



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 4PE5 / pdb_00004pe5
Title : Crystal Structure of GluN1a/GluN2B NMDA Receptor Ion Channel
Authors : Karakas, E.; Furukawa, H.
Deposited on : 2014-04-22
Resolution : 3.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

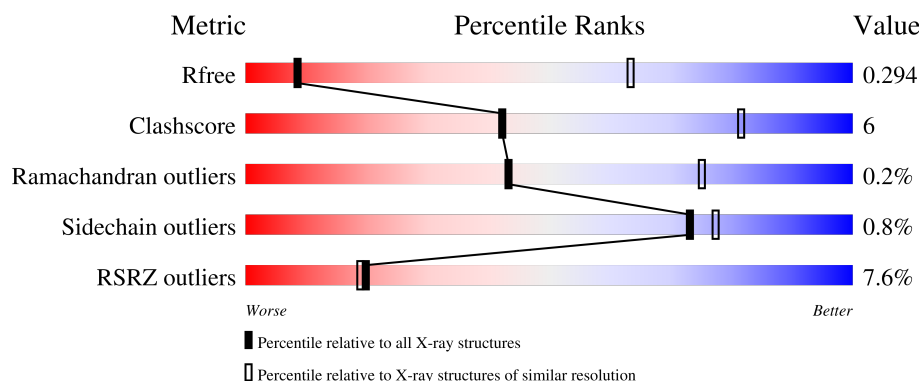
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	825	7% 79% 11% 10%
1	C	825	8% 81% 10% 9%
2	B	820	6% 77% 10% 12%
2	D	820	7% 77% 11% 11%
3	E	4	75% 25%

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Mol	Chain	Length	Quality of chain
3	I	4	
3	J	4	
4	F	6	
5	G	6	
6	H	2	

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
5	MAN	G	5	-	-	X	-
5	MAN	G	6	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20246 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5049	3173	884	967	25			
1	C	754	Total	C	N	O	S	0	0	0
			5026	3175	874	954	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP P35439
A	239	ASP	ASN	engineered mutation	UNP P35439
A	350	GLN	ASN	engineered mutation	UNP P35439
A	471	GLN	ASN	engineered mutation	UNP P35439
A	491	GLN	ASN	engineered mutation	UNP P35439
A	561	CYS	THR	engineered mutation	UNP P35439
A	594	GLN	GLU	engineered mutation	UNP P35439
A	595	SER	GLU	engineered mutation	UNP P35439
A	597	SER	GLU	engineered mutation	UNP P35439
A	598	THR	GLU	engineered mutation	UNP P35439
A	771	GLN	ASN	engineered mutation	UNP P35439
A	810	CYS	PHE	engineered mutation	UNP P35439
A	844	ASN	ARG	engineered mutation	UNP P35439
A	845	GLY	ARG	engineered mutation	UNP P35439
A	846	ALA	LYS	engineered mutation	UNP P35439
C	61	GLN	ASN	engineered mutation	UNP P35439
C	239	ASP	ASN	engineered mutation	UNP P35439
C	350	GLN	ASN	engineered mutation	UNP P35439
C	471	GLN	ASN	engineered mutation	UNP P35439
C	491	GLN	ASN	engineered mutation	UNP P35439
C	561	CYS	THR	engineered mutation	UNP P35439
C	594	GLN	GLU	engineered mutation	UNP P35439
C	595	SER	GLU	engineered mutation	UNP P35439
C	597	SER	GLU	engineered mutation	UNP P35439
C	598	THR	GLU	engineered mutation	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	GLN	ASN	engineered mutation	UNP P35439
C	810	CYS	PHE	engineered mutation	UNP P35439
C	844	ASN	ARG	engineered mutation	UNP P35439
C	845	GLY	ARG	engineered mutation	UNP P35439
C	846	ALA	LYS	engineered mutation	UNP P35439

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	720	Total	C	N	O	S	0	0	0
			4798	3048	788	933	29			
2	D	727	Total	C	N	O	S	0	0	0
			4777	3027	809	912	29			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	214	CYS	SER	engineered mutation	UNP Q00960
B	348	ASP	ASN	engineered mutation	UNP Q00960
B	?	-	CYS	deletion	UNP Q00960
B	?	-	PRO	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	?	-	GLU	deletion	UNP Q00960
B	557	CYS	ASP	engineered mutation	UNP Q00960
B	588	SER	CYS	engineered mutation	UNP Q00960
B	815	CYS	ILE	engineered mutation	UNP Q00960
B	838	SER	CYS	engineered mutation	UNP Q00960
B	849	SER	CYS	engineered mutation	UNP Q00960
D	214	CYS	SER	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960
D	?	-	CYS	deletion	UNP Q00960
D	?	-	PRO	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	?	-	GLU	deletion	UNP Q00960
D	557	CYS	ASP	engineered mutation	UNP Q00960
D	588	SER	CYS	engineered mutation	UNP Q00960
D	815	CYS	ILE	engineered mutation	UNP Q00960
D	838	SER	CYS	engineered mutation	UNP Q00960

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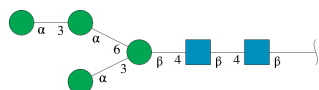
Chain	Residue	Modelled	Actual	Comment	Reference
D	849	SER	CYS	engineered mutation	UNP Q00960

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
4	F	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

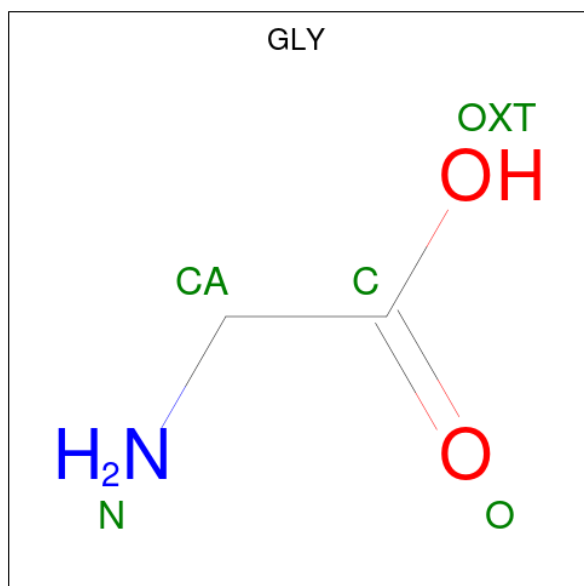


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is TUNGSTEN ION (CCD ID: W) (formula: W).

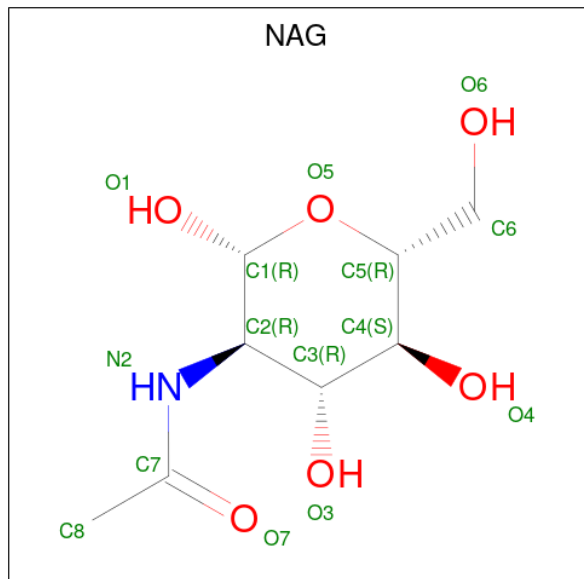
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	37	Total	W	0	0
			37	37		
7	B	11	Total	W	0	0
			11	11		
7	C	36	Total	W	0	0
			36	36		

- Molecule 8 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



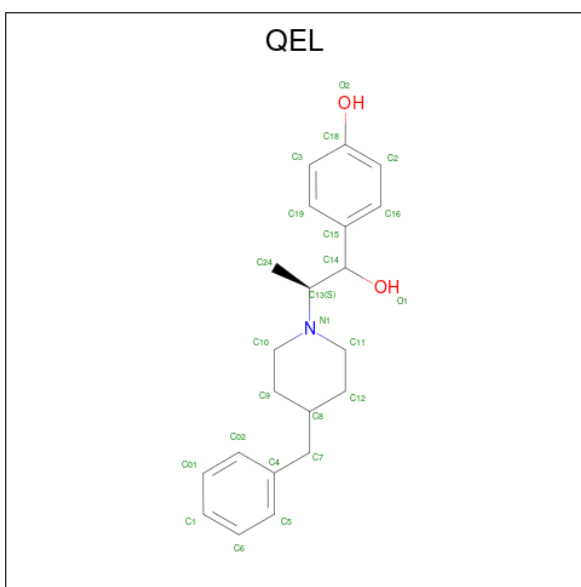
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			5	2	1	2		
8	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



