
2	MLY	D	218	2	7,8,11	0.60	0	3,8,13	0.25	0
2	MLY	B	329	2	7,8,11	0.44	0	3,8,13	0.49	0
2	MLY	D	54	2	7,8,11	0.45	0	3,8,13	0.27	0
2	MLY	B	267	2	7,8,11	0.55	0	3,8,13	0.34	0
2	MLY	B	207	2	7,8,11	0.57	0	3,8,13	0.42	0
2	MLY	D	327	2	7,8,11	0.53	0	3,8,13	0.45	0
2	MLY	F	267	2	7,8,11	0.50	0	3,8,13	0.63	0
1	MLY	E	102	1	7,8,11	0.46	0	3,8,13	0.42	0
1	MLY	A	102	1	7,8,11	0.51	0	3,8,13	0.45	0
1	MLY	C	85	1	9,10,11	0.57	0	6,11,13	0.82	0
2	MLY	F	235	2	7,8,11	0.61	0	3,8,13	0.27	0
2	MLY	B	154	2	7,8,11	0.53	0	3,8,13	0.29	0
2	MLY	F	107	2	7,8,11	0.53	0	3,8,13	0.25	0
2	MLY	F	54	2	9,10,11	0.75	0	6,11,13	0.74	0
2	MLY	B	248	2	7,8,11	0.47	0	3,8,13	0.41	0
2	MLY	B	146	2	7,8,11	0.64	0	3,8,13	0.23	0
2	MLY	F	248	2	9,10,11	0.55	0	6,11,13	0.62	0
2	MLY	F	207	2	7,8,11	0.72	0	3,8,13	0.79	0
1	MLY	A	115	1	7,8,11	0.50	0	3,8,13	0.42	0
2	MLY	F	154	2	9,10,11	0.66	0	6,11,13	0.67	0
2	MLY	F	74	2	7,8,11	0.64	0	3,8,13	0.23	0
1	MLY	A	101	1	7,8,11	0.45	0	3,8,13	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	325	2	7,8,11	0.60	0	3,8,13	1.40	1 (33%)
2	MLY	B	107	2	9,10,11	0.64	0	6,11,13	1.29	1 (16%)
2	MLY	B	205	2	7,8,11	0.57	0	3,8,13	0.37	0
2	MLY	B	327	2	7,8,11	0.49	0	3,8,13	0.56	0
2	MLY	F	218	2	7,8,11	0.61	0	3,8,13	0.42	0
1	MLY	C	115	1	7,8,11	0.58	0	3,8,13	0.37	0
2	MLY	D	262	2	7,8,11	0.44	0	3,8,13	0.28	0
1	MLY	A	44	1	7,8,11	0.53	0	3,8,13	0.24	0
1	MLY	E	115	1	3,4,11	0.65	0	2,4,13	0.78	0
2	MLY	F	188	2	9,10,11	0.59	0	6,11,13	0.88	0
2	MLY	D	107	2	7,8,11	0.54	0	3,8,13	0.56	0
2	MLY	F	205	2	7,8,11	0.56	0	3,8,13	0.32	0
1	MLY	C	102	1	9,10,11	0.56	0	6,11,13	0.74	0
2	MLY	B	237	2	7,8,11	0.55	0	3,8,13	0.21	0
2	MLY	F	237	2	7,8,11	0.46	0	3,8,13	0.34	0
2	MLY	B	235	2	7,8,11	0.57	0	3,8,13	0.28	0
2	MLY	D	205	2	7,8,11	0.50	0	3,8,13	0.45	0
2	MLY	D	329	2	7,8,11	0.50	0	3,8,13	0.26	0
2	MLY	F	262	2	7,8,11	0.47	0	3,8,13	0.37	0
2	MLY	D	267	2	7,8,11	0.59	0	3,8,13	0.48	0
2	MLY	B	355	2	9,10,11	0.52	0	6,11,13	0.87	0
2	MLY	B	262	2	9,10,11	0.49	0	6,11,13	1.00	0
1	MLY	A	85	1	9,10,11	0.60	0	6,11,13	0.77	0
2	MLY	D	188	2	7,8,11	0.65	0	3,8,13	0.15	0
2	MLY	D	235	2	7,8,11	0.55	0	3,8,13	0.24	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	355	2	-	0/9/9/11	-
2	MLY	D	207	2	-	1/6/7/11	-
2	MLY	D	237	2	-	0/6/7/11	-
2	MLY	D	146	2	-	3/6/7/11	-
1	MLY	C	44	1	-	0/6/7/11	-
1	MLY	C	31	1	-	1/6/7/11	-
2	MLY	B	74	2	-	1/6/7/11	-
2	MLY	B	54	2	-	0/6/7/11	-
2	MLY	D	325	2	-	0/6/7/11	-
2	MLY	D	248	2	-	3/6/7/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	E	85	1	-	2/6/7/11	-
2	MLY	B	218	2	-	4/6/7/11	-
1	MLY	C	101	1	-	4/8/9/11	-
2	MLY	D	154	2	-	1/6/7/11	-
2	MLY	D	74	2	-	2/8/9/11	-
1	MLY	E	101	1	-	2/6/7/11	-
1	MLY	E	44	1	-	2/6/7/11	-
2	MLY	B	188	2	-	1/6/7/11	-
2	MLY	D	218	2	-	1/6/7/11	-
2	MLY	B	329	2	-	0/6/7/11	-
2	MLY	D	54	2	-	0/6/7/11	-
2	MLY	B	267	2	-	0/6/7/11	-
2	MLY	B	207	2	-	2/6/7/11	-
2	MLY	D	327	2	-	1/6/7/11	-
2	MLY	F	267	2	-	2/6/7/11	-
1	MLY	E	102	1	-	2/6/7/11	-
1	MLY	A	102	1	-	1/6/7/11	-
1	MLY	C	85	1	-	2/8/9/11	-
2	MLY	F	235	2	-	1/6/7/11	-
2	MLY	B	154	2	-	0/6/7/11	-
2	MLY	F	107	2	-	1/6/7/11	-
2	MLY	F	54	2	-	2/8/9/11	-
2	MLY	B	248	2	-	0/6/7/11	-
2	MLY	B	146	2	-	2/6/7/11	-
2	MLY	F	248	2	-	2/8/9/11	-
2	MLY	F	207	2	-	2/6/7/11	-
1	MLY	A	115	1	-	0/6/7/11	-
2	MLY	F	154	2	-	1/8/9/11	-
2	MLY	F	74	2	-	0/6/7/11	-
1	MLY	A	101	1	-	2/6/7/11	-
2	MLY	B	325	2	-	0/6/7/11	-
2	MLY	B	107	2	-	3/8/9/11	-
2	MLY	B	205	2	-	1/6/7/11	-
2	MLY	B	327	2	-	2/6/7/11	-
2	MLY	F	218	2	-	0/6/7/11	-
1	MLY	C	115	1	-	3/6/7/11	-
2	MLY	D	262	2	-	2/6/7/11	-
1	MLY	A	44	1	-	3/6/7/11	-

