



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 06:10 AM UTC

PDB ID : 2C11 / pdb_00002c11
Title : Crystal structure of the 2-hydrazinopyridine of semicarbazide- sensitive amine oxidase
Authors : Jakobsson, E.; Kleywegt, G.J.
Deposited on : 2005-09-09
Resolution : 2.90 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
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

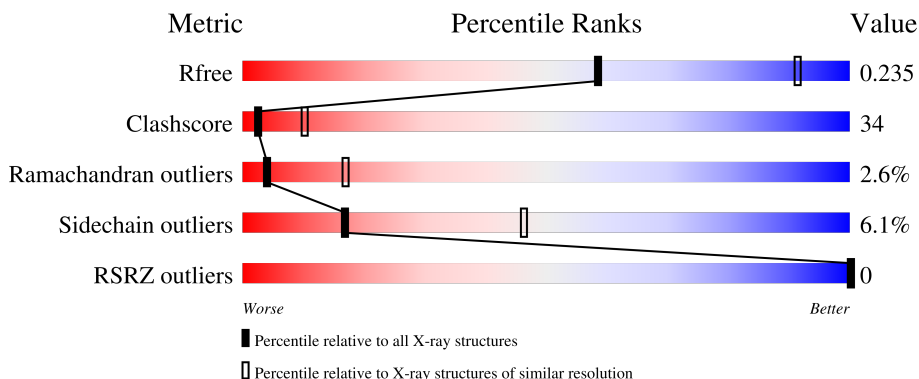
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	735	
1	B	735	
1	C	735	
1	D	735	
2	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	2	 100%
3	F	2	 50% 50%
4	G	3	 33% 67%
4	K	3	 67% 33%
5	H	5	 80% 20%
5	L	5	 20% 80%
6	J	3	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PAQ	A	471	X	-	-	-
1	PAQ	B	471	X	-	-	-
1	PAQ	C	471	X	-	-	-
1	PAQ	D	471	X	-	-	-
3	FUC	F	2	X	-	-	-
5	NAG	H	1	X	-	-	-
5	FUC	H	5	X	-	-	-
5	NAG	L	1	X	-	-	-
5	FUC	L	5	X	-	-	-
6	FUC	J	3	X	-	-	-
7	NAG	D	1736	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21917 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 MEMBRANE COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	672	5340	3434	924	965	17	0	0	1
1	B	672	5340	3434	924	965	17	0	0	1
1	C	672	5340	3434	924	965	17	0	0	1
1	D	672	5340	3434	924	965	17	0	0	1

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



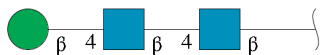
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0
2	I	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



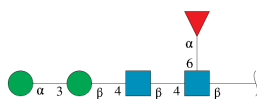
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	24	14	1	9	0	0	0

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



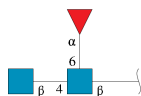
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	3	39	22	2	15	0	0	0
4	K	3	39	22	2	15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	H	5	60	34	2	24	0	0	0
5	L	5	60	34	2	24	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	J	3	38	22	2	14	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
8	A	2	2	2	0	0
8	B	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	2	Total Ca 2 2	0	0
8	D	2	Total Ca 2 2	0	0

- Molecule 9 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	7	Total Cu 7 7	0	0
9	B	8	Total Cu 8 8	0	0
9	C	8	Total Cu 8 8	0	0
9	D	7	Total Cu 7 7	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Cl 2 2	0	0
10	C	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

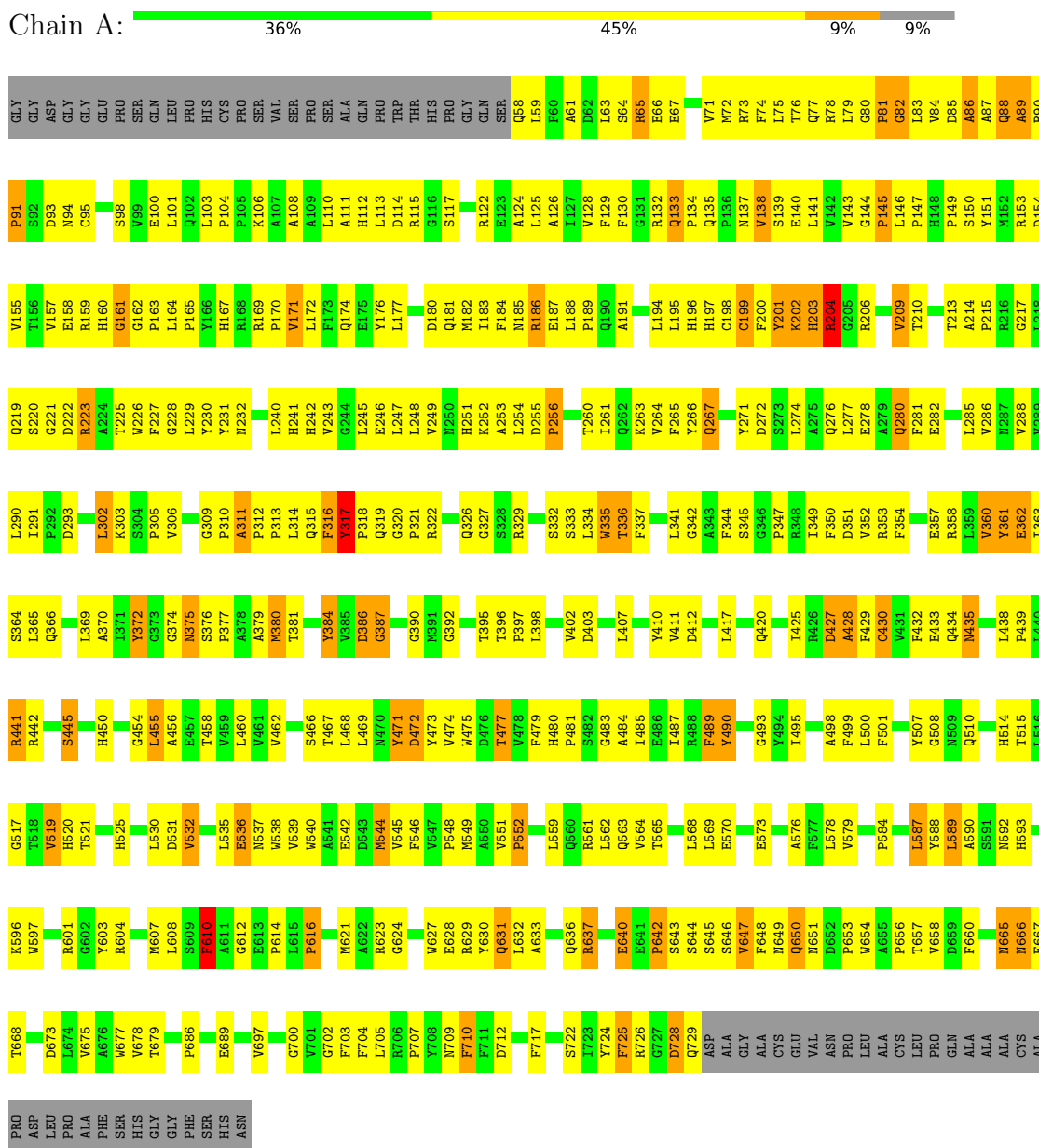
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	19	Total O 19 19	0	0
11	B	20	Total O 20 20	0	0
11	C	11	Total O 11 11	0	0
11	D	9	Total O 9 9	0	0

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: MEMBRANE COPPER AMINE OXIDASE