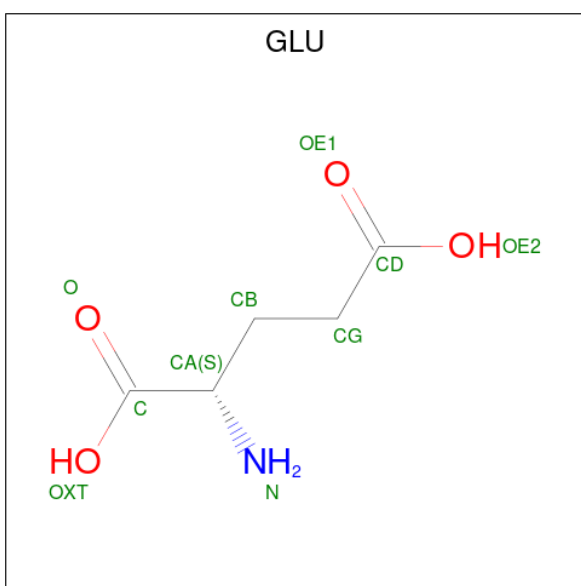
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1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

- Molecule 10 is 4-[(1R,2S)-2-(4-benzylpiperidin-1-yl)-1-hydroxypropyl]phenol (CCD ID: QEL) (formula: $C_{21}H_{27}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			24	21	1	2		
10	C	1	Total	C	N	O	0	0
			24	21	1	2		

- Molecule 11 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).

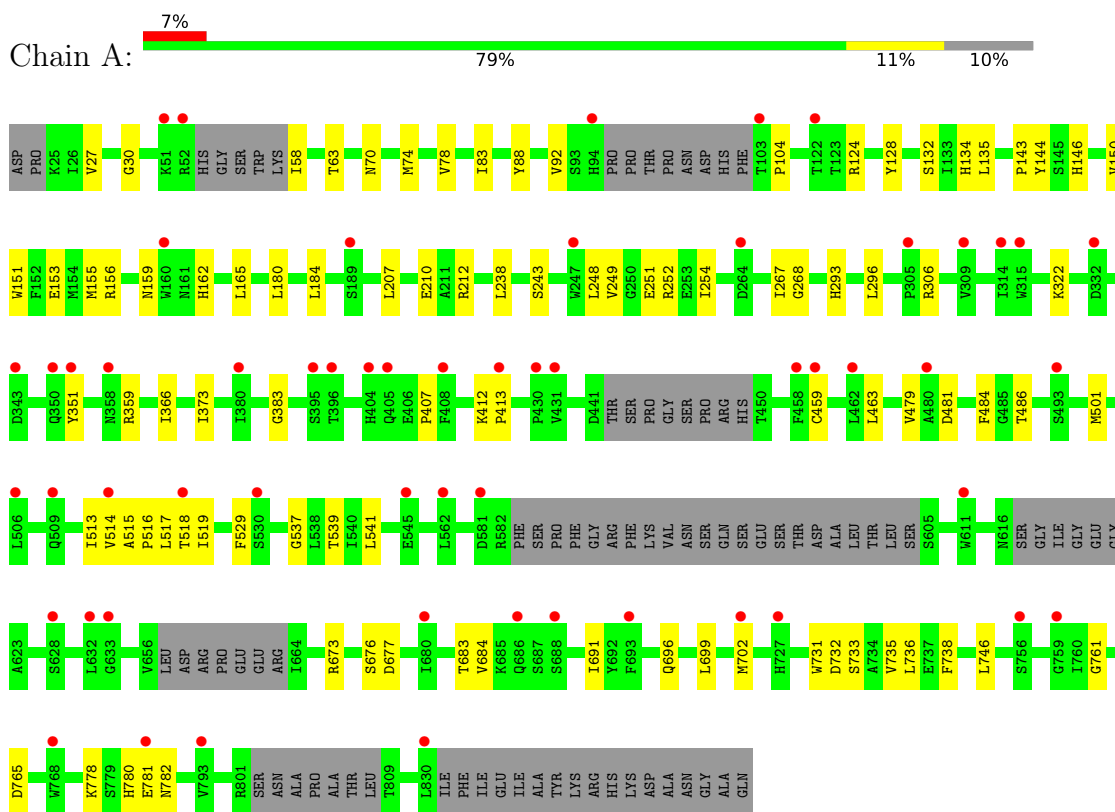


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			10	5	1	4		
11	D	1	Total	C	N	O	0	0
			10	5	1	4		

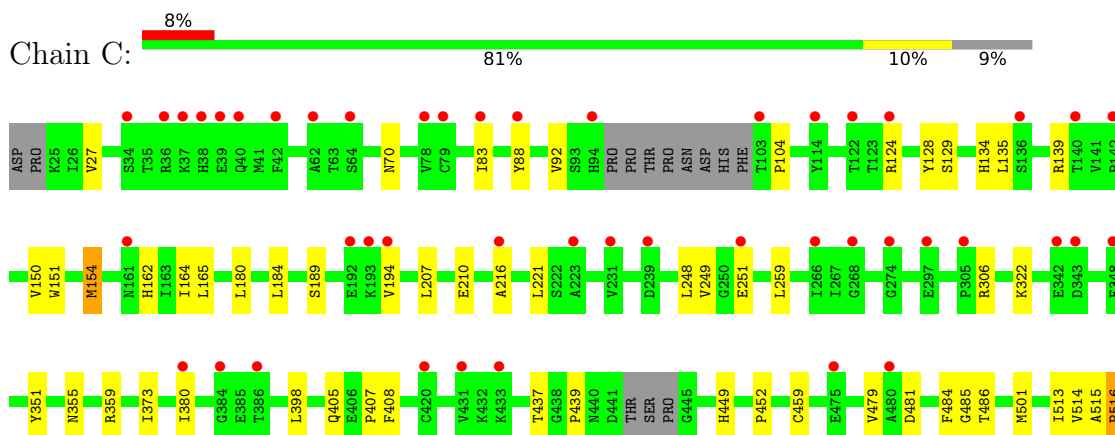
3 Residue-property plots

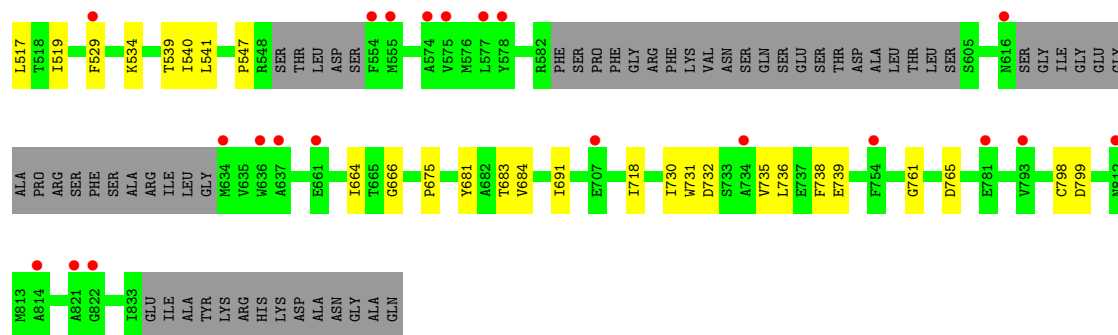
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate receptor ionotropic, NMDA 1

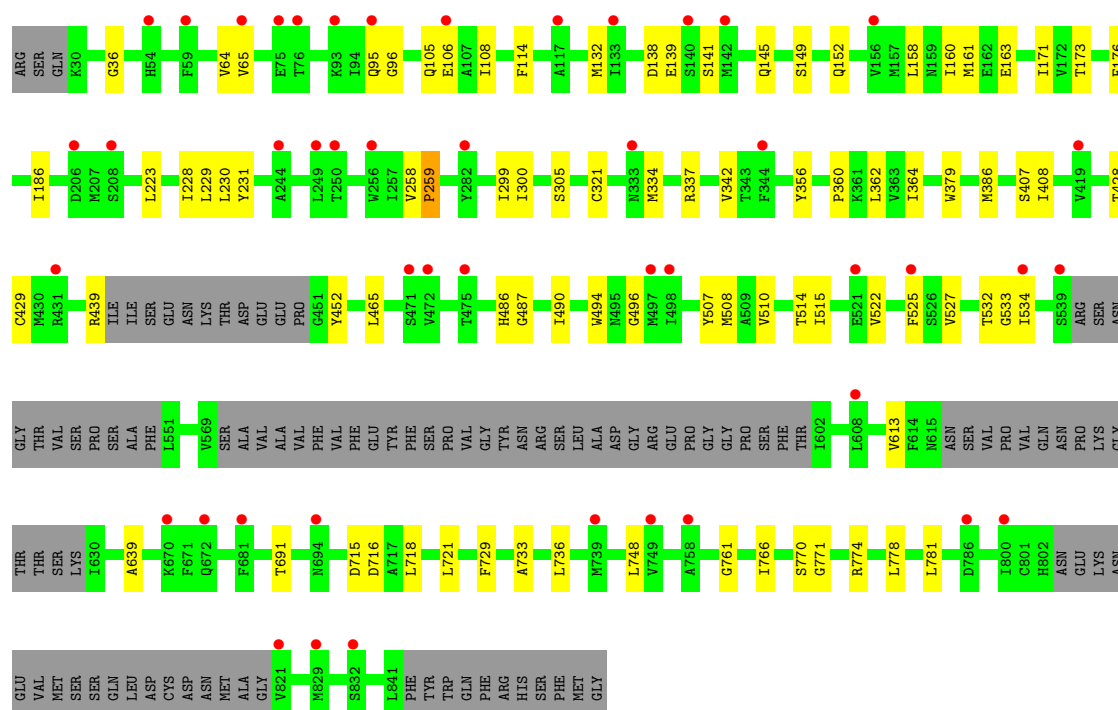
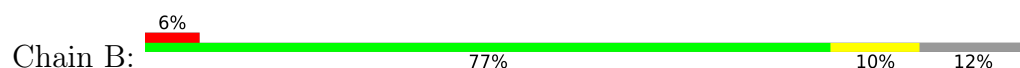