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	355	MLY	OXT-C	-2.15	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	355	MLY	OXT-C-O	-2.81	117.71	124.08
2	B	107	MLY	CD-CE-NZ	-2.41	107.49	113.71
2	B	325	MLY	CD-CG-CB	-2.39	104.63	113.62

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	101	MLY	O-C-CA-CB
2	B	74	MLY	C-CA-CB-CG
2	B	107	MLY	O-C-CA-CB
2	B	146	MLY	O-C-CA-CB
2	B	205	MLY	C-CA-CB-CG

There are no ring outliers.

19 monomers are involved in 26 short contacts:

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

5.5 Carbohydrates [i](#)

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	1.35	3 (17%)
3	NAG	G	2	3	14,14,15	0.93	0	17,19,21	2.37	4 (23%)
3	NAG	H	1	3,2	14,14,15	0.81	0	17,19,21	1.88	5 (29%)
3	NAG	H	2	3	14,14,15	1.04	2 (14%)	17,19,21	1.12	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	-	6/6/23/26	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 (2) 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
3	H	2	NAG	C2-N2	2.03	1.49	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C2-N2-C7	7.27	132.64	122.90
3	H	1	NAG	C1-C2-N2	4.73	117.89	110.43
3	G	2	NAG	O5-C1-C2	-3.22	106.32	111.29
3	G	2	NAG	C8-C7-N2	3.12	121.30	116.12
3	G	2	NAG	C1-C2-N2	3.07	115.26	110.43

There are no chirality outliers.

5 of 14 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	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2