- Molecule 1: MEMBRANE COPPER AMINE OXIDASE

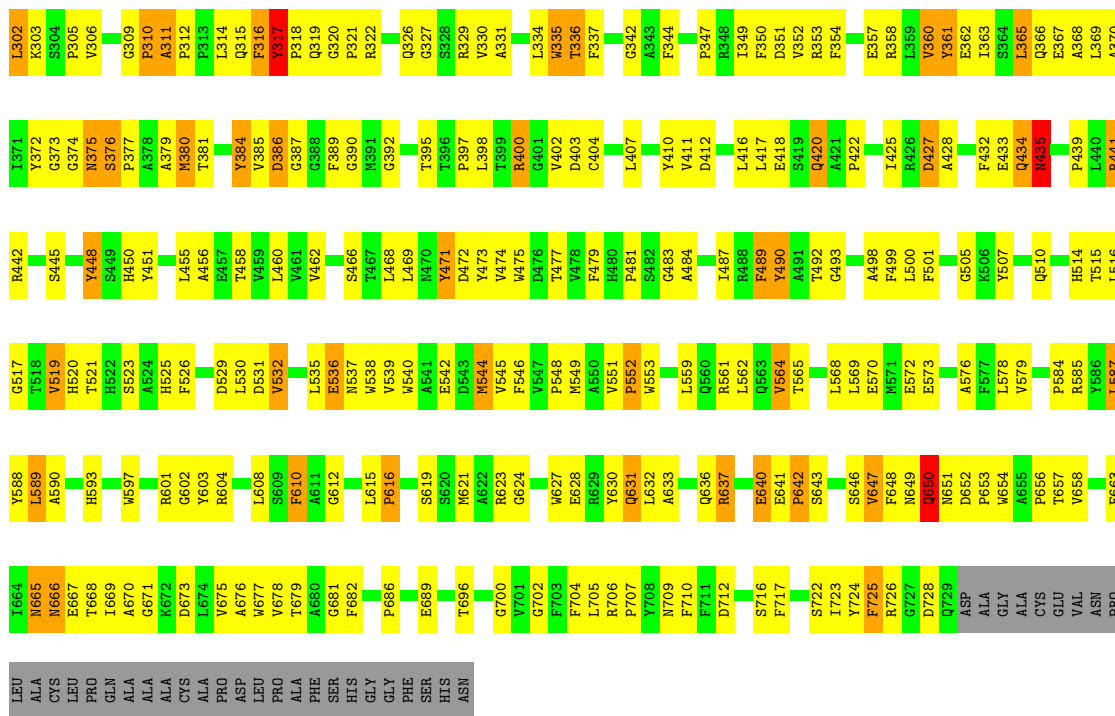
Chain B: 43% 43% 5% 9%

GLY	GLY	ASP	GLY	GLY	GLY	PRO	SER	GLN	LEU	PRO	HIS	CYS	SER	VAL	SER	PRO	SER	ALA	GLN	TRP	THR	HIS	PRO	GLY	GLN	SER	Q58	D62	L63	S64	R65	E66	E67	L68	T69	M72	R73	F74	L75	T76	Q77	R78	P81	G82	L83	V84	A89	R90	P91	N94	S98																																																																																																						
V99	E100	L101	Q102	K106	G116	A124	L125	A126	I127	V128	L129	F130	G131	R132	O133	P134	Q135	P136	M137	V138	L141	V142	V143	G144	P145	L146	L147	H148	P149	S150	Y151	M152	R153	D154	V155	T156	V157	E158	G162	P163	L164	P165	Y166	H167	R168	R169	P170	F173	L174	E175	V176	L177	D178																																																																																																				
I179	D180	Q181	M182	F184	N185	R186	E187	C198	G199	R199	F200	O133	P134	Y201	K202	H203	R204	G205	R206	N207	L208	V209	V143	T210	R211	T212	T213	A214	P215	R216	G217	L218	G221	D222	R223	A224	T225	V226	F227	G228	L229	Y230	S234	G235	A236	G237	F238	F239	H241	H242	V243	G244																																																																																																					
L245	E246	L247	N250	L254	D255	Q262	K263	V264	F265	Y266	Q267	G268	R269	Y270	L274	A275	Q276	L277	E278	Q280	F281	E282	L285	Y288	V289	L290	D293	T296	G297	G298	S299	W300	T225	S304	P308	G309	L310	A311	P312	P313	L314	Q315	F316	Y317	P318	Q319	R322	Q326	G327	S328	S333	L334	F334	F337	L341	L342	L343	F344	T349	R353	G354	R358	L359	Y360	Y361	E362	L363	L369	A370	L371	Y372	G373	G374	S375	P377	A378	K380	T381	R383	Y384	V385	D386	G387	G388	F389	G390	K391	G392	T395	T396	P397	L398	V402	D403	Y406	L407																																																									
A408	D412	W413	L417	L425	R426	D427	G505	G506	Y507	F432	E433	Q434	N435	Q436	G437	P439	L440	R441	R442	H443	Y448	Y451	F452	G453	G454	L455	A456	E457	V462	R463	S466	T467	L468	L469	M470	Y471	D472	Y473	Y474	M475	D476	T477	V478	F479	H480	F486	L487	R488	F489	Y490	G493	S497	L500	F501	T504	G505	G506	Y507	L508	N509	E513	H514	T515	L516	G517	W518	H519	H520	Y521	H525	V528	D529	L530	D531	V532	A533	G534	L535	V538	V539	W540	A541	E542	D543	N544	V545	F546	V547	P548	P549	P552	H553	S554	P555	E556	L559	R561	L562	S563	F564	R566	E570	N571	E572	P584	R585	Y586	L587	Y588	L589	A590	S591	N592	H593	S594	N595	Y596	W597	H598	G599	H599	R600	G601	G602	Y603	R604	M607	L608	S609	P610	E613	P614	L615	P616	S626	W627	E628	R629	Y630	Q631	L632	A633	Q636	R637	K638	F639	E640	E641	P642	S645	S646	V647	F648
W649	Q650	D652	T657	F660	S661	D662	F663	L664	N665	N666	E667	T668	L669	D673	L674	V675	A676	W677	P686	H687	A688	E689	D690	N693	V697	P707	F710	D714	F717	Y718	S719	A720	D721	S722	I723	Y724	R725	R726	G727	D728	Q729	ALA	GLY	ALA	CYS	GLU	VAL	R566	E570	N571	E572	P584	R585	Y586	L587	Y588	L589	A590	S591	N592	H593	S594	N595	Y596	W597	H598	G599	H599	R600	G601	G602	Y603	R604	M607	L608	S609	P610	E613	P614	L615	P616	S626	W627	E628	R629	Y630	Q631	L632	A633	Q636	R637	K638	F639	E640	E641	P642	S645	S646	V647	F648																																																					
ASN	PRO	LEU	ALA	CYS	LEU	PRO	GLN	ALA	ALA	ALA	CYS	ALA	PRO	ASP	LEU	VAL	PRO	ALA	ALA	PHE	SER	HIS	GLY	GLY	PHE	SER	HIS	ASN	Q58	A61	D62	L63	S64	R65	E66	E67	L68	V71	M72	R73	F74	L75	T76	Q77	R78	L79	G80	P81	G82	L83	V84	A89	R90	P91	N94	S98																																																																																																	

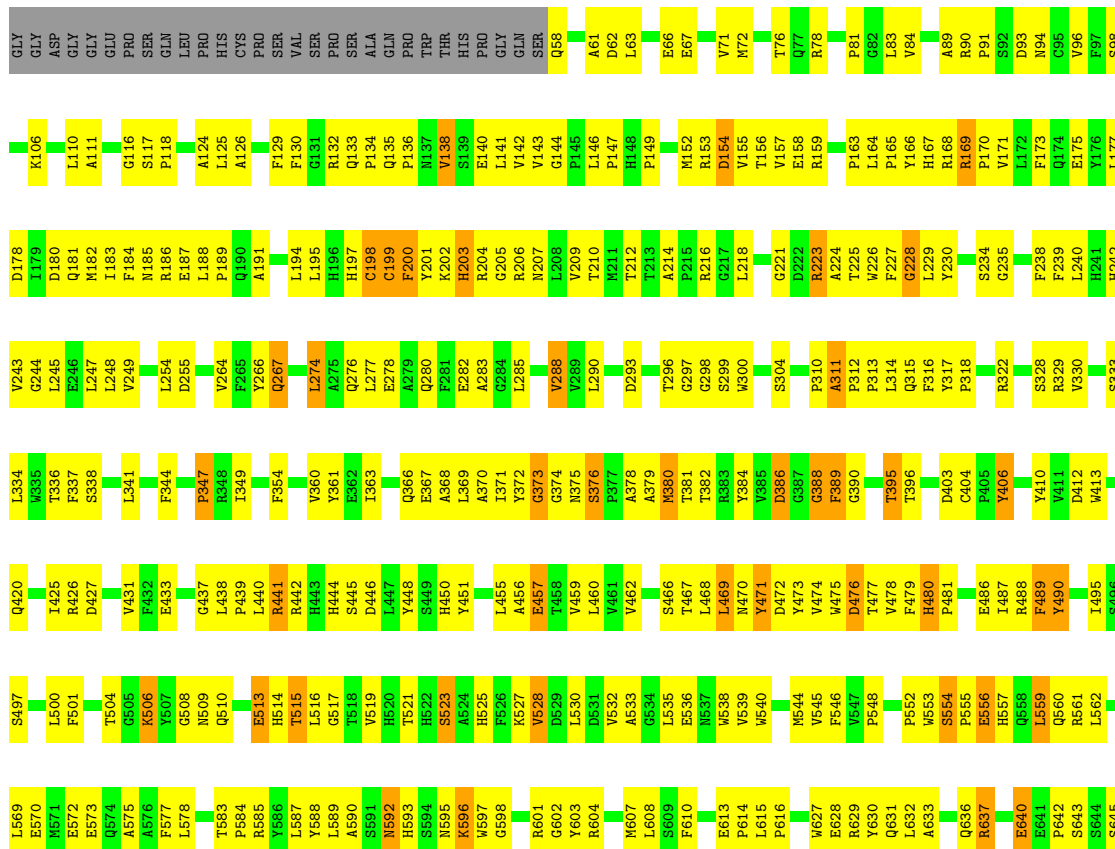
● Molecule 1: MEMBRANE COPPER AMINE OXIDASE

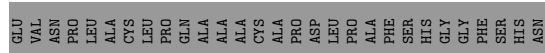
Chain C: 36% 47% 8% 9%

GLY	GLY	ASP	GLY	GLY	GLY	PRO	SER	GLN	LEU	PRO	HIS	CYS	PRO	SER	VAL	VAL	SER	PRO	ALA	GLN	TRP	THR	HIS	PRO	GLY	GLN	SER	Q58	A61	D62	L63	S64	R65	E66	E67	L68	V71	M72	R73	F74	L75	T76	Q77	R78	L79	G80	P81	G82	L83	V84	A89	R90						
P81	S92	D93	N94	C95	V96	F97	S98	L101	Q102	P103	L104	C105	K106	L107	A108	A109	A110	A111	H112	L113	D114	R115	G116	S117	P118	P119	R122	E123	A124	L125	V128	F129	Q133	P134	Q135	V138	S139	E140	V143	G144	P145	L146	Y151	M152	R153	D154	V155	D156	A87	Q88	R89	H160						
G161	G162	P163	L164	P165	G166	H167	R168	R169	V170	P171	L172	F173	Q174	E175	V176	L177	D180	Q181	M182	I183	N250	F184	H251	N185	R186	E187	L188	P189	Q190	A191	S192	G193	L194	L195	H196	H197	C198	G199	F200	Y201	K202	H203	R204	G205	R206	V209	T210	M211	T212	A214	L218	G217	L219	Q219	S220	G221	D222	R223
A224	T225	F227	G228	L229	Y230	Y231	S234	L240	H241	H242	V243	G244	L245	E246	L247	L248	V249	H250	H251	K252	A253	L254	D255	P256	W259	T260	I261	Q262	K263	L264	F265	Y266	C198	G199	Y271	S272	S273	L274	A275	Q276	L277	E278	A279	F281	T212	E282	V288	V289	L290	I291	F292	D293	S301					



● Molecule 1: MEMBRANE COPPER AMINE OXIDASE





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

Chain E: 100%



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

Chain I: 100%



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%



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

Chain G: 33% 67%



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

Chain K: 67% 33%




- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 80% 20%

MAG1
MAG2
BMA3
MAN4
FUC5

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  20% 80%

MAG1
MAG2
BMA3
MAN4
FUC5

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	127.40Å 127.40Å 219.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.90) 94.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.276 0.234 , 0.235	Depositor DCC
R_{free} test set	4335 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtrriage
Anisotropy	0.549	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21917	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: CL, CU, FUC, MAN, PAQ, NAG, CA, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	1/5488 (0.0%)	1.09	41/7481 (0.5%)
1	B	0.56	0/5488	1.09	40/7481 (0.5%)
1	C	0.57	1/5488 (0.0%)	1.09	38/7481 (0.5%)
1	D	0.56	1/5488 (0.0%)	1.07	33/7481 (0.4%)
All	All	0.57	3/21952 (0.0%)	1.08	152/29924 (0.5%)