- Molecule 1: Glutamate receptor ionotropic, NMDA 1

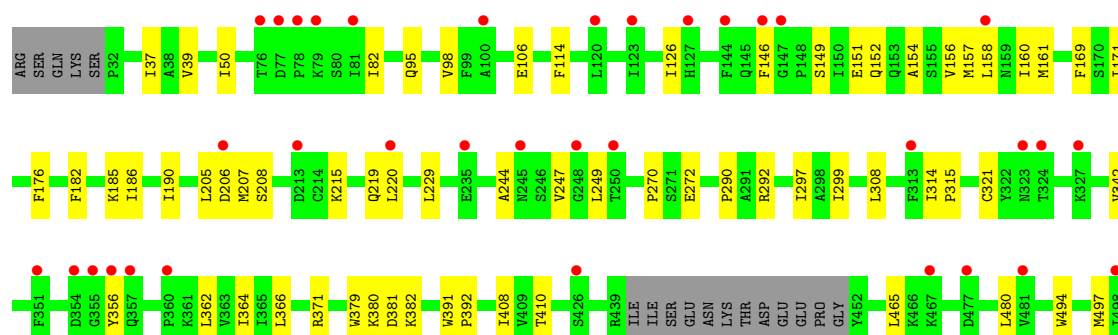
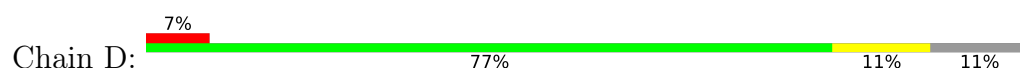


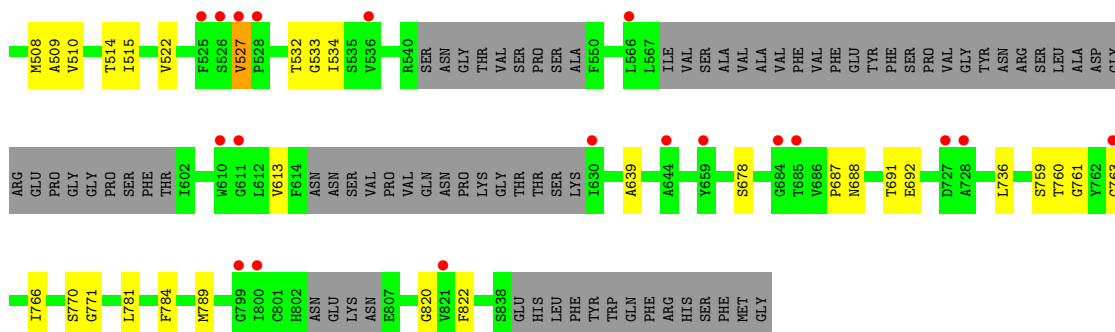


• Molecule 2: Glutamate receptor ionotropic, NMDA 2B



• Molecule 2: Glutamate receptor ionotropic, NMDA 2B





- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 75% 25%



- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 25% 75%



- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 75% 25%



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

Chain F: 17% 83%



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 33% 67%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.83Å 163.19Å 163.14Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	29.72 – 3.96 29.72 – 3.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.72-3.96) 98.1 (29.72-3.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.256 , 0.295 0.259 , 0.294	Depositor DCC
R_{free} test set	2627 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	196.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 107.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20246	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: MAN, NAG, W, BMA, QEL

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	0.29	0/5138	0.78	0/7050
1	C	0.29	0/5118	0.79	0/7035
2	B	0.26	0/4884	0.71	0/6718
2	D	0.29	0/4862	0.76	5/6682 (0.1%)
All	All	0.28	0/20002	0.76	5/27485 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	220	LEU	N-CA-C	-6.91	103.76	111.71
2	D	308	LEU	N-CA-C	-5.71	105.04	112.23
2	D	247	VAL	N-CA-C	-5.43	107.44	112.43
2	D	678	SER	CA-C-N	-5.24	114.98	120.38
2	D	678	SER	C-N-CA	-5.24	114.98	120.38

There are no chirality outliers.

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	5049	0	4271	57	0
1	C	5026	0	4204	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4798	0	3981	52	0
2	D	4777	0	3881	61	0
3	E	50	0	43	1	0
3	I	50	0	43	4	0
3	J	50	0	43	1	0
4	F	72	0	61	0	0
5	G	72	0	61	12	0
6	H	28	0	25	2	0
7	A	37	0	0	0	0
7	B	11	0	0	0	0
7	C	36	0	0	0	0
8	A	5	0	2	2	0
8	C	5	0	2	0	0
9	A	42	0	39	0	0
9	B	28	0	26	0	0
9	C	14	0	13	0	0
9	D	28	0	26	0	0
10	B	24	0	26	6	0
10	C	24	0	26	6	0
11	B	10	0	5	2	0
11	D	10	0	5	2	0
All	All	20246	0	16783	233	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 6.