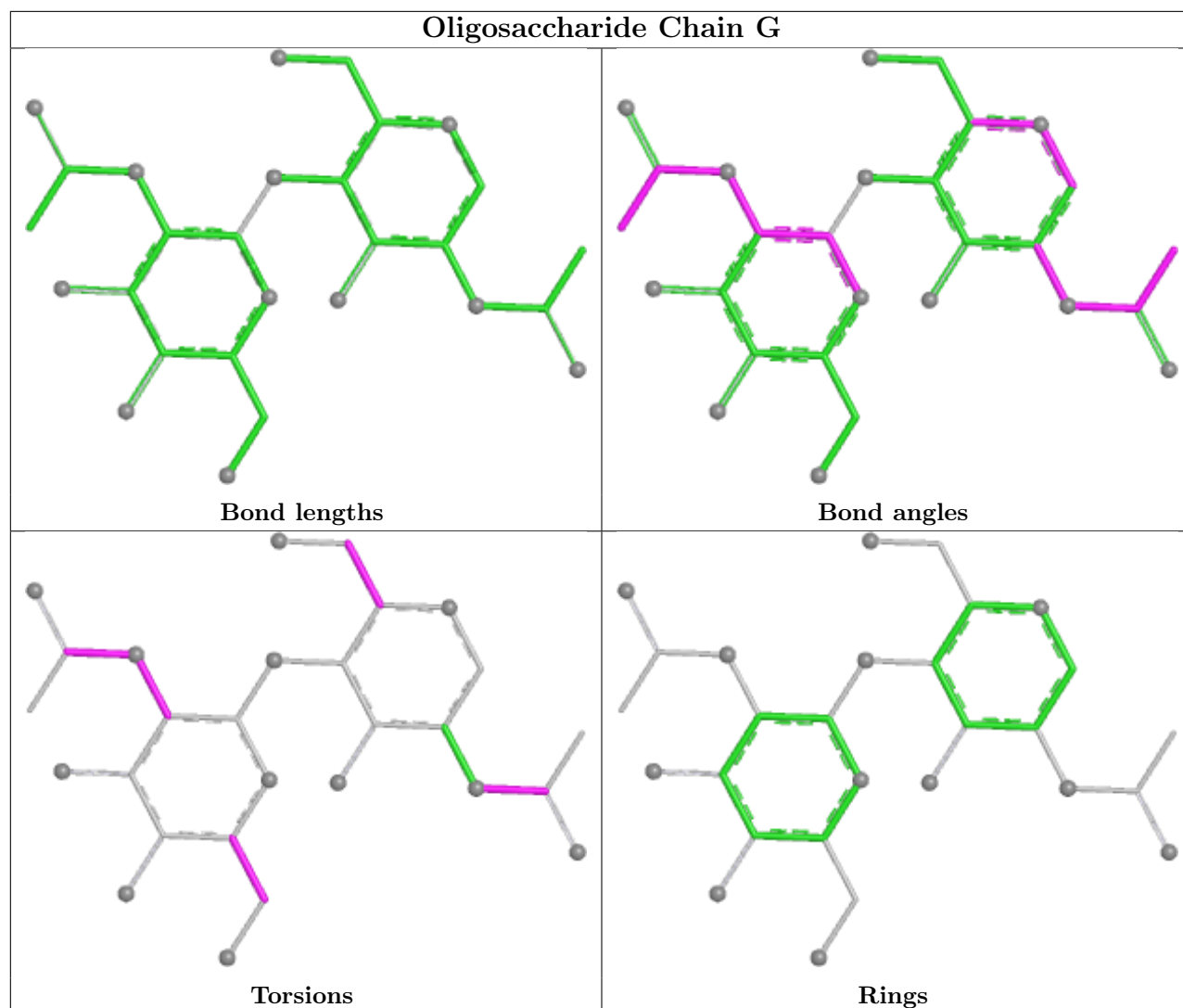
There are no ring outliers.