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
1	A	1	0
1	B	1	0
1	C	1	0
1	D	1	0
All	All	4	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	728	ASP	C-N	-5.28	1.25	1.33
1	C	728	ASP	C-N	-5.27	1.25	1.33
1	D	728	ASP	C-N	-5.06	1.26	1.33

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLY	N-CA-C	11.56	125.24	112.29
1	B	631	GLN	N-CA-C	-10.10	101.09	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	ARG	N-CA-C	9.96	125.78	109.95
1	A	204	ARG	N-CA-C	9.84	125.15	108.23
1	C	631	GLN	N-CA-C	-9.84	100.82	113.12

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5340	0	5113	432	0
1	B	5340	0	5111	340	0
1	C	5340	0	5113	424	0
1	D	5340	0	5111	364	0
2	E	28	0	25	3	0
2	I	28	0	25	3	0
3	F	24	0	22	4	0
4	G	39	0	34	1	0
4	K	39	0	34	5	0
5	H	60	0	52	3	0
5	L	60	0	52	0	0
6	J	38	0	34	5	0
7	A	28	0	26	4	0
7	B	42	0	39	3	0
7	C	28	0	26	2	0
7	D	42	0	39	2	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
9	A	7	0	0	0	0
9	B	8	0	0	0	0
9	C	8	0	0	0	0
9	D	7	0	0	0	0
10	A	2	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
11	A	19	0	0	5	0
11	B	20	0	0	5	0
11	C	11	0	0	5	0
11	D	9	0	0	4	0
All	All	21917	0	20856	1471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 1471 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:B:360:VAL:HG11	1:B:363:ILE:HG13	1.37	1.04
1:C:90:ARG:HG2	1:C:91:PRO:HD2	1.42	1.02
1:B:106:LYS:HB2	1:B:637:ARG:HH21	1.27	0.99
1:A:90:ARG:HG2	1:A:91:PRO:HD2	1.43	0.96
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.45	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	669/735 (91%)	571 (85%)	72 (11%)	26 (4%)	2	10
1	B	669/735 (91%)	585 (87%)	76 (11%)	8 (1%)	10	34
1	C	669/735 (91%)	575 (86%)	69 (10%)	25 (4%)	2	11
1	D	669/735 (91%)	587 (88%)	71 (11%)	11 (2%)	7	27
All	All	2676/2940 (91%)	2318 (87%)	288 (11%)	70 (3%)	4	17

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	MET
1	A	637	ARG
1	B	267	GLN
1	B	386	ASP
1	B	596	LYS

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	562/609 (92%)	523 (93%)	39 (7%)	14	41
1	B	562/609 (92%)	530 (94%)	32 (6%)	18	49
1	C	562/609 (92%)	523 (93%)	39 (7%)	14	41
1	D	562/609 (92%)	534 (95%)	28 (5%)	22	53
All	All	2248/2436 (92%)	2110 (94%)	138 (6%)	17	46

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	223	ARG
1	D	406	TYR
1	D	556	GLU
1	B	326	GLN
1	B	282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	650	GLN
1	D	510	GLN
1	C	693	ASN
1	D	280	GLN
1	D	618	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](#)

4 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
1	PAQ	D	471	1	19,22,23	2.01	6 (31%)	18,29,31	2.57	5 (27%)
1	PAQ	B	471	1	19,22,23	2.01	6 (31%)	18,29,31	2.58	5 (27%)
1	PAQ	C	471	1	19,22,23	2.04	6 (31%)	18,29,31	2.64	5 (27%)
1	PAQ	A	471	1	19,22,23	2.01	6 (31%)	18,29,31	2.63	4 (22%)

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
1	PAQ	D	471	1	1/1/5/10	5/8/27/29	0/2/2/2
1	PAQ	B	471	1	1/1/5/10	5/8/27/29	0/2/2/2
1	PAQ	C	471	1	1/1/5/10	6/8/27/29	0/2/2/2
1	PAQ	A	471	1	1/1/5/10	6/8/27/29	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	PAQ	CG-CD2	-5.80	1.39	1.50
1	D	471	PAQ	CG-CD2	-5.77	1.39	1.50
1	C	471	PAQ	CG-CD2	-5.76	1.39	1.50
1	B	471	PAQ	CG-CD2	-5.75	1.39	1.50
1	C	471	PAQ	CE1-CD1	-3.56	1.39	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	PAQ	CB-CG-CD1	6.79	120.61	111.13
1	A	471	PAQ	CB-CG-CD1	6.72	120.53	111.13
1	B	471	PAQ	CB-CG-CD1	6.39	120.06	111.13
1	D	471	PAQ	CB-CG-CD1	6.32	119.97	111.13
1	D	471	PAQ	CD2-CG-CD1	6.27	119.02	104.64

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	471	PAQ	CG
1	B	471	PAQ	CG
1	C	471	PAQ	CG
1	D	471	PAQ	CG

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	PAQ	N-CA-CB-CG
1	A	471	PAQ	CA-CB-CG-CD1
1	A	471	PAQ	C2-C1-N2-N1
1	A	471	PAQ	N3-C1-N2-N1
1	B	471	PAQ	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	471	PAQ	4	0
1	B	471	PAQ	5	0
1	C	471	PAQ	4	0
1	A	471	PAQ	5	0

5.5 Carbohydrates i

25 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
2	NAG	E	1	2,1	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	0.85	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	0.98	1 (5%)
3	FUC	F	2	3	10,10,11	0.61	0	14,14,16	0.81	0
4	NAG	G	1	4,1	14,14,15	0.77	0	17,19,21	0.87	0
4	NAG	G	2	4	14,14,15	0.97	0	17,19,21	0.99	2 (11%)
4	BMA	G	3	4	11,11,12	0.91	0	15,15,17	0.55	0
5	NAG	H	1	1,5	14,14,15	0.82	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	H	2	5	14,14,15	0.70	0	17,19,21	0.91	0
5	BMA	H	3	5	11,11,12	0.91	0	15,15,17	1.04	1 (6%)
5	MAN	H	4	5	11,11,12	0.72	0	15,15,17	0.84	1 (6%)
5	FUC	H	5	5	10,10,11	0.73	0	14,14,16	0.56	0
2	NAG	I	1	2,1	14,14,15	0.61	0	17,19,21	0.75	1 (5%)
2	NAG	I	2	2	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.65	0	17,19,21	1.22	2 (11%)
6	NAG	J	2	6	14,14,15	0.46	0	17,19,21	0.71	0
6	FUC	J	3	6	10,10,11	0.49	0	14,14,16	0.58	0
4	NAG	K	1	4,1	14,14,15	0.55	0	17,19,21	0.73	0
4	NAG	K	2	4	14,14,15	0.74	0	17,19,21	0.76	0
4	BMA	K	3	4	11,11,12	0.63	0	15,15,17	0.72	1 (6%)
5	NAG	L	1	1,5	14,14,15	0.79	0	17,19,21	1.12	1 (5%)
5	NAG	L	2	5	14,14,15	0.87	1 (7%)	17,19,21	0.92	1 (5%)
5	BMA	L	3	5	11,11,12	1.02	1 (9%)	15,15,17	0.57	0
5	MAN	L	4	5	11,11,12	0.96	1 (9%)	15,15,17	0.65	1 (6%)
5	FUC	L	5	5	10,10,11	0.81	0	14,14,16	0.54	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	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	F	2	3	1/1/4/5	-	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	FUC	H	5	5	1/1/4/5	-	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	6/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	6/6/23/26	0/1/1/1
6	FUC	J	3	6	1/1/4/5	-	0/1/1/1
4	NAG	K	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	5/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
5	NAG	L	1	1,5	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	1/1/1/1
5	FUC	L	5	5	1/1/4/5	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	3	BMA	C2-C3	2.46	1.56	1.52
3	F	1	NAG	C1-C2	2.33	1.55	1.52
5	L	4	MAN	C2-C3	2.22	1.55	1.52
5	L	2	NAG	C1-C2	2.16	1.55	1.52
5	H	1	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	NAG	C4-C3-C2	-4.13	104.97	111.02
5	H	3	BMA	C1-C2-C3	3.67	114.98	109.64
5	H	1	NAG	C3-C4-C5	-3.17	104.49	110.23
6	J	1	NAG	C4-C3-C2	-3.14	106.42	111.02
5	H	4	MAN	C1-O5-C5	2.96	116.15	112.19

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	2	FUC	C1
5	H	1	NAG	C1
5	H	5	FUC	C1
5	L	1	NAG	C1
5	L	5	FUC	C1

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	4	MAN	C1-C2-C3-C4-C5-O5

16 monomers are involved in 24 short contacts:

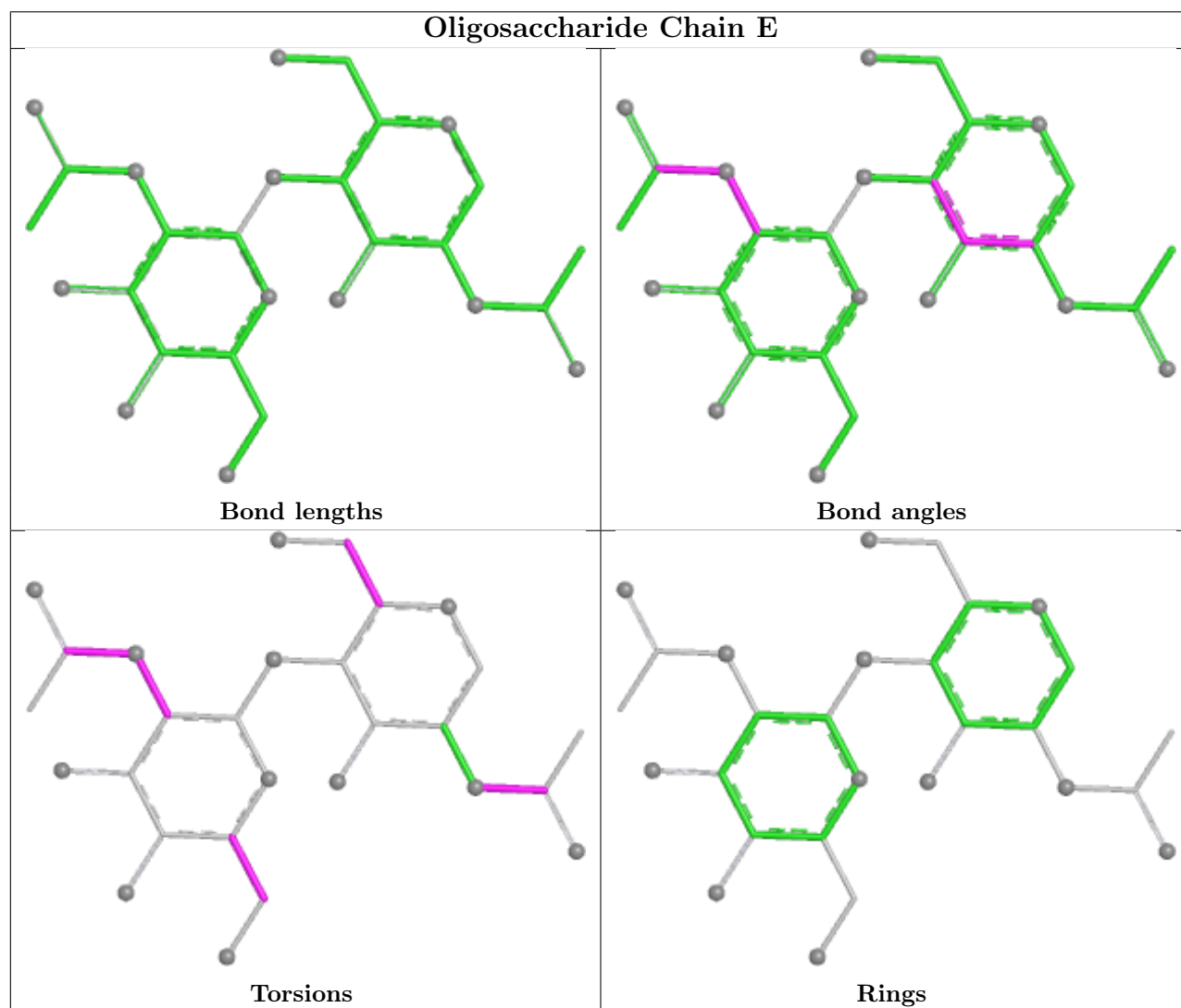
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	FUC	4	0
5	H	2	NAG	2	0
2	E	2	NAG	2	0
6	J	2	NAG	3	0
6	J	3	FUC	2	0
2	I	2	NAG	3	0
2	E	1	NAG	3	0
3	F	1	NAG	2	0
6	J	1	NAG	5	0
2	I	1	NAG	3	0
4	G	1	NAG	1	0

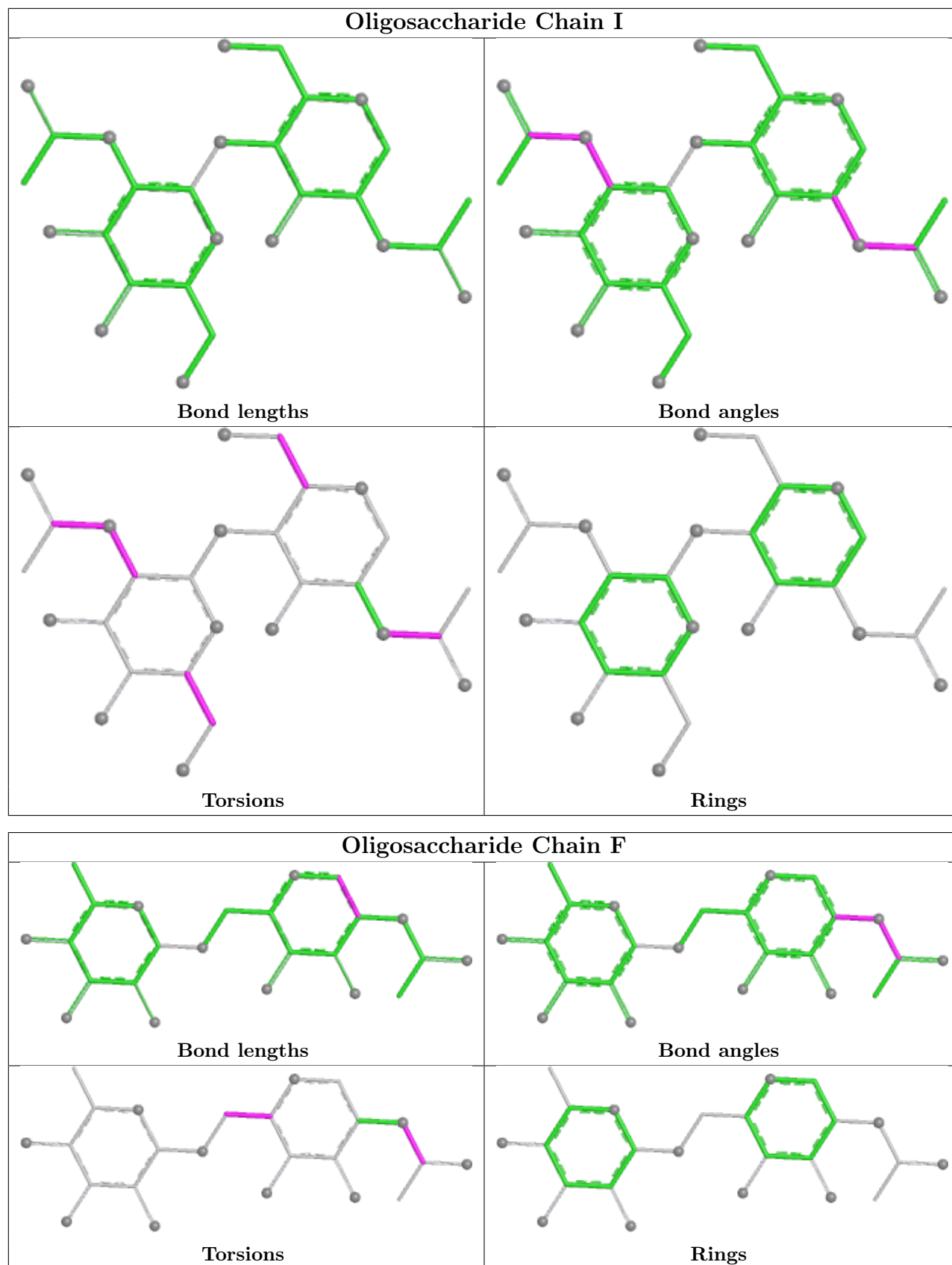
Continued on next page...

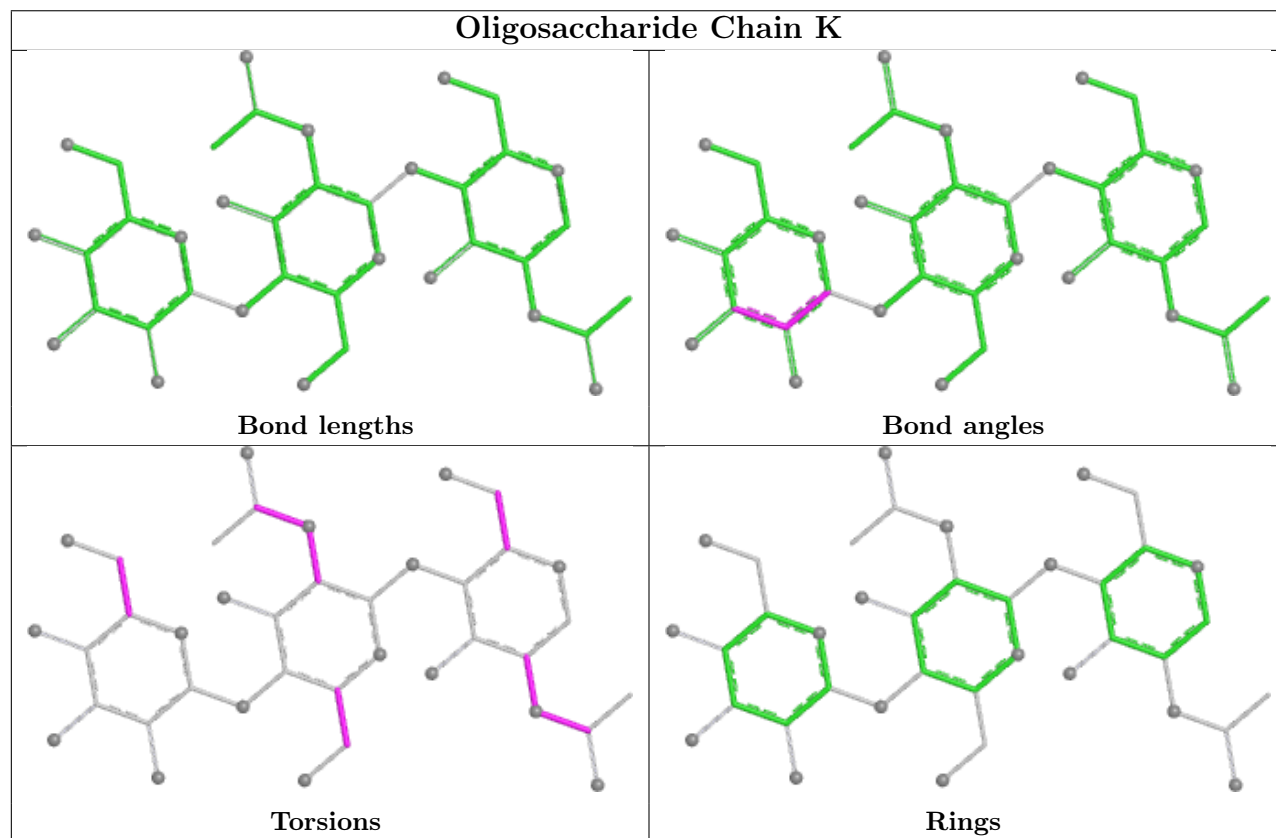
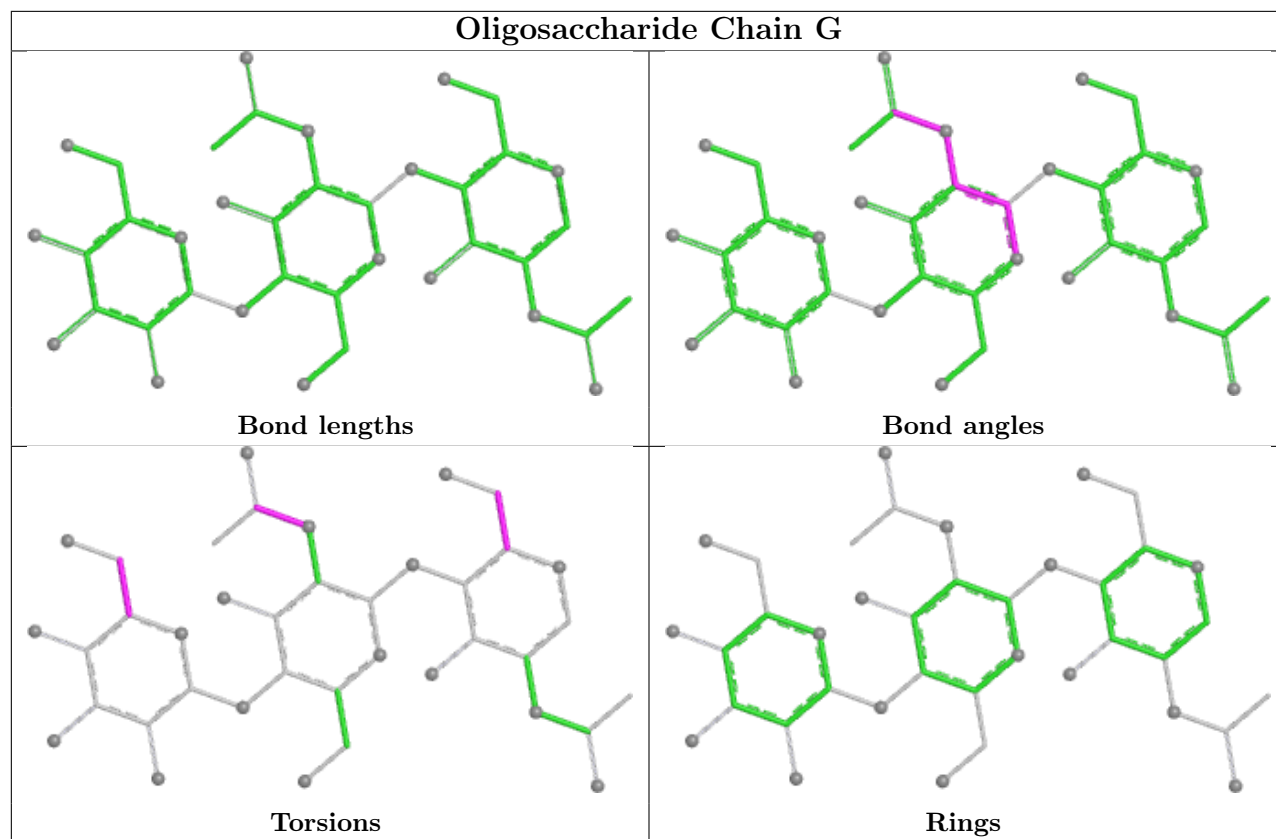
Continued from previous page...