All (233) 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)
5:G:5:MAN:H61	5:G:6:MAN:H3	1.37	1.00
5:G:5:MAN:H61	5:G:6:MAN:C3	2.00	0.86
2:B:114:PHE:CB	10:B:920:QEL:H6	2.10	0.80
2:D:514:THR:HG1	11:D:907:GLU:N	1.80	0.78
3:I:2:NAG:C3	3:I:3:BMA:H2	2.16	0.75
2:B:114:PHE:CG	10:B:920:QEL:H6	2.20	0.75
5:G:3:BMA:H4	5:G:4:MAN:C1	2.17	0.75
10:C:939:QEL:H6	2:D:114:PHE:CB	2.18	0.73
1:C:70:ASN:ND2	2:D:321:CYS:O	2.21	0.73
5:G:5:MAN:C6	5:G:6:MAN:H5	2.19	0.71
1:C:408:PHE:HD2	1:C:516:PRO:HG3	1.57	0.70
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:THR:HG1	8:A:942:GLY:N	1.90	0.69
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.76	0.67
2:D:95:GLN:NE2	2:D:315:PRO:O	2.25	0.67
3:I:2:NAG:H3	3:I:3:BMA:H2	1.76	0.67
1:C:798:CYS:SG	1:C:799:ASP:N	2.67	0.66
1:A:58:ILE:HD13	1:A:296:LEU:HD12	1.79	0.65
2:D:270:PRO:O	2:D:371:ARG:NH2	2.29	0.65
2:B:114:PHE:HB2	10:B:920:QEL:H6	1.80	0.64
5:G:5:MAN:H61	5:G:6:MAN:H5	1.79	0.64
2:B:514:THR:HG1	11:B:921:GLU:N	1.94	0.64
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.79	0.63
3:I:2:NAG:O3	3:I:3:BMA:H2	1.99	0.62
1:A:212:ARG:NH2	1:A:238:LEU:O	2.31	0.62
1:C:154:MET:HE3	1:C:248:LEU:HD11	1.82	0.61
1:C:162:HIS:NE2	1:C:765:ASP:O	2.31	0.60
2:B:223:LEU:HD13	2:B:228:ILE:HD13	1.85	0.59
1:A:92:VAL:HG11	1:A:104:PRO:HB3	1.83	0.59
1:A:407:PRO:HG3	1:A:735:VAL:HA	1.85	0.59
2:B:171:ILE:HD11	2:B:186:ILE:HG21	1.85	0.58
1:A:162:HIS:NE2	1:A:765:ASP:O	2.34	0.58
1:C:129:SER:OG	1:C:139:ARG:NH2	2.35	0.58
2:B:465:LEU:HD13	2:B:510:VAL:HG11	1.86	0.57
1:A:153:GLU:OE1	1:A:156:ARG:NH1	2.37	0.57
5:G:5:MAN:H61	5:G:6:MAN:C5	2.34	0.57
2:B:158:LEU:HA	2:B:161:MET:HE3	1.85	0.57
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.88	0.56
1:C:407:PRO:HG3	1:C:735:VAL:HA	1.87	0.56
1:C:135:LEU:HD11	10:C:939:QEL:C2	2.36	0.55
2:B:299:ILE:HA	2:B:342:VAL:HG11	1.87	0.55
1:C:519:ILE:HG23	1:C:529:PHE:HD2	1.72	0.55
2:D:687:PRO:HG2	3:J:1:NAG:H82	1.89	0.55
10:C:939:QEL:H6	2:D:114:PHE:CG	2.42	0.55
2:B:718:LEU:HD11	2:B:748:LEU:HG	1.89	0.54
5:G:5:MAN:C6	5:G:6:MAN:C5	2.85	0.54
2:D:534:ILE:HG12	2:D:691:THR:HG22	1.89	0.54
1:C:124:ARG:NH1	1:C:251:GLU:OE1	2.40	0.54
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.90	0.54
1:A:243:SER:HA	1:A:383:GLY:HA3	1.88	0.54
2:B:534:ILE:HG12	2:B:691:THR:HG22	1.89	0.54
1:C:484:PHE:O	1:C:501:MET:N	2.35	0.54
2:D:760:THR:OG1	2:D:761:GLY:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASN:ND2	2:B:321:CYS:O	2.35	0.54
1:A:780:HIS:ND1	2:D:759:SER:O	2.40	0.53
1:A:484:PHE:O	1:A:501:MET:N	2.34	0.53
2:D:366:LEU:HD13	2:D:391:TRP:HZ2	1.72	0.53
2:D:532:THR:OG1	2:D:533:GLY:N	2.39	0.53
2:D:688:ASN:N	2:D:692:GLU:OE2	2.41	0.53
2:B:132:MET:O	2:B:145:GLN:NE2	2.37	0.53
2:B:527:VAL:HG21	2:B:781:LEU:HD21	1.90	0.53
2:D:527:VAL:HG21	2:D:781:LEU:HD21	1.91	0.53
5:G:5:MAN:C6	5:G:6:MAN:H3	2.26	0.53
2:B:465:LEU:HD22	2:B:510:VAL:HG21	1.91	0.52
2:B:64:VAL:HG12	2:B:305:SER:HB2	1.90	0.52
1:A:778:LYS:O	1:A:782:ASN:ND2	2.42	0.52
2:B:532:THR:OG1	2:B:533:GLY:N	2.36	0.52
2:D:408:ILE:HG12	2:D:508:MET:HB2	1.90	0.52
2:B:106:GLU:HG3	2:B:176:PHE:CE1	2.45	0.52
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.92	0.51
1:A:135:LEU:HD11	10:B:920:QEL:C2	2.40	0.51
1:A:683:THR:OG1	1:A:684:VAL:N	2.42	0.51
1:A:519:ILE:HG23	1:A:529:PHE:HD2	1.75	0.51
1:C:683:THR:OG1	1:C:684:VAL:N	2.43	0.51
2:B:152:GLN:HE22	2:B:360:PRO:HD2	1.76	0.51
2:B:138:ASP:HB3	2:B:141:SER:HB2	1.93	0.51
1:C:407:PRO:HB3	1:C:738:PHE:CG	2.46	0.51
1:A:124:ARG:NH1	1:A:251:GLU:OE1	2.43	0.50
1:C:180:LEU:O	1:C:184:LEU:HG	2.11	0.50
1:C:373:ILE:HD11	6:H:1:NAG:O5	2.11	0.50
1:A:165:LEU:HD22	1:A:180:LEU:HD23	1.94	0.50
2:B:106:GLU:HG3	2:B:176:PHE:HE1	1.76	0.50
2:D:465:LEU:HD22	2:D:510:VAL:HG21	1.94	0.50
1:A:479:VAL:HG22	1:A:481:ASP:H	1.76	0.49
2:B:149:SER:HB3	2:B:356:TYR:CD1	2.47	0.49
2:D:158:LEU:HA	2:D:161:MET:HE3	1.93	0.49
2:D:784:PHE:HE1	2:D:789:MET:HG2	1.77	0.49
2:D:820:GLY:O	2:D:822:PHE:N	2.41	0.49
2:B:160:ILE:HD11	2:B:364:ILE:HG12	1.93	0.49
2:B:161:MET:HE1	2:B:229:LEU:HD11	1.95	0.49
10:C:939:QEL:H6	2:D:114:PHE:HB2	1.94	0.49
2:B:494:TRP:HE1	2:B:522:VAL:HG11	1.76	0.49
1:A:58:ILE:HG21	1:A:296:LEU:HD13	1.94	0.48
1:C:405:GLN:HG2	1:C:516:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:GLY:HA2	2:B:496:GLY:HA3	1.96	0.48
2:B:486:HIS:CE1	11:B:921:GLU:HB2	2.49	0.48
1:A:180:LEU:O	1:A:184:LEU:HG	2.13	0.48
1:A:673:ARG:HD3	1:A:702:MET:HE3	1.95	0.48
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.78	0.48
2:D:205:LEU:HB3	2:D:207:MET:HE3	1.96	0.47
1:A:463:LEU:HD13	1:A:514:VAL:HG21	1.97	0.47
1:C:539:THR:HG23	1:C:736:LEU:HD12	1.96	0.47
1:C:479:VAL:HG22	1:C:481:ASP:H	1.79	0.47
1:C:486:THR:HG22	1:C:691:ILE:HD11	1.96	0.47
2:D:613:VAL:HA	2:D:639:ALA:HB1	1.97	0.47
2:B:408:ILE:HG12	2:B:508:MET:HB2	1.96	0.47
2:D:465:LEU:HD13	2:D:510:VAL:HG11	1.96	0.47
2:D:494:TRP:HE1	2:D:522:VAL:HG11	1.79	0.47
2:B:231:TYR:HD1	2:B:259:PRO:HG2	1.79	0.47
1:A:537:GLY:O	1:A:733:SER:N	2.42	0.47
1:A:696:GLN:HB3	1:A:699:LEU:HB2	1.97	0.47
2:B:407:SER:O	2:B:507:TYR:N	2.48	0.47
5:G:5:MAN:C6	5:G:6:MAN:C3	2.86	0.47
1:A:128:TYR:HA	1:A:134:HIS:CD2	2.50	0.46
2:D:206:ASP:OD1	2:D:208:SER:OG	2.28	0.46
1:A:539:THR:HG23	1:A:736:LEU:HD12	1.97	0.46
2:D:244:ALA:HB1	2:D:249:LEU:HB2	1.96	0.46
1:A:207:LEU:O	1:A:210:GLU:HB2	2.15	0.46
1:A:778:LYS:HD2	1:A:781:GLU:HG2	1.97	0.46
2:D:152:GLN:O	2:D:156:VAL:HG23	2.16	0.46
1:C:664:ILE:HG22	1:C:666:GLY:H	1.80	0.46
1:A:486:THR:HG22	1:A:691:ILE:HD11	1.97	0.46
1:C:459:CYS:HB3	1:C:514:VAL:HG12	1.96	0.46
1:A:58:ILE:HD11	1:A:293:HIS:CD2	2.50	0.46
2:D:514:THR:OG1	11:D:907:GLU:N	2.44	0.46
1:C:135:LEU:HD22	2:D:208:SER:HB3	1.98	0.45
1:C:398:LEU:HD23	1:C:398:LEU:H	1.80	0.45
1:A:254:ILE:HD13	1:A:268:GLY:HA3	1.97	0.45
1:C:221:LEU:HB3	1:C:249:VAL:HG12	1.99	0.45
1:A:513:ILE:HB	1:A:761:GLY:HA3	1.98	0.45
1:C:27:VAL:HG13	1:C:88:TYR:CD1	2.51	0.45
2:D:126:ILE:O	2:D:292:ARG:NH1	2.45	0.45
1:C:128:TYR:HA	1:C:134:HIS:CD2	2.50	0.45
1:C:437:THR:HA	1:C:452:PRO:HA	1.97	0.45
2:D:508:MET:HG2	2:D:766:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG21	1:A:351:TYR:CD2	2.52	0.45
1:A:373:ILE:HD11	3:E:1:NAG:O5	2.17	0.45
1:A:459:CYS:HB3	1:A:514:VAL:HG12	1.99	0.45
2:D:37:ILE:HD12	2:D:297:ILE:HG23	1.98	0.45
2:B:149:SER:HB3	2:B:356:TYR:CG	2.52	0.45
1:A:366:ILE:HD11	1:A:373:ILE:HD12	1.99	0.45
2:B:163:GLU:HG2	2:B:386:MET:HG3	1.99	0.45
2:D:497:MET:HE2	2:D:509:ALA:HB1	1.99	0.45
2:B:770:SER:OG	2:B:771:GLY:N	2.49	0.45
1:C:150:VAL:HG21	1:C:351:TYR:CD2	2.52	0.45
1:C:731:TRP:CG	1:C:732:ASP:H	2.34	0.45
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.99	0.45
1:A:27:VAL:HG13	1:A:88:TYR:CD1	2.52	0.44
1:A:407:PRO:HB3	1:A:738:PHE:CG	2.51	0.44
2:B:105:GLN:HB2	2:B:108:ILE:HG13	1.97	0.44
2:D:39:VAL:HG22	2:D:98:VAL:HB	2.00	0.44
2:D:515:ILE:HD11	2:D:763:GLY:HA3	1.99	0.44
2:D:391:TRP:HA	2:D:392:PRO:HD3	1.85	0.44
2:D:770:SER:OG	2:D:771:GLY:N	2.48	0.44
1:A:143:PRO:HG2	1:A:146:HIS:CD2	2.52	0.44
2:B:230:LEU:HB3	2:B:258:VAL:HG12	2.00	0.44
1:A:83:ILE:HG22	1:A:306:ARG:O	2.17	0.44
1:A:132:SER:O	10:B:920:QEL:H19	2.16	0.44
1:C:355:ASN:ND2	1:C:380:ILE:H	2.16	0.44
2:D:151:GLU:HB3	2:D:185:LYS:HG2	1.99	0.44
2:D:126:ILE:HG22	2:D:146:PHE:CD1	2.53	0.44
2:B:36:GLY:O	2:B:95:GLN:N	2.50	0.44
2:B:138:ASP:OD1	2:B:139:GLU:N	2.50	0.44
2:B:613:VAL:HA	2:B:639:ALA:HB1	2.00	0.44
1:C:135:LEU:HD11	10:C:939:QEL:C18	2.47	0.44
1:A:515:ALA:O	1:A:517:LEU:N	2.51	0.43
2:D:106:GLU:HG3	2:D:176:PHE:CE1	2.53	0.43
2:B:428:THR:OG1	2:B:429:CYS:N	2.51	0.43
2:B:508:MET:HG2	2:B:766:ILE:HG22	2.00	0.43
2:B:774:ARG:HE	2:B:778:LEU:HD11	1.82	0.43
1:C:83:ILE:HG22	1:C:306:ARG:O	2.18	0.43
5:G:5:MAN:H4	5:G:6:MAN:H3	2.01	0.43
1:A:135:LEU:HD11	10:B:920:QEL:C18	2.49	0.43
2:D:380:LYS:O	2:D:382:LYS:N	2.52	0.43
1:A:30:GLY:HA2	1:A:63:THR:O	2.18	0.43
2:B:532:THR:HG22	2:B:761:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ILE:HG13	1:C:216:ALA:HB3	2.00	0.43
1:C:165:LEU:HB3	1:C:194:VAL:HG12	2.00	0.43
10:C:939:QEL:H6	2:D:114:PHE:HB3	1.99	0.43
1:C:439:PRO:HA	1:C:449:HIS:O	2.18	0.43
1:C:675:PRO:HB3	1:C:681:TYR:HE1	1.83	0.43
1:A:249:VAL:HG22	1:A:267:ILE:O	2.19	0.43
1:A:155:MET:O	1:A:159:ASN:N	2.52	0.43
1:A:541:LEU:HD11	1:A:746:LEU:HB3	1.99	0.43
2:B:96:GLY:HA3	2:B:300:ILE:HD13	2.01	0.43
1:C:515:ALA:O	1:C:517:LEU:N	2.52	0.43
1:C:259:LEU:HD12	1:C:259:LEU:HA	1.83	0.42
1:A:732:ASP:OD2	8:A:942:GLY:N	2.53	0.42
6:H:1:NAG:O4	6:H:1:NAG:N2	2.49	0.42
1:A:144:TYR:CE2	1:A:252:ARG:HD3	2.54	0.42
2:D:149:SER:HB3	2:D:356:TYR:CD1	2.54	0.42
1:C:541:LEU:HB2	1:C:736:LEU:HD22	2.02	0.42
2:D:157:MET:HE1	2:D:182:PHE:HZ	1.85	0.42
2:D:169:PHE:CZ	2:D:190:ILE:HD11	2.54	0.42
2:D:171:ILE:HD11	2:D:186:ILE:HG21	2.02	0.42
1:A:412:LYS:HA	1:A:413:PRO:HD3	1.93	0.42
2:D:149:SER:HB3	2:D:356:TYR:CG	2.55	0.42
2:D:154:ALA:HB1	2:D:186:ILE:HD11	2.01	0.42
1:A:150:VAL:HG21	1:A:351:TYR:HD2	1.85	0.42
2:D:784:PHE:CE1	2:D:789:MET:HG2	2.54	0.42
5:G:5:MAN:H62	5:G:6:MAN:H5	2.00	0.42
1:C:150:VAL:HG21	1:C:351:TYR:HD2	1.85	0.42
1:A:731:TRP:CG	1:A:732:ASP:H	2.38	0.42
2:D:410:THR:HG23	2:D:480:LEU:HD23	2.02	0.42
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.89	0.41
1:A:676:SER:OG	1:A:677:ASP:N	2.50	0.41
2:B:299:ILE:HG23	2:B:342:VAL:HG21	2.01	0.41
1:C:207:LEU:O	1:C:210:GLU:HB2	2.20	0.41
5:G:3:BMA:C4	5:G:4:MAN:C1	2.86	0.41
1:C:151:TRP:HA	1:C:248:LEU:HD21	2.01	0.41
1:C:154:MET:HE2	1:C:154:MET:HB2	1.86	0.41
2:B:334:MET:O	2:B:337:ARG:HG2	2.20	0.41
1:C:184:LEU:HA	1:C:189:SER:HB2	2.03	0.41
1:A:58:ILE:O	1:A:58:ILE:HG13	2.20	0.41
2:B:439:ARG:HA	2:B:452:TYR:HA	2.03	0.41
2:B:533:GLY:O	2:B:733:ALA:N	2.54	0.41
1:C:540:ILE:HG23	1:C:730:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:LYS:O	2:D:219:GLN:HG3	2.21	0.41
1:A:74:MET:O	1:A:78:VAL:HG23	2.21	0.41
1:C:184:LEU:HB3	1:C:189:SER:O	2.20	0.41
1:C:718:ILE:HD13	1:C:739:GLU:HG3	2.03	0.41
2:D:532:THR:HG22	2:D:761:GLY:HA2	2.03	0.41
1:C:513:ILE:HB	1:C:761:GLY:HA3	2.03	0.41
2:D:182:PHE:O	2:D:186:ILE:HG12	2.21	0.41
2:B:721:LEU:HD11	2:B:729:PHE:HB2	2.02	0.40
2:D:160:ILE:HD11	2:D:364:ILE:HG12	2.03	0.40
1:A:151:TRP:HA	1:A:248:LEU:HD21	2.03	0.40
2:B:715:ASP:OD1	2:B:716:ASP:N	2.54	0.40
2:D:156:VAL:O	2:D:160:ILE:HG13	2.21	0.40
3:I:2:NAG:C3	3:I:3:BMA:C2	2.86	0.40
2:D:50:ILE:HA	2:D:290:PRO:HB3	2.04	0.40
2:D:314:ILE:HA	2:D:315:PRO:HD3	1.96	0.40
2:B:515:ILE:HG12	2:B:525:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