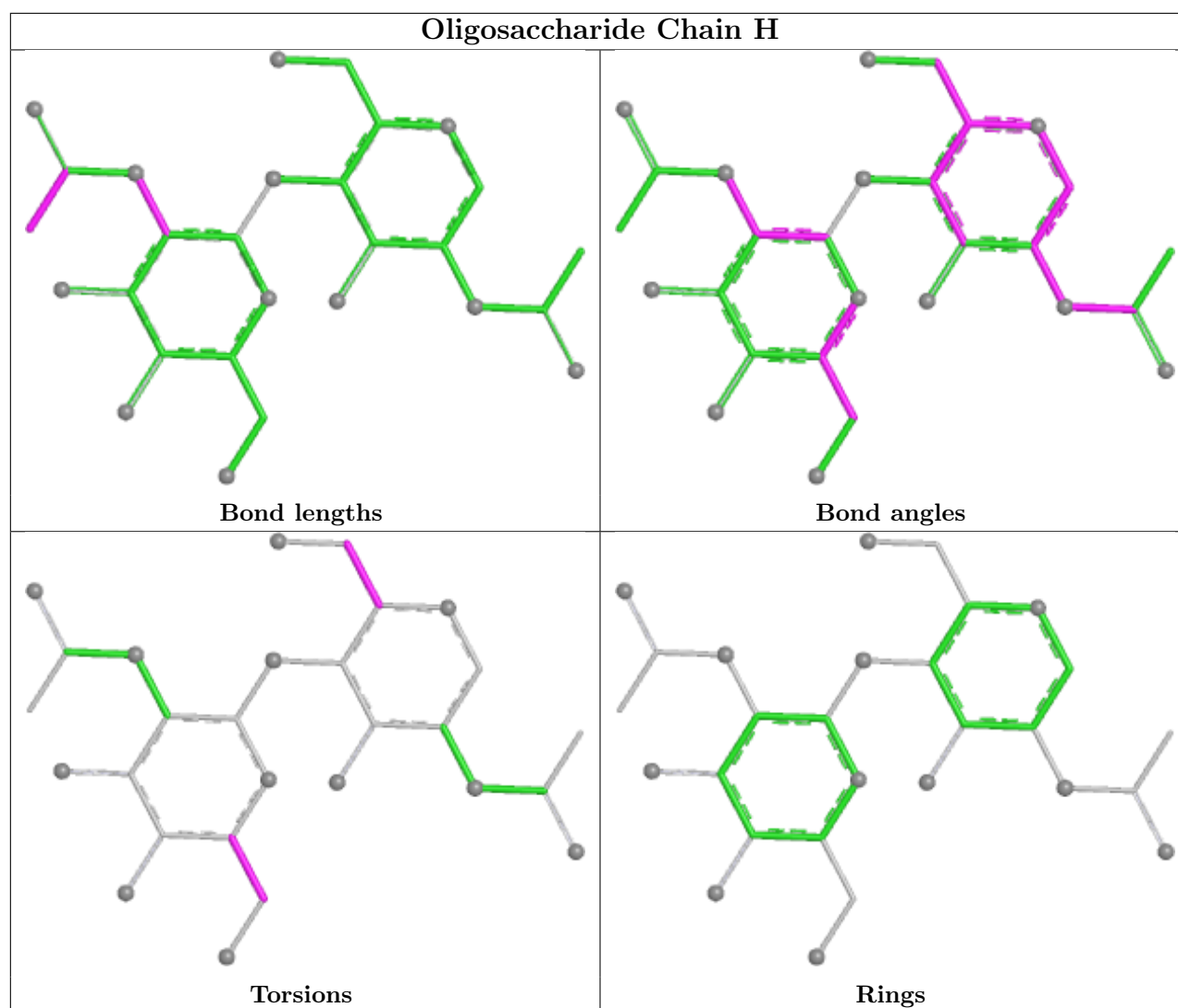
1 monomer is involved in 1 short contact:

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 [i](#)

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	$\# Z > 2$
4	NAG	A	500	1	14,14,15	0.82	0	17,19,21	0.92	1 (5%)
4	NAG	E	500	1	14,14,15	0.81	0	17,19,21	0.88	1 (5%)
4	NAG	B	404	2	14,14,15	0.79	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	500	2	14,14,15	0.84	0	17,19,21	1.36	3 (17%)
4	NAG	D	403	2	14,14,15	0.80	0	17,19,21	0.86	0
6	PAM	D	404	2	6,7,17	0.54	0	5,6,17	0.79	0
6	PAM	B	405	2	16,16,17	0.86	1 (6%)	15,15,17	0.81	0
4	NAG	C	500	1	14,14,15	0.79	0	17,19,21	0.87	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
4	NAG	A	500	1	-	2/6/23/26	0/1/1/1
4	NAG	E	500	1	-	0/6/23/26	0/1/1/1
4	NAG	B	404	2	-	0/6/23/26	0/1/1/1
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
6	PAM	D	404	2	-	3/5/5/15	-
6	PAM	B	405	2	-	7/14/14/15	-
4	NAG	C	500	1	-	0/6/23/26	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	-3.19	1.25	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	500	NAG	C1-O5-C5	3.07	116.30	112.19
4	A	500	NAG	C4-C3-C2	-2.80	106.92	111.02
4	F	500	NAG	C6-C5-C4	-2.28	107.42	113.02
4	F	500	NAG	O5-C5-C6	-2.22	103.34	107.66
4	B	404	NAG	C2-N2-C7	-2.11	120.08	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	404	PAM	O2-C1-C2-C3