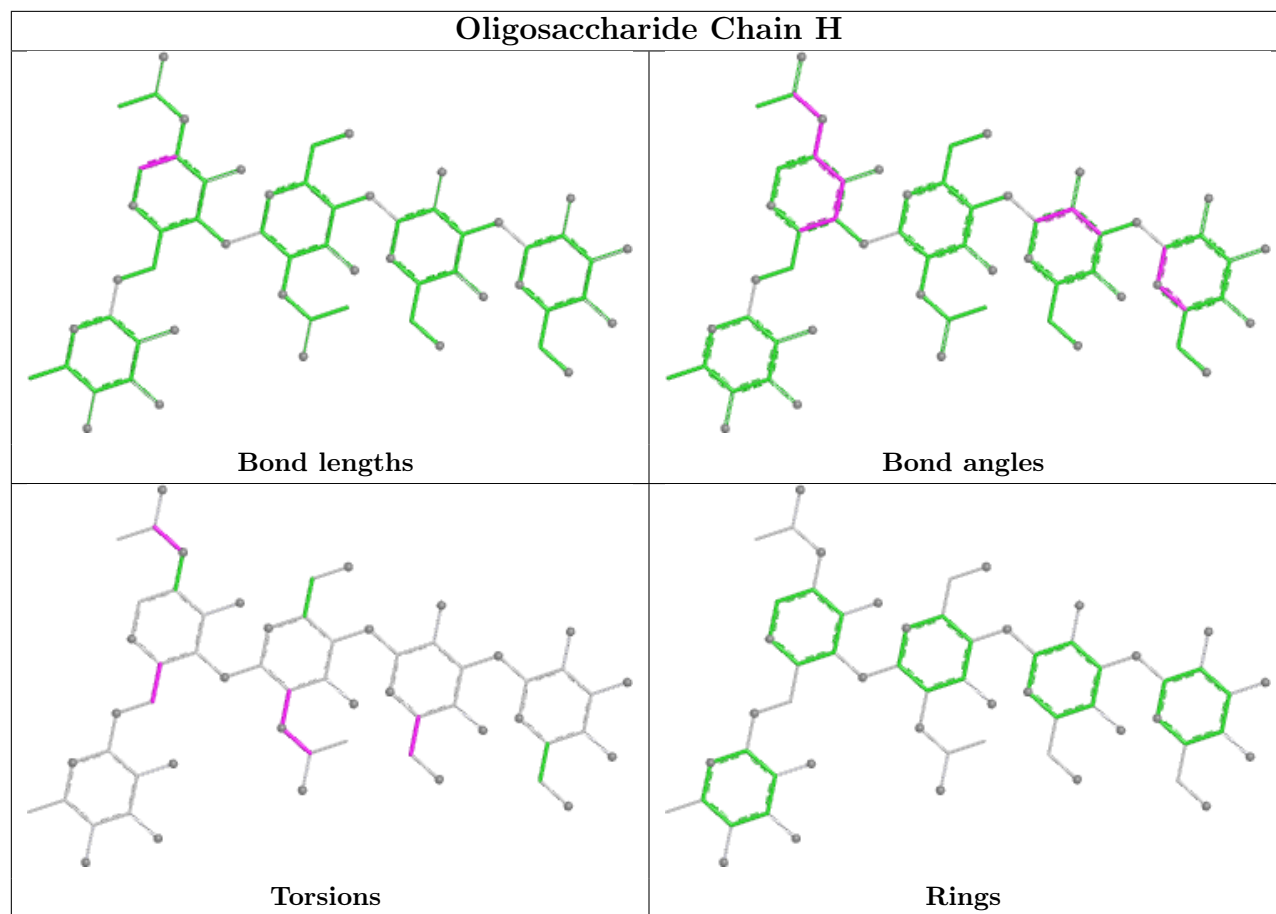
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	3	0
4	K	2	NAG	3	0
5	H	1	NAG	2	0
4	K	3	BMA	1	0
5	H	5	FUC	1	0

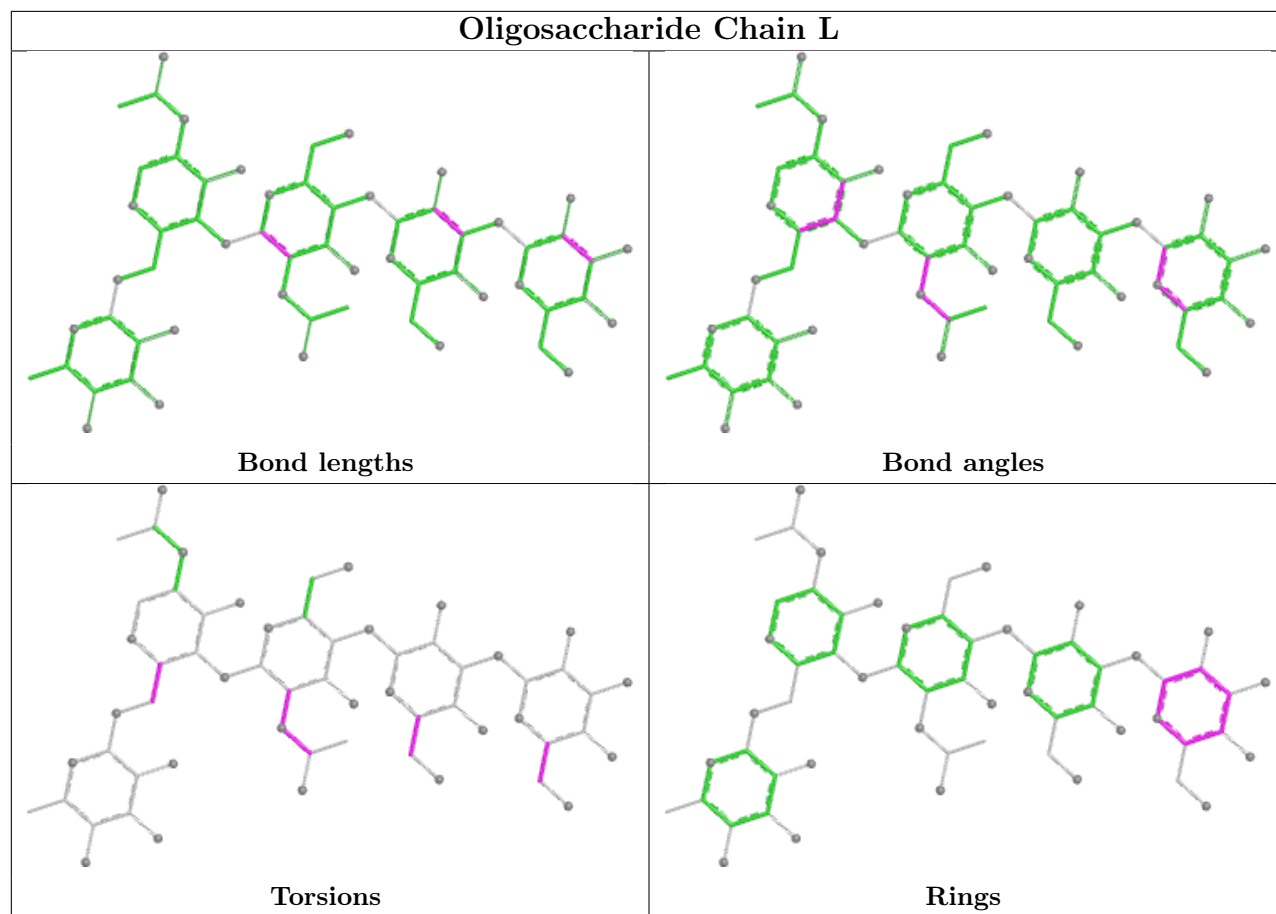
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