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	727/825 (88%)	667 (92%)	59 (8%)	1 (0%)	48	81
1	C	742/825 (90%)	681 (92%)	58 (8%)	3 (0%)	30	65
2	B	708/820 (86%)	656 (93%)	50 (7%)	2 (0%)	36	69
2	D	715/820 (87%)	656 (92%)	58 (8%)	1 (0%)	48	81
All	All	2892/3290 (88%)	2660 (92%)	225 (8%)	7 (0%)	43	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	547	PRO
2	B	490	ILE
2	D	381	ASP
2	B	259	PRO
1	C	516	PRO
1	A	516	PRO
1	C	485	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/710 (59%)	420 (100%)	2 (0%)	81	82
1	C	402/710 (57%)	398 (99%)	4 (1%)	68	76
2	B	394/716 (55%)	392 (100%)	2 (0%)	81	82
2	D	368/716 (51%)	364 (99%)	4 (1%)	65	74
All	All	1586/2852 (56%)	1574 (99%)	12 (1%)	73	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LYS
1	A	359	ARG
2	B	65	VAL
2	B	736	LEU
1	C	154	MET
1	C	322	LYS
1	C	359	ARG
1	C	534	LYS
2	D	82	ILE
2	D	272	GLU
2	D	527	VAL
2	D	736	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	355	ASN
1	A	494	ASN
2	B	152	GLN
2	B	159	ASN
2	B	486	HIS
1	C	355	ASN
1	C	521	ASN
1	C	674	ASN
2	D	486	HIS
2	D	703	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