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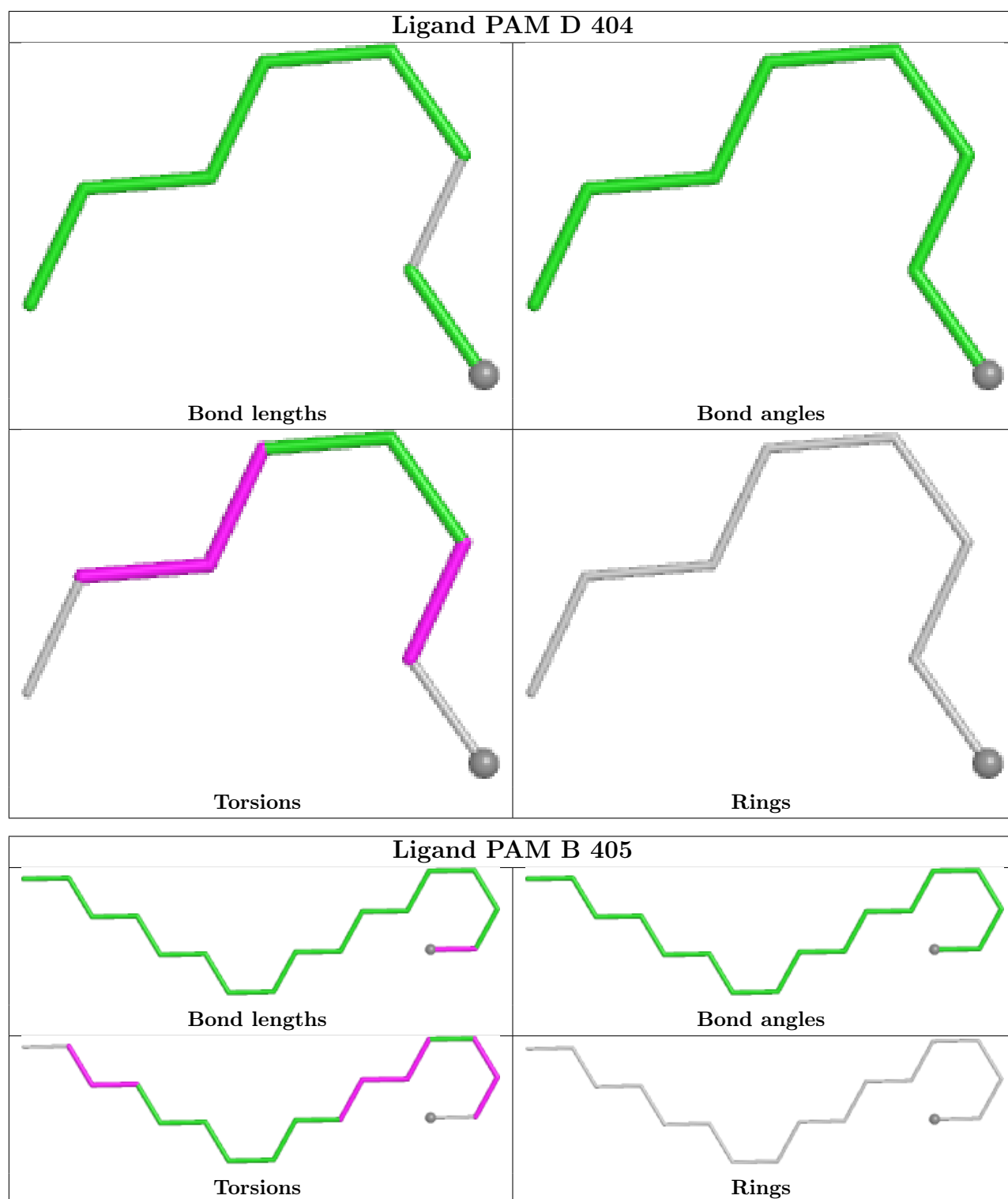
Mol	Chain	Res	Type	Atoms
4	D	403	NAG	O5-C5-C6-O6
4	D	403	NAG	C4-C5-C6-O6
6	B	405	PAM	C3-C4-C5-C6
6	D	404	PAM	C3-C4-C5-C6

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 [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	115/141 (81%)	-0.15	1 (0%) 81 74	53, 76, 113, 131	0
1	C	116/141 (82%)	0.03	3 (2%) 57 47	52, 81, 132, 170	0
1	E	107/141 (75%)	0.90	16 (14%) 5 4	84, 147, 191, 204	0
2	B	295/319 (92%)	0.08	9 (3%) 51 41	43, 77, 136, 200	0
2	D	291/319 (91%)	0.20	12 (4%) 41 33	50, 89, 164, 192	0
2	F	262/319 (82%)	0.15	12 (4%) 37 29	51, 79, 147, 184	0
All	All	1186/1380 (85%)	0.17	53 (4%) 38 30	43, 84, 166, 204	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	318	GLY	4.7
1	E	52	TYR	4.1
2	F	293	PHE	4.0
2	F	148	PRO	4.0
2	D	291	GLY	3.8