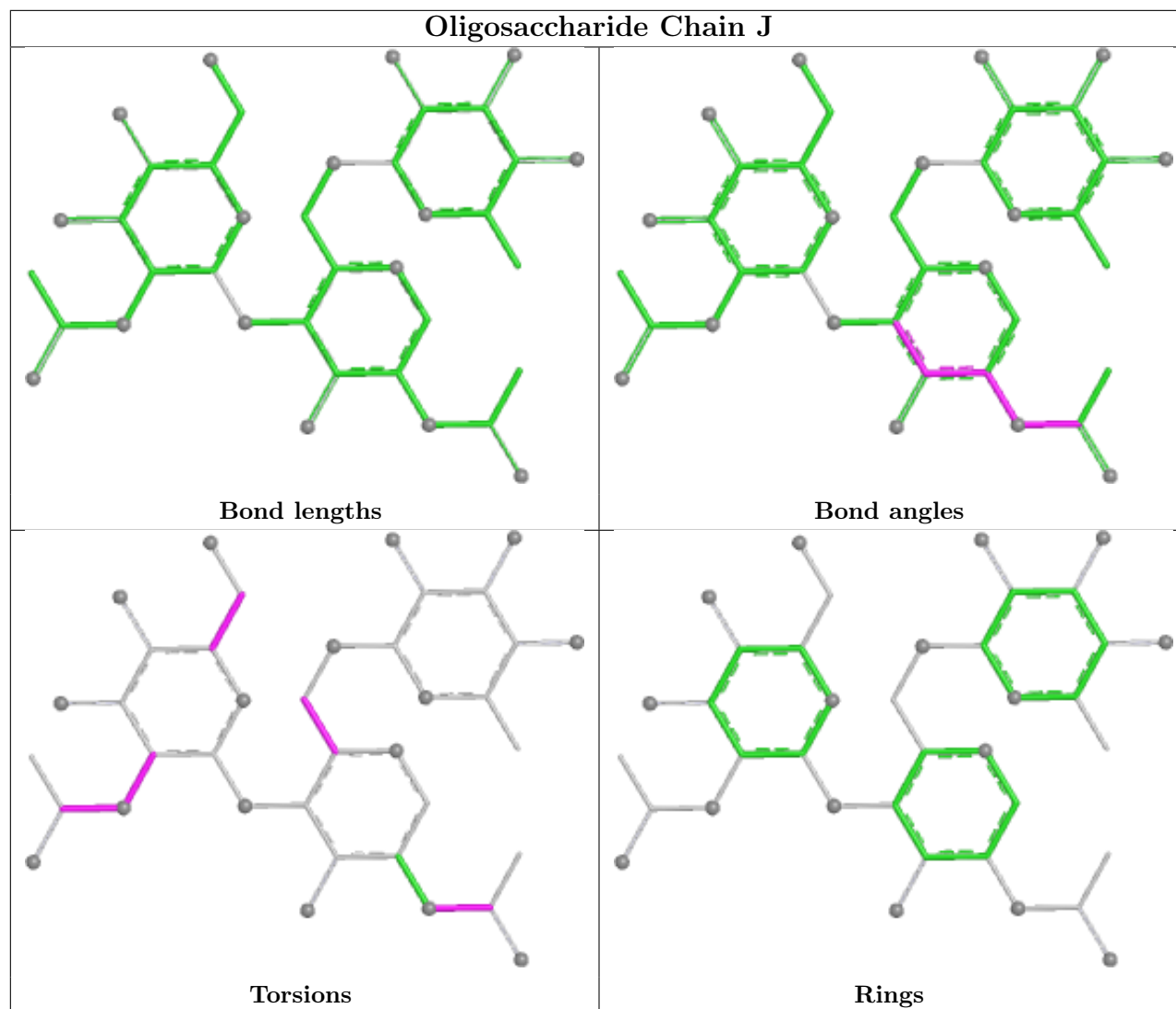












5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 42 are monoatomic - leaving 10 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
7	NAG	D	1738	1	14,14,15	1.07	1 (7%)	17,19,21	0.85	0
7	NAG	B	1736	1	14,14,15	0.89	1 (7%)	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	1736	1	14,14,15	0.75	0	17,19,21	0.73	1 (5%)
7	NAG	B	1735	1	14,14,15	0.71	0	17,19,21	0.81	0
7	NAG	A	1734	1	14,14,15	0.71	0	17,19,21	0.63	0
7	NAG	A	1735	1	14,14,15	0.66	0	17,19,21	0.68	0
7	NAG	D	1735	1	14,14,15	0.88	1 (7%)	17,19,21	0.67	0
7	NAG	C	1735	1	14,14,15	0.82	1 (7%)	17,19,21	0.67	0
7	NAG	B	1738	1	14,14,15	0.80	1 (7%)	17,19,21	0.58	0
7	NAG	C	1736	1	14,14,15	0.81	1 (7%)	17,19,21	0.75	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
7	NAG	D	1738	1	-	5/6/23/26	0/1/1/1
7	NAG	B	1736	1	-	5/6/23/26	0/1/1/1
7	NAG	D	1736	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	B	1735	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1734	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1735	1	-	5/6/23/26	0/1/1/1
7	NAG	D	1735	1	-	4/6/23/26	0/1/1/1
7	NAG	C	1735	1	-	6/6/23/26	0/1/1/1
7	NAG	B	1738	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1736	1	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1738	NAG	C1-C2	3.27	1.56	1.52
7	B	1736	NAG	C1-C2	2.77	1.56	1.52
7	C	1735	NAG	C1-C2	2.34	1.55	1.52
7	C	1736	NAG	C1-C2	2.29	1.55	1.52
7	D	1735	NAG	C1-C2	2.26	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1736	NAG	C2-N2-C7	-2.16	120.01	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1736	NAG	C2-N2-C7	-2.06	120.14	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	1736	NAG	C1

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1734	NAG	C8-C7-N2-C2
7	A	1734	NAG	O7-C7-N2-C2
7	A	1735	NAG	C8-C7-N2-C2
7	A	1735	NAG	O7-C7-N2-C2
7	B	1736	NAG	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1735	NAG	2	0
7	A	1734	NAG	4	0
7	D	1735	NAG	2	0
7	C	1735	NAG	2	0
7	B	1738	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	671/735 (91%)	-1.48	0 100 100	43, 64, 79, 87	0
1	B	671/735 (91%)	-1.49	0 100 100	41, 60, 75, 81	0
1	C	671/735 (91%)	-1.52	0 100 100	43, 64, 79, 88	0
1	D	671/735 (91%)	-1.53	0 100 100	41, 60, 75, 81	0
All	All	2684/2940 (91%)	-1.51	0 100 100	41, 62, 77, 88	0

There are no RSRZ outliers to report.

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	PAQ	D	471	21/22	0.98	0.06	54,59,60,61	0
1	PAQ	B	471	21/22	0.99	0.07	55,59,61,61	0
1	PAQ	C	471	21/22	0.99	0.03	56,59,61,61	0
1	PAQ	A	471	21/22	0.99	0.04	56,59,60,63	0

6.3 Carbohydrates [i](#)

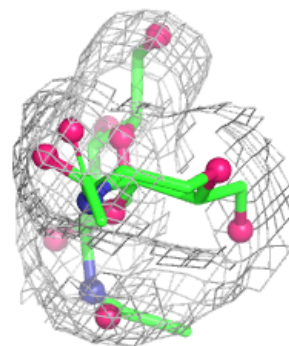
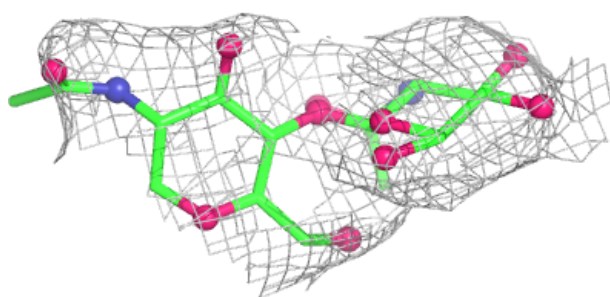
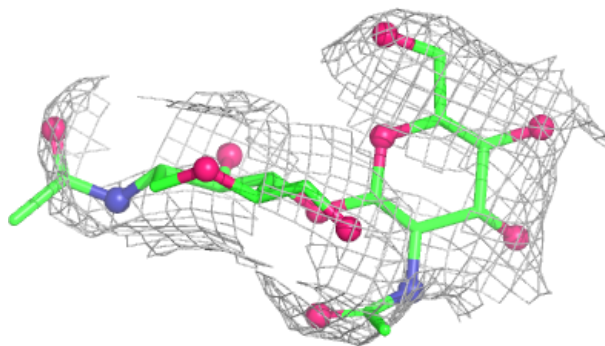
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BMA	G	3	11/12	0.93	0.06	94,94,95,95	0
5	NAG	H	2	14/15	0.97	0.04	95,97,98,98	0
5	BMA	H	3	11/12	0.97	0.03	97,97,98,98	0
5	FUC	H	5	10/11	0.97	0.06	91,93,94,95	0
5	NAG	L	2	14/15	0.97	0.04	92,95,96,97	0
6	NAG	J	2	14/15	0.97	0.05	91,92,93,93	0
4	NAG	K	2	14/15	0.98	0.04	83,85,87,89	0
4	BMA	K	3	11/12	0.98	0.04	89,90,91,91	0
2	NAG	I	1	14/15	0.98	0.05	74,75,77,80	0
2	NAG	I	2	14/15	0.98	0.04	82,84,85,85	0
5	MAN	H	4	11/12	0.98	0.03	96,98,99,99	0
3	NAG	F	1	14/15	0.98	0.05	80,81,83,85	0
5	NAG	L	1	14/15	0.98	0.05	76,79,84,88	0
3	FUC	F	2	10/11	0.98	0.03	78,79,80,80	0
5	BMA	L	3	11/12	0.98	0.04	97,98,98,98	0
5	MAN	L	4	11/12	0.98	0.03	96,98,98,98	0
5	FUC	L	5	10/11	0.98	0.05	84,85,86,86	0
2	NAG	E	2	14/15	0.98	0.04	88,91,92,92	0
2	NAG	E	1	14/15	0.99	0.03	75,77,80,84	0
4	NAG	K	1	14/15	0.99	0.04	75,76,78,81	0
4	NAG	G	1	14/15	0.99	0.04	72,75,77,80	0
4	NAG	G	2	14/15	0.99	0.04	85,86,89,92	0
6	NAG	J	1	14/15	0.99	0.03	80,83,86,89	0
5	NAG	H	1	14/15	0.99	0.03	82,86,91,93	0
6	FUC	J	3	10/11	0.99	0.04	82,83,84,84	0