26 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	E	1	1,3	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.55	0
3	BMA	E	3	3	11,11,12	0.26	0	15,15,17	0.52	0
3	MAN	E	4	3	11,11,12	0.25	0	15,15,17	0.52	0
4	NAG	F	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	0.37	0
4	BMA	F	3	4	11,11,12	1.06	1 (9%)	15,15,17	1.80	4 (26%)
4	MAN	F	4	4	11,11,12	0.68	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	F	5	4	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
4	MAN	F	6	4	11,11,12	0.67	0	15,15,17	1.01	2 (13%)
5	NAG	G	1	5,2	14,14,15	0.29	0	17,19,21	0.42	0
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.39	0
5	BMA	G	3	5	11,11,12	0.26	0	15,15,17	0.52	0
5	MAN	G	4	5	11,11,12	0.25	0	15,15,17	0.52	0
5	MAN	G	5	5	11,11,12	0.27	0	15,15,17	0.52	0
5	MAN	G	6	5	11,11,12	0.25	0	15,15,17	0.64	0
6	NAG	H	1	1,6	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
6	NAG	H	2	6	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	I	1	1,3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	I	2	3	14,14,15	0.41	0	17,19,21	0.87	0
3	BMA	I	3	3	11,11,12	0.27	0	15,15,17	0.68	0
3	MAN	I	4	3	11,11,12	0.67	0	15,15,17	0.99	2 (13%)
3	NAG	J	1	3,2	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	0.56	0
3	BMA	J	3	3	11,11,12	0.27	0	15,15,17	0.52	0
3	MAN	J	4	3	11,11,12	0.26	0	15,15,17	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	2/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	G	6	5	-	2/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	3	BMA	C4-C5	2.35	1.58	1.53
4	F	1	NAG	C1-C2	2.29	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	O5-C5-C6	3.44	114.36	107.66
6	H	1	NAG	C1-O5-C5	2.87	116.04	112.19
4	F	1	NAG	C1-O5-C5	2.83	115.97	112.19
4	F	3	BMA	O2-C2-C1	2.72	115.46	109.22
4	F	3	BMA	O2-C2-C3	2.61	115.56	110.15
4	F	6	MAN	C1-O5-C5	2.40	115.41	112.19
4	F	5	MAN	C1-O5-C5	2.37	115.37	112.19
4	F	4	MAN	C1-O5-C5	2.32	115.29	112.19
3	I	4	MAN	C1-O5-C5	2.30	115.27	112.19
3	I	4	MAN	O2-C2-C3	-2.19	105.62	110.15
4	F	5	MAN	O2-C2-C3	-2.19	105.62	110.15
4	F	3	BMA	O3-C3-C2	2.14	114.43	110.05
4	F	6	MAN	O2-C2-C3	-2.14	105.71	110.15
4	F	4	MAN	O2-C2-C3	-2.14	105.72	110.15

There are no chirality outliers.

All (20) torsion outliers are listed below:

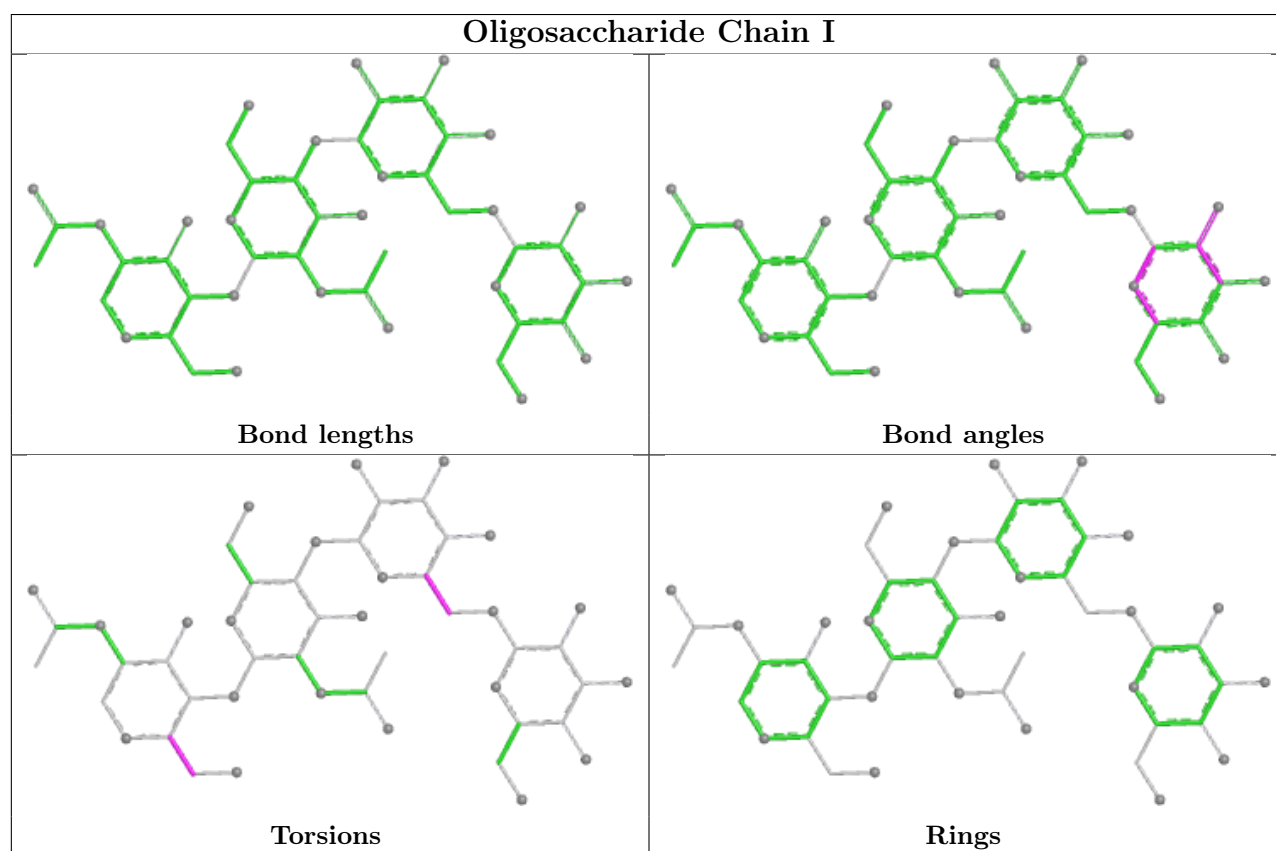
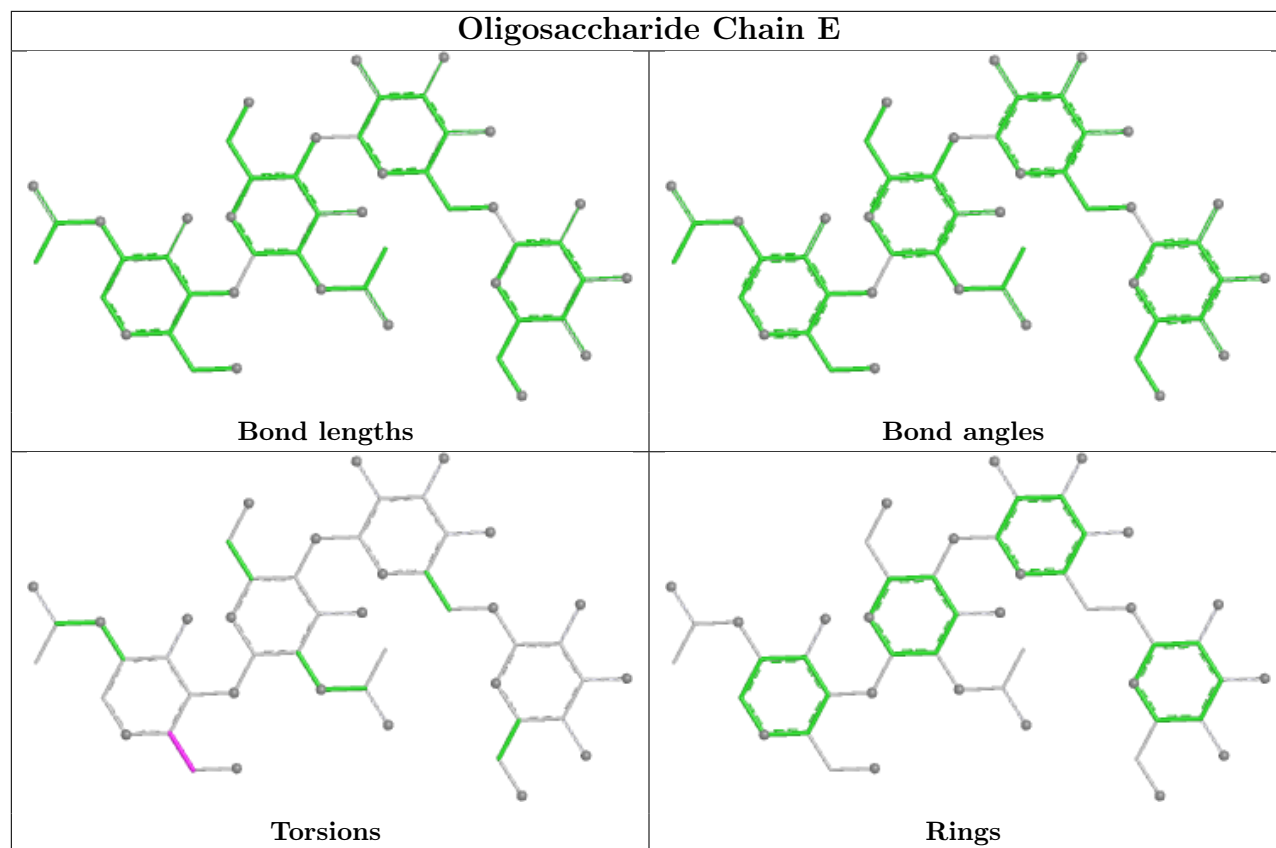
Mol	Chain	Res	Type	Atoms
5	G	6	MAN	O5-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
5	G	5	MAN	C4-C5-C6-O6
5	G	6	MAN	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6