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
1	MLY	C	31	9/12	0.38	0.12	130,137,140,149	0
2	MLY	D	267	9/12	0.48	0.21	151,155,162,162	0
2	MLY	D	248	9/12	0.52	0.21	139,148,154,155	0
1	MLY	E	102	9/12	0.62	0.22	148,150,161,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLY	B	325	9/12	0.63	0.19	130,139,157,158	0
2	MLY	D	54	9/12	0.73	0.21	108,117,137,138	0
1	MLY	E	101	9/12	0.74	0.11	123,132,146,168	0
2	MLY	B	355	11/12	0.80	0.21	98,102,107,108	0
1	MLY	E	85	9/12	0.80	0.23	111,125,135,135	0
1	MLY	E	115	5/12	0.80	0.11	152,157,163,165	0
2	MLY	B	146	9/12	0.81	0.20	126,132,139,140	0
1	MLY	A	102	9/12	0.81	0.16	79,85,91,91	0
2	MLY	B	329	9/12	0.81	0.14	93,101,104,105	0
2	MLY	B	327	9/12	0.82	0.10	110,116,124,126	0
2	MLY	D	107	9/12	0.82	0.20	133,146,161,165	0
2	MLY	F	154	11/12	0.82	0.18	93,98,108,109	0
2	MLY	D	146	9/12	0.85	0.14	80,105,122,123	0
2	MLY	D	329	9/12	0.86	0.11	74,77,91,95	0
2	MLY	F	218	9/12	0.87	0.15	88,98,113,114	0
2	MLY	B	248	9/12	0.89	0.13	90,103,117,118	0
2	MLY	D	355	10/12	0.89	0.14	98,105,128,131	0
1	MLY	C	101	11/12	0.90	0.11	73,82,94,97	0
2	MLY	F	54	11/12	0.90	0.18	61,76,111,117	0
2	MLY	F	267	9/12	0.90	0.10	71,82,85,87	0
2	MLY	B	262	11/12	0.91	0.14	73,79,102,105	0
2	MLY	B	267	9/12	0.91	0.12	74,83,111,114	0
2	MLY	F	205	9/12	0.91	0.11	66,84,97,104	0
1	MLY	A	44	9/12	0.91	0.12	63,81,99,100	0
1	MLY	E	44	9/12	0.91	0.11	93,100,111,122	0
2	MLY	B	74	9/12	0.92	0.10	44,61,94,101	0
1	MLY	A	101	9/12	0.92	0.09	68,80,100,101	0
2	MLY	B	218	9/12	0.92	0.10	59,67,73,76	0
2	MLY	D	154	9/12	0.92	0.11	64,73,98,100	0
1	MLY	A	85	11/12	0.92	0.13	46,62,75,79	0
2	MLY	F	262	9/12	0.92	0.09	62,67,74,80	0
1	MLY	C	102	11/12	0.92	0.14	91,98,108,110	0
2	MLY	D	188	9/12	0.93	0.10	69,80,85,90	0
2	MLY	B	188	9/12	0.93	0.12	56,69,96,98	0
2	MLY	F	188	11/12	0.93	0.14	54,62,91,96	0
2	MLY	D	262	9/12	0.93	0.12	107,110,131,133	0
2	MLY	F	207	9/12	0.93	0.09	68,76,92,105	0
2	MLY	B	107	11/12	0.93	0.12	65,83,108,120	0
2	MLY	F	235	9/12	0.93	0.11	70,79,92,95	0
2	MLY	F	248	11/12	0.93	0.13	52,59,98,106	0
2	MLY	D	327	9/12	0.93	0.12	78,85,101,101	0
1	MLY	C	85	11/12	0.93	0.12	56,65,82,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLY	B	205	9/12	0.94	0.10	47,52,77,79	0
2	MLY	B	207	9/12	0.94	0.11	52,54,85,86	0
2	MLY	D	207	9/12	0.94	0.09	51,61,72,74	0
2	MLY	D	235	9/12	0.94	0.12	65,77,89,93	0
1	MLY	A	115	9/12	0.94	0.09	55,62,69,78	0
2	MLY	D	74	11/12	0.94	0.15	52,73,106,106	0
1	MLY	C	44	9/12	0.94	0.10	59,74,85,87	0
2	MLY	B	54	9/12	0.94	0.10	60,72,84,89	0
2	MLY	F	74	9/12	0.94	0.09	60,64,84,92	0
1	MLY	C	115	9/12	0.95	0.10	70,85,92,98	0
2	MLY	D	205	9/12	0.95	0.10	45,72,90,95	0
2	MLY	F	107	9/12	0.95	0.09	64,78,86,100	0
2	MLY	B	154	9/12	0.95	0.10	65,73,95,99	0
2	MLY	F	237	9/12	0.96	0.07	64,67,85,88	0
2	MLY	D	325	9/12	0.96	0.08	60,66,82,84	0
2	MLY	D	237	9/12	0.96	0.10	70,77,90,93	0
2	MLY	D	218	9/12	0.96	0.11	65,70,76,77	0
2	MLY	B	235	9/12	0.97	0.09	56,63,71,82	0
2	MLY	B	237	9/12	0.98	0.06	53,56,67,70	0