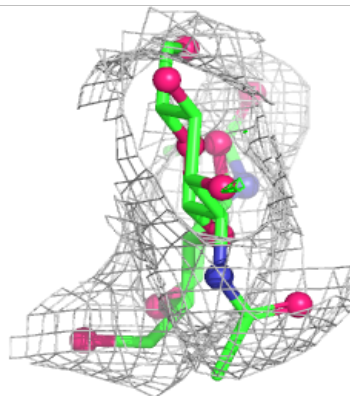
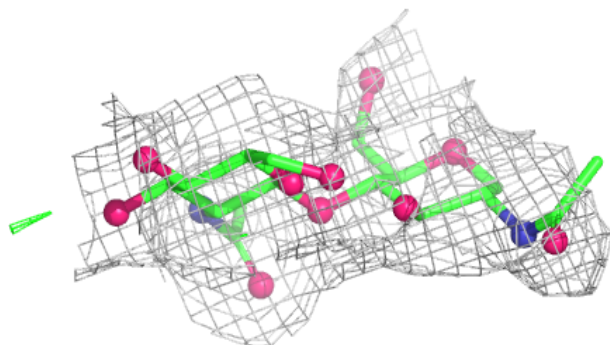
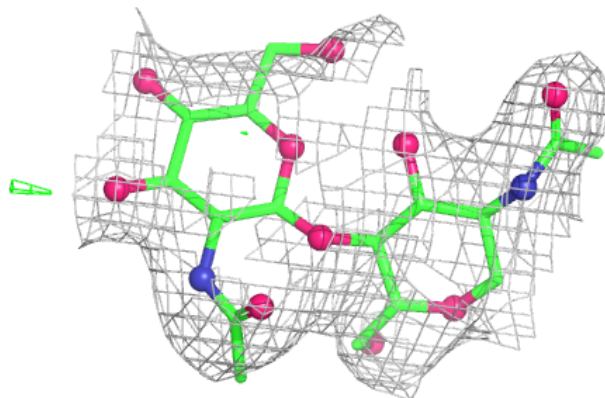
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

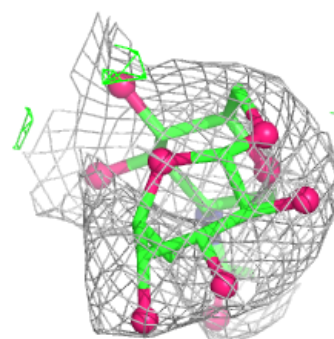
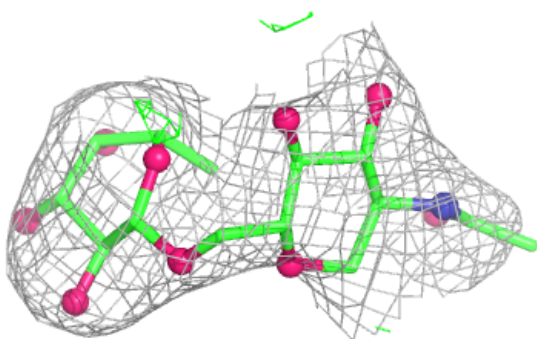
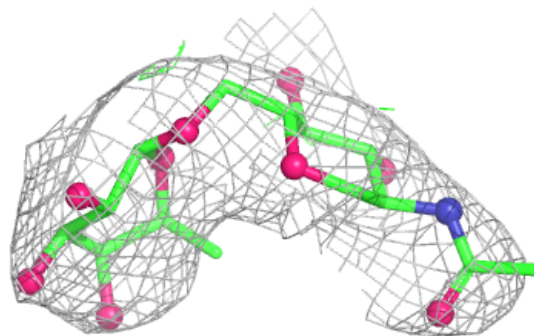
**Electron density around Chain I:**

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

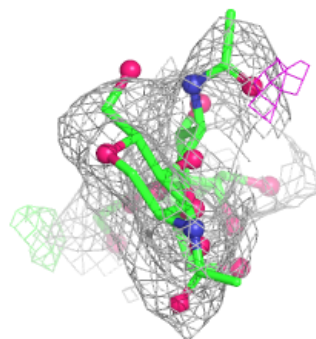
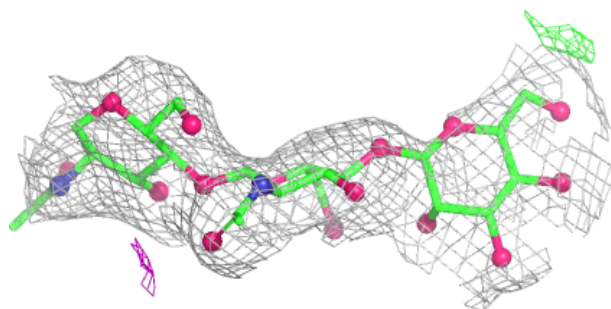
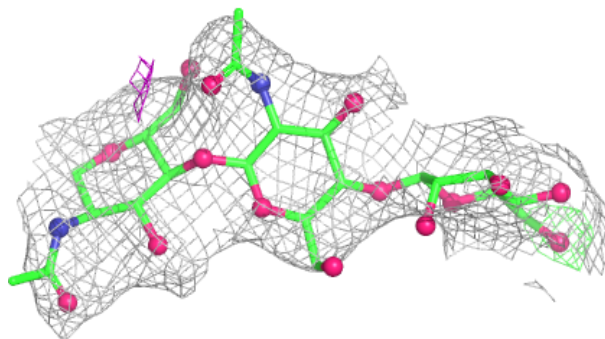


Electron density around Chain F:

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

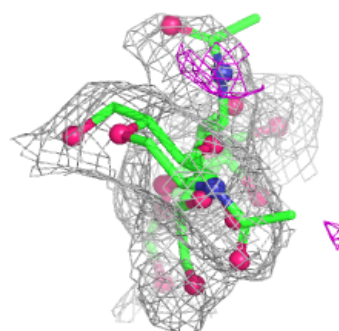
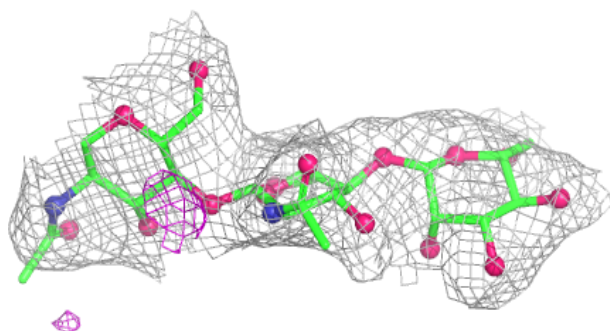
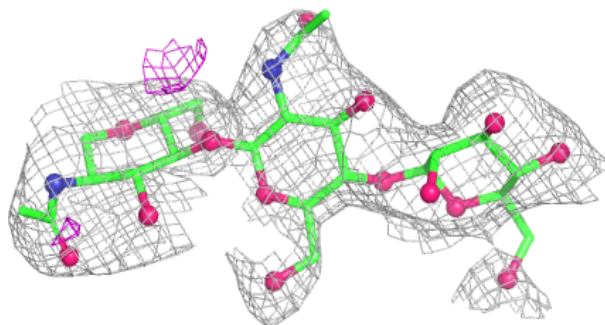
**Electron density around Chain G:**

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

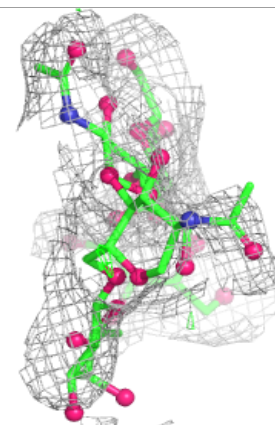
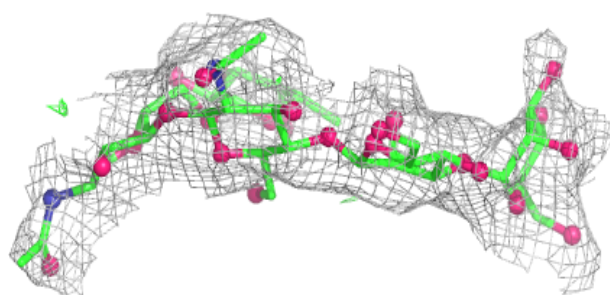
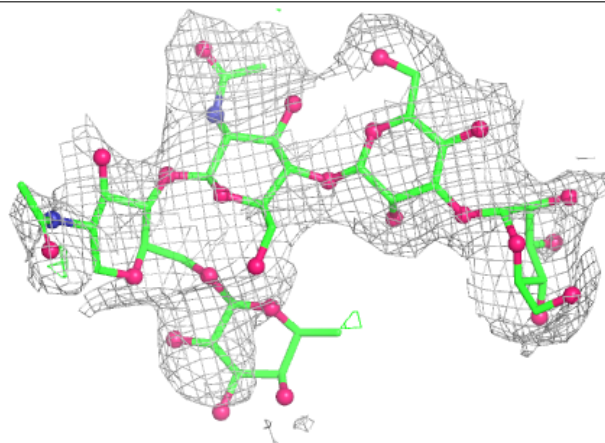