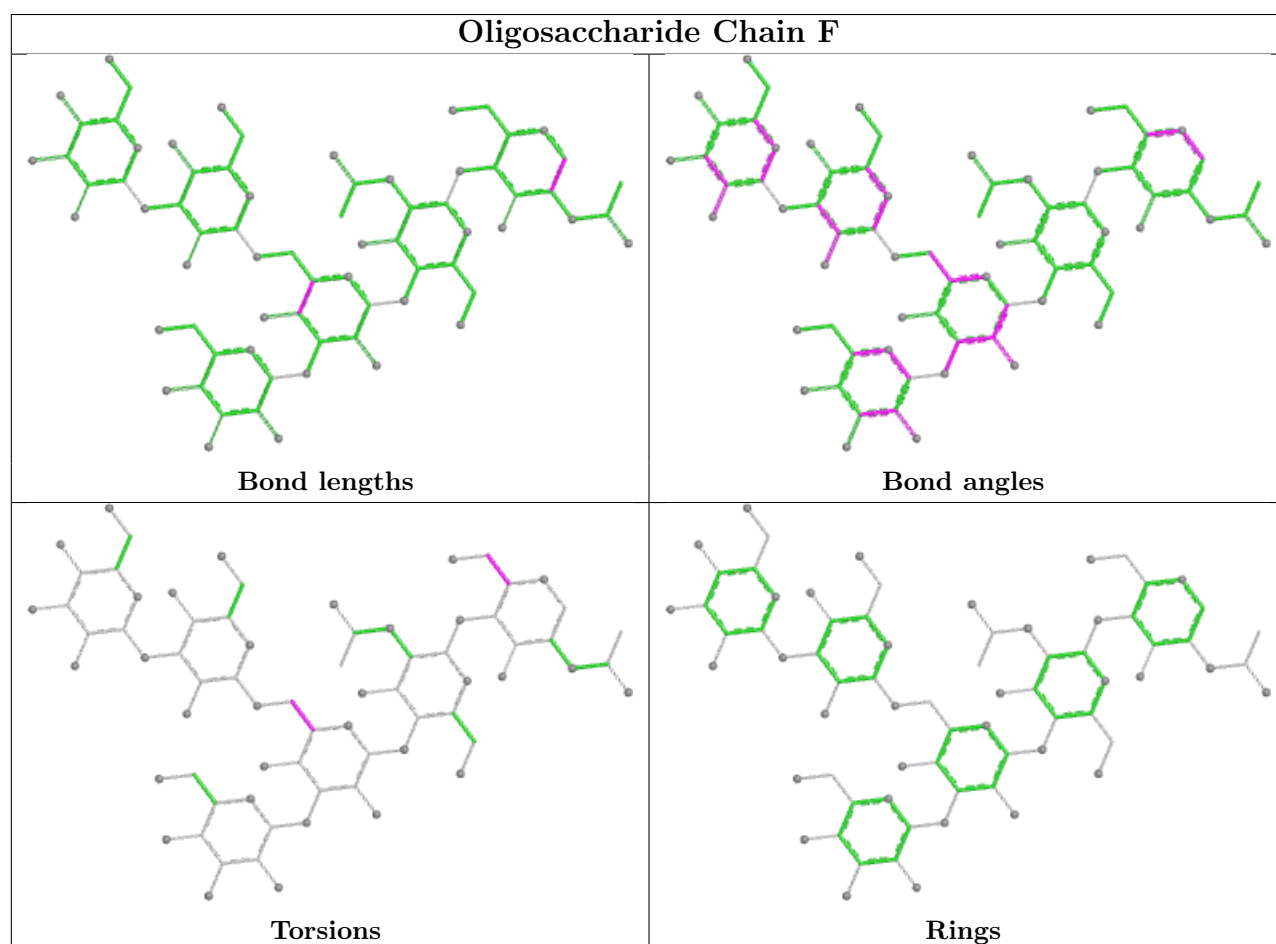
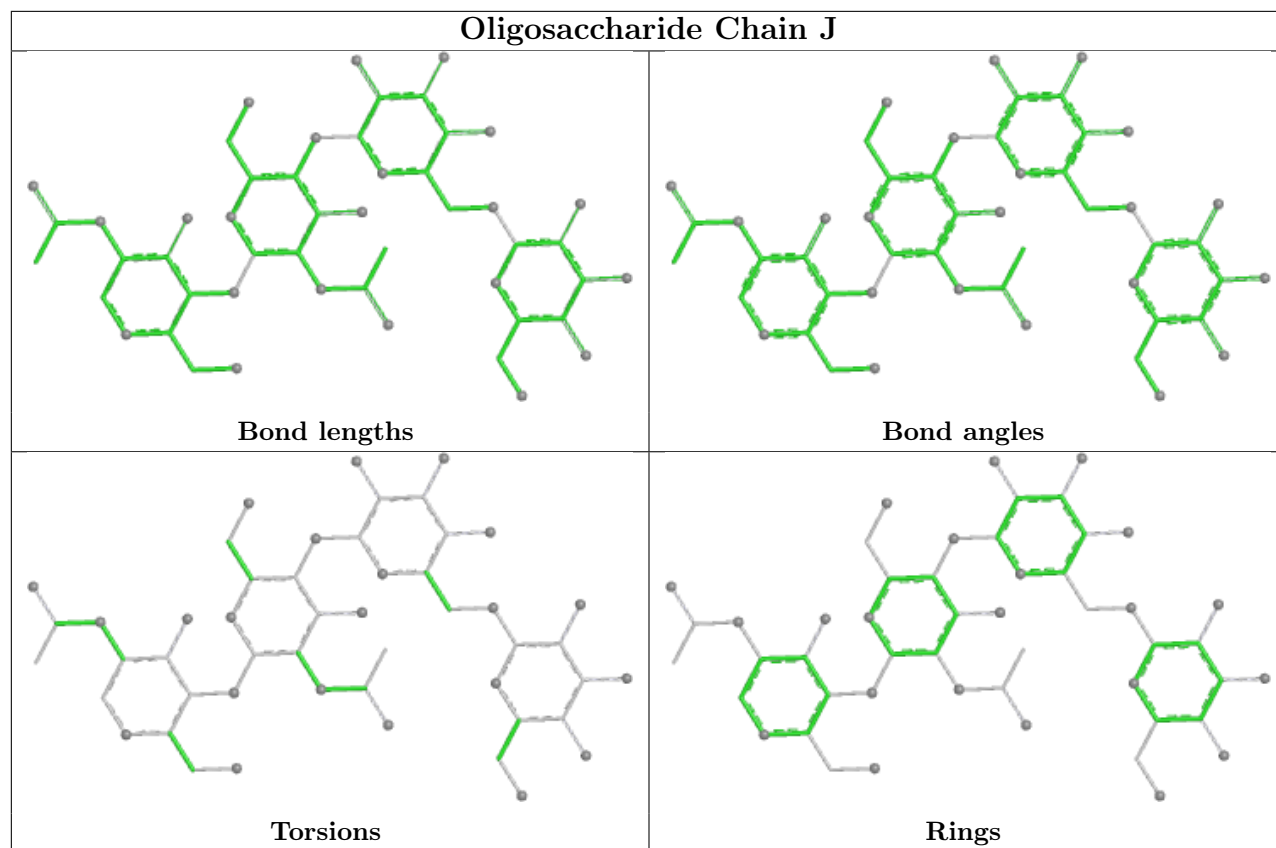
There are no ring outliers.