6.3 Carbohydrates

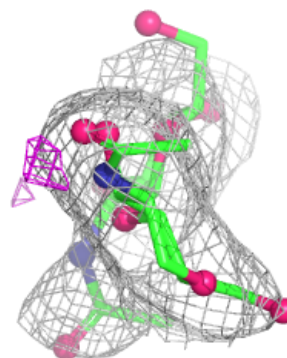
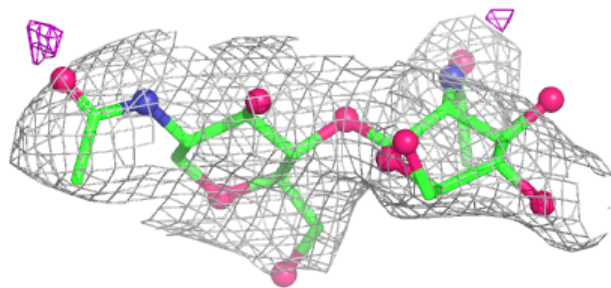
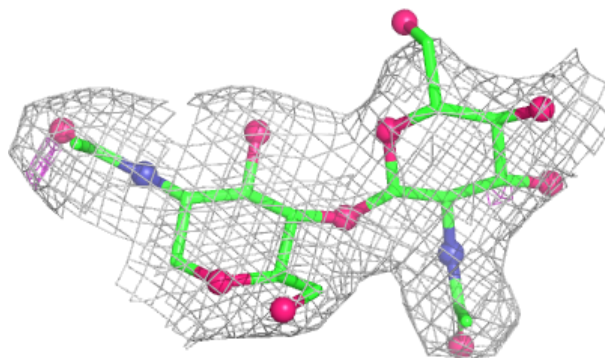
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	G	2	14/15	0.71	0.14	119,125,128,129	0
3	NAG	H	2	14/15	0.82	0.16	102,108,112,113	14
3	NAG	G	1	14/15	0.91	0.09	59,69,94,97	0
3	NAG	H	1	14/15	0.94	0.10	53,71,99,102	0

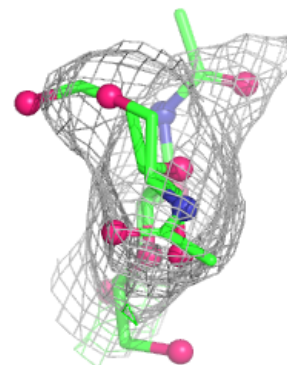
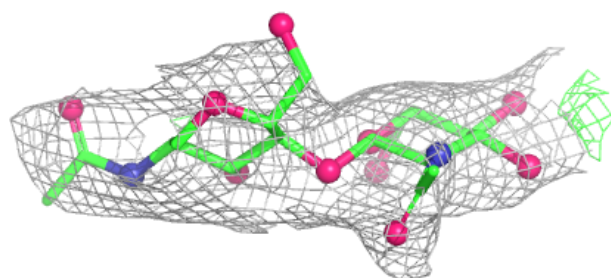
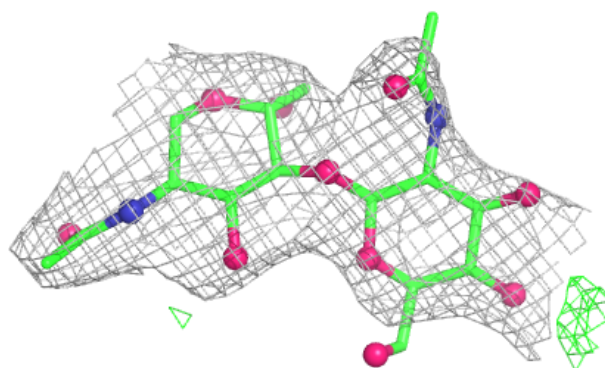
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain 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)