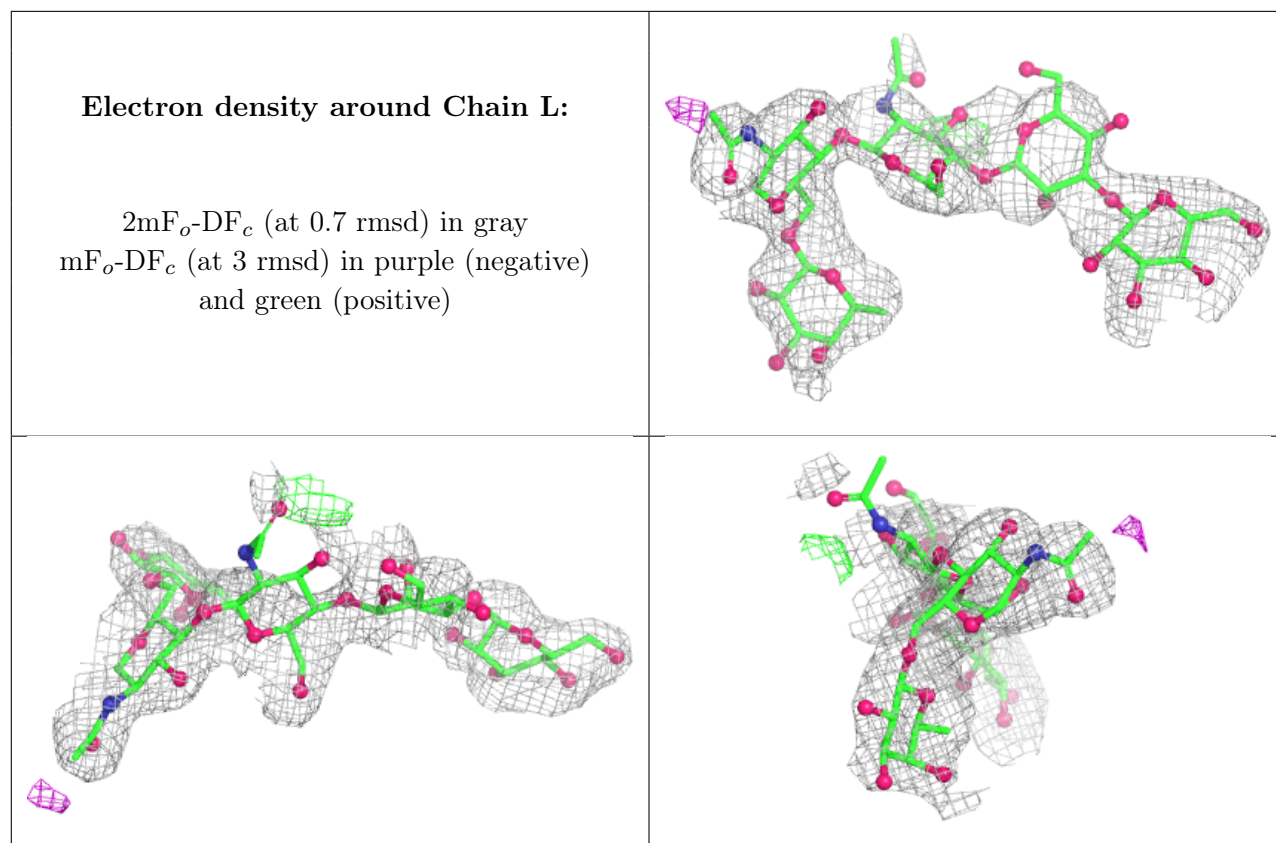
Electron density around Chain K:

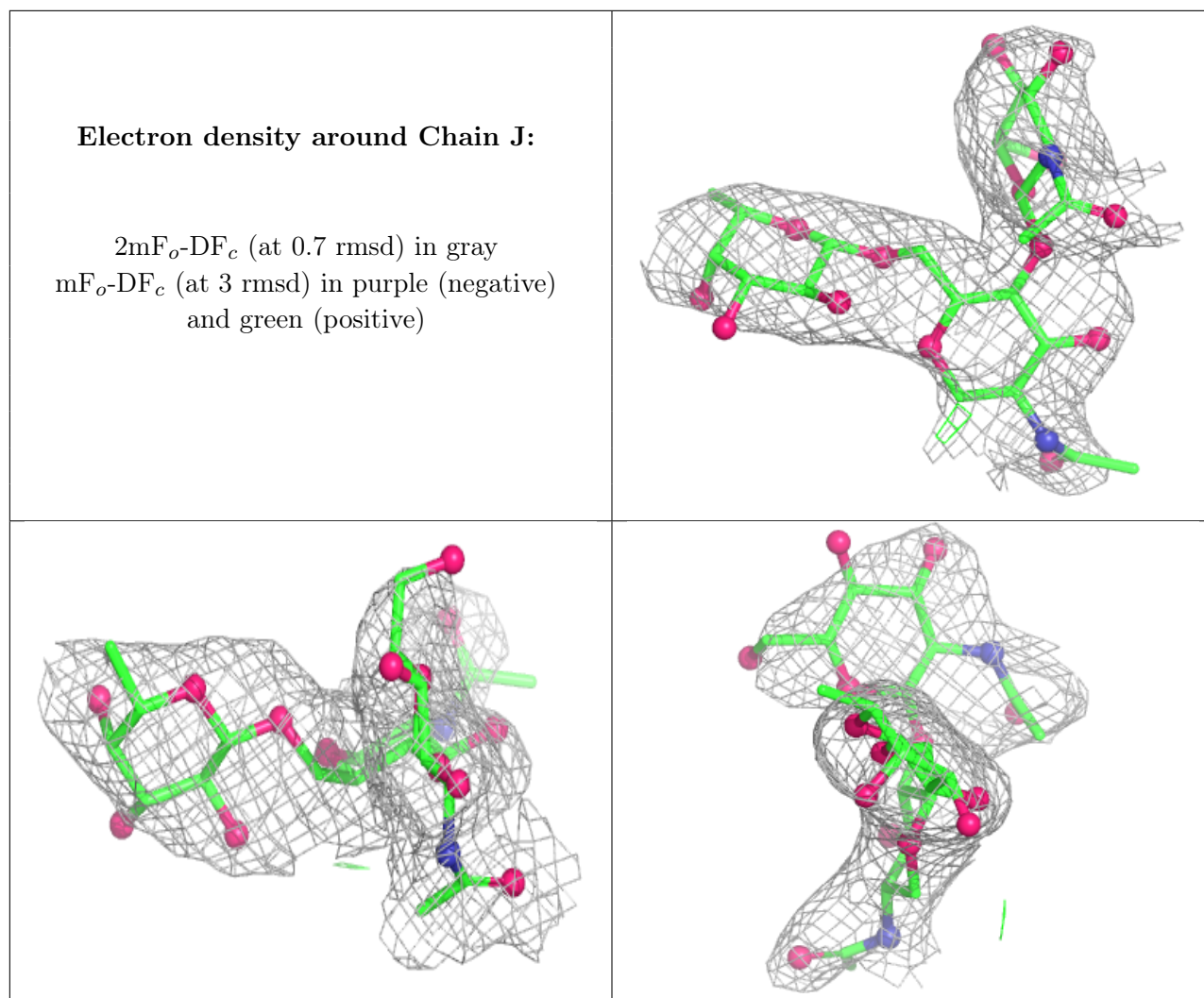
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain H:**

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







6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	1736	14/15	0.94	0.05	84,86,88,88	0
7	NAG	B	1738	14/15	0.94	0.05	81,83,84,85	0
7	NAG	C	1735	14/15	0.96	0.04	70,72,73,74	0
7	NAG	D	1738	14/15	0.96	0.05	81,83,85,85	0
7	NAG	D	1736	14/15	0.97	0.03	83,84,86,86	0
7	NAG	A	1735	14/15	0.98	0.03	84,86,88,89	0
7	NAG	C	1736	14/15	0.98	0.04	82,85,88,88	0
7	NAG	D	1735	14/15	0.99	0.03	71,74,76,77	0
7	NAG	A	1734	14/15	0.99	0.03	71,73,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	B	1735	14/15	0.99	0.04	69,70,73,73	0
8	CA	D	1743	1/1	0.99	0.02	46,46,46,46	0
9	CU	A	1740	1/1	0.99	0.02	81,81,81,81	0
9	CU	A	1743	1/1	0.99	0.02	84,84,84,84	0
9	CU	A	1744	1/1	0.99	0.02	74,74,74,74	0
9	CU	B	1747	1/1	0.99	0.02	81,81,81,81	0
9	CU	B	1748	1/1	0.99	0.02	66,66,66,66	0
9	CU	B	1750	1/1	0.99	0.02	63,63,63,63	0
9	CU	C	1742	1/1	0.99	0.03	84,84,84,84	0
9	CU	C	1744	1/1	0.99	0.03	90,90,90,90	0
9	CU	C	1747	1/1	0.99	0.02	84,84,84,84	0
9	CU	D	1745	1/1	0.99	0.02	79,79,79,79	0
9	CU	D	1746	1/1	0.99	0.02	78,78,78,78	0
9	CU	D	1747	1/1	0.99	0.07	82,82,82,82	0
8	CA	B	1743	1/1	1.00	0.02	47,47,47,47	0
9	CU	A	1745	1/1	1.00	0.02	80,80,80,80	0
9	CU	B	1742	1/1	1.00	0.01	55,55,55,55	0
9	CU	B	1744	1/1	1.00	0.02	76,76,76,76	0
9	CU	B	1745	1/1	1.00	0.01	75,75,75,75	0
9	CU	B	1746	1/1	1.00	0.01	71,71,71,71	0
8	CA	C	1737	1/1	1.00	0.01	50,50,50,50	0
8	CA	C	1739	1/1	1.00	0.01	50,50,50,50	0
9	CU	B	1749	1/1	1.00	0.03	69,69,69,69	0
8	CA	D	1741	1/1	1.00	0.01	47,47,47,47	0
9	CU	C	1738	1/1	1.00	0.01	49,49,49,49	0
9	CU	C	1741	1/1	1.00	0.01	79,79,79,79	0
8	CA	A	1736	1/1	1.00	0.02	52,52,52,52	0
9	CU	C	1743	1/1	1.00	0.02	73,73,73,73	0
9	CU	A	1737	1/1	1.00	0.01	49,49,49,49	0
9	CU	C	1745	1/1	1.00	0.02	77,77,77,77	0
9	CU	C	1746	1/1	1.00	0.03	67,67,67,67	0
8	CA	A	1738	1/1	1.00	0.02	49,49,49,49	0
9	CU	D	1742	1/1	1.00	0.02	52,52,52,52	0
9	CU	A	1741	1/1	1.00	0.02	83,83,83,83	0
9	CU	A	1742	1/1	1.00	0.02	77,77,77,77	0
8	CA	B	1741	1/1	1.00	0.02	46,46,46,46	0
9	CU	D	1748	1/1	1.00	0.01	74,74,74,74	0
9	CU	D	1749	1/1	1.00	0.01	67,67,67,67	0
9	CU	D	1750	1/1	1.00	0.02	67,67,67,67	0
10	CL	A	1739	1/1	1.00	0.03	47,47,47,47	0
10	CL	A	1746	1/1	1.00	0.03	47,47,47,47	0
10	CL	C	1740	1/1	1.00	0.03	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	CL	D	1744	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.