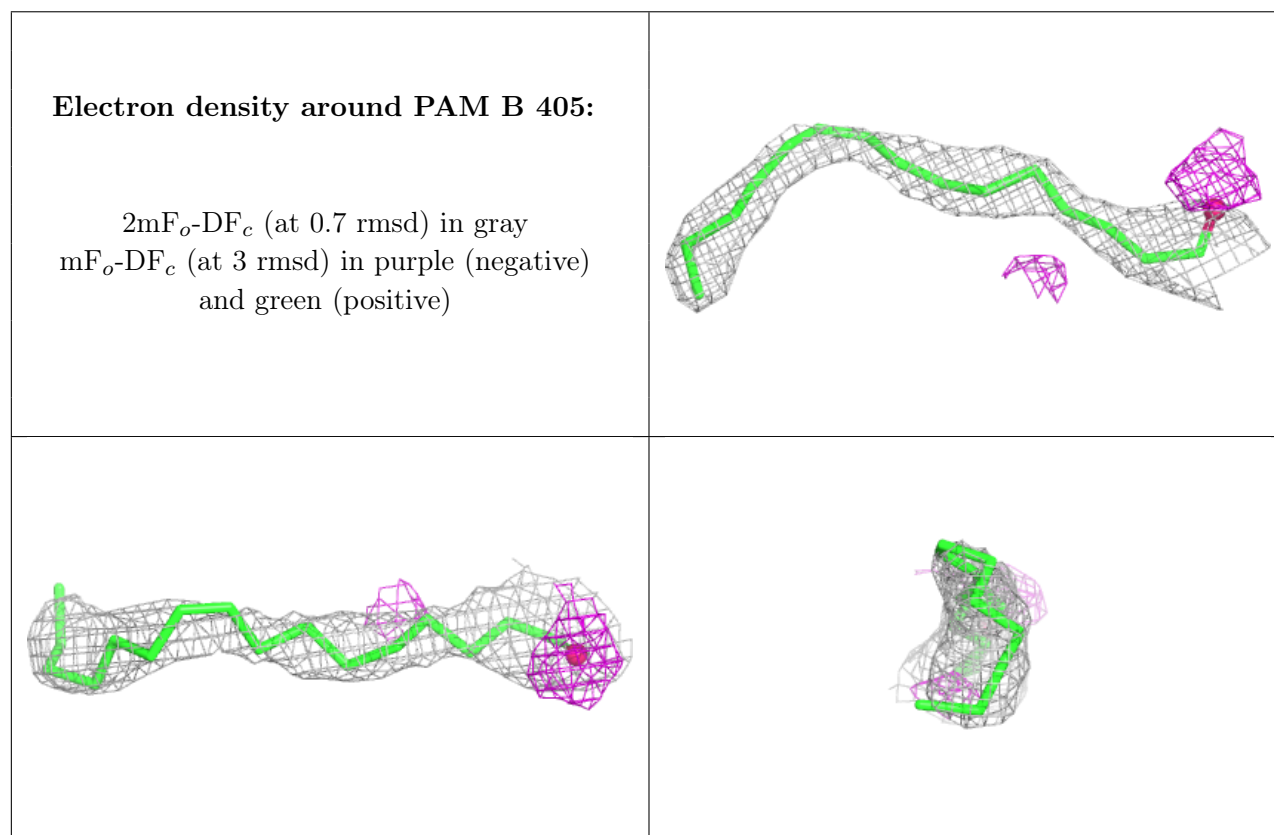


6.4 Ligands ⓘ

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

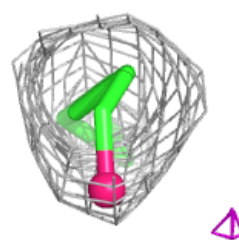
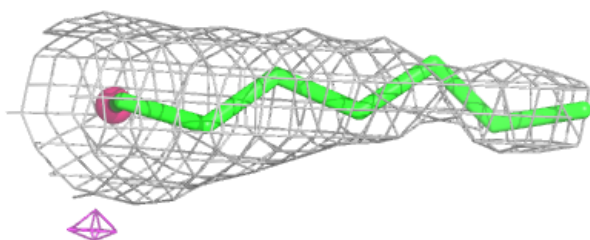
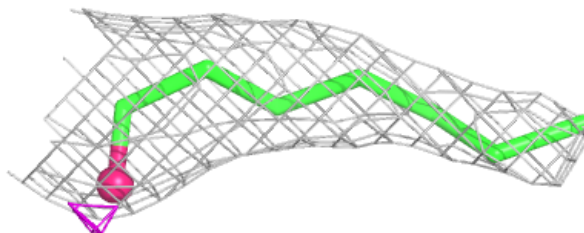
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	500	14/15	0.61	0.17	88,114,119,120	14
4	NAG	C	500	14/15	0.76	0.17	81,110,119,121	14
4	NAG	D	403	14/15	0.80	0.13	78,113,123,123	0
4	NAG	A	500	14/15	0.84	0.10	106,126,139,140	0
4	NAG	B	404	14/15	0.86	0.12	93,100,104,105	0
4	NAG	F	500	14/15	0.89	0.12	72,95,106,108	0
6	PAM	B	405	17/18	0.93	0.20	54,82,105,113	0
6	PAM	D	404	8/18	0.95	0.14	60,68,78,79	0
5	CL	B	401	1/1	0.98	0.07	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 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.