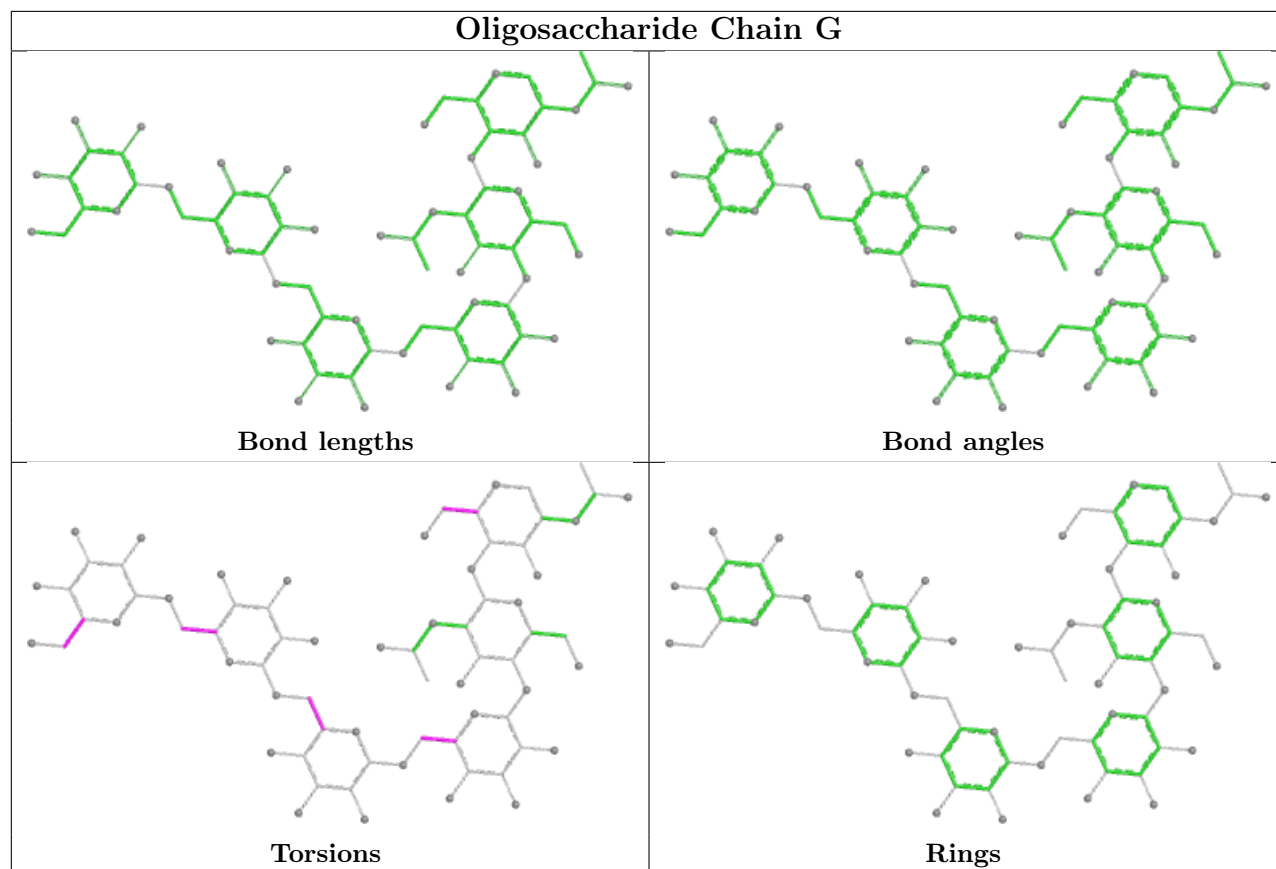
9 monomers are involved in 20 short contacts:

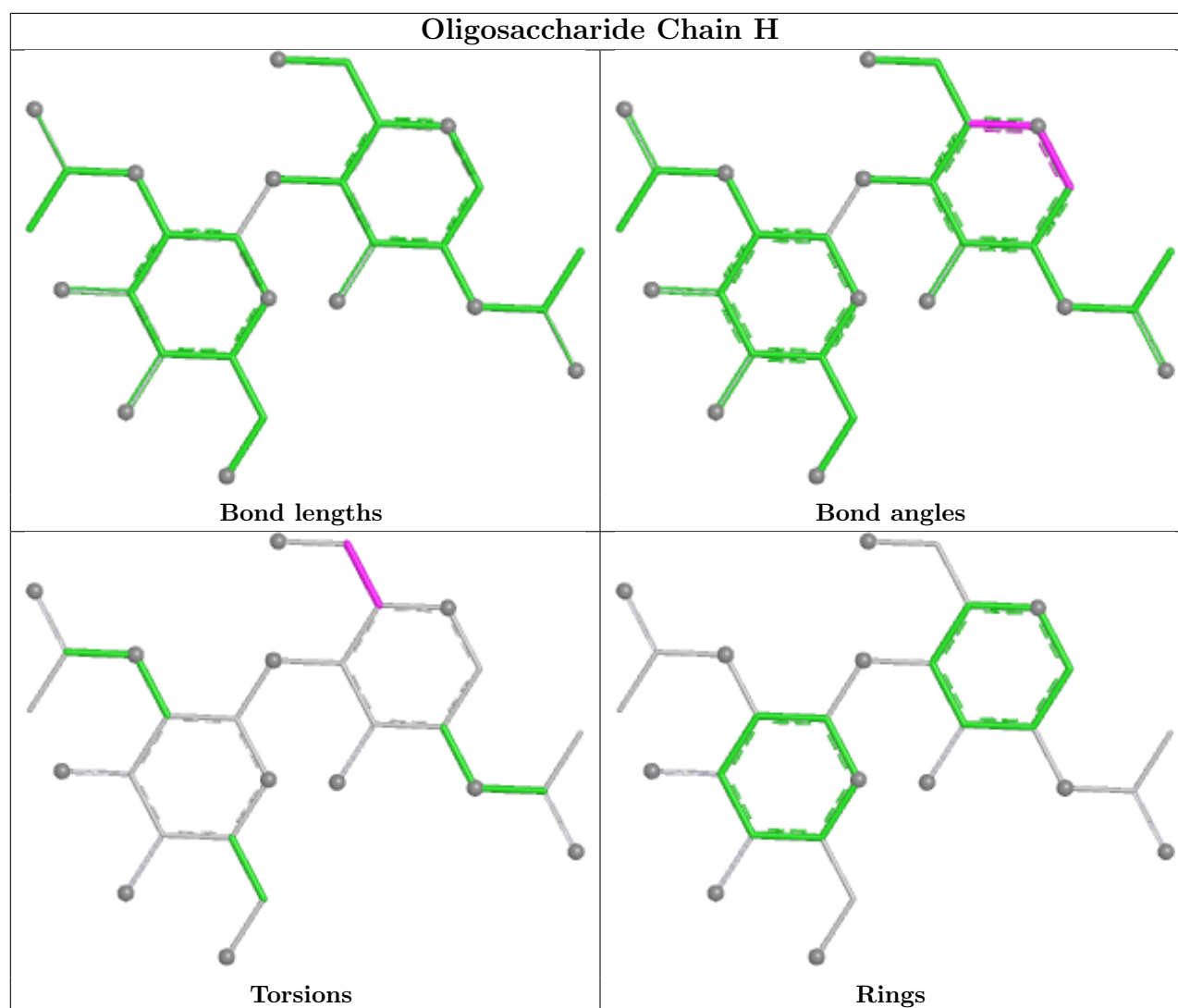
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	4	MAN	2	0
3	E	1	NAG	1	0
5	G	6	MAN	10	0
5	G	5	MAN	10	0
3	J	1	NAG	1	0
3	I	2	NAG	4	0
3	I	3	BMA	4	0
6	H	1	NAG	2	0
5	G	3	BMA	2	0

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 98 ligands modelled in this entry, 84 are monoatomic - leaving 14 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	$\# Z > 2$
9	NAG	D	902	2	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
10	QEL	B	920	-	26,26,26	2.76	9 (34%)	35,35,35	1.75	7 (20%)
11	GLU	D	907	-	8,9,9	1.10	1 (12%)	8,11,11	1.21	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	945	1	14,14,15	0.25	0	17,19,21	0.63	1 (5%)
9	NAG	C	941	1	14,14,15	0.24	0	17,19,21	0.44	0
8	GLY	A	942	-	4,4,4	1.15	1 (25%)	3,4,4	1.64	1 (33%)
10	QEL	C	939	-	26,26,26	2.60	9 (34%)	35,35,35	1.86	7 (20%)
9	NAG	A	944	1	14,14,15	0.22	0	17,19,21	0.38	0
8	GLY	C	940	-	4,4,4	1.16	1 (25%)	3,4,4	1.67	1 (33%)
9	NAG	B	913	2	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	B	912	2	14,14,15	0.21	0	17,19,21	0.36	0
9	NAG	D	901	2	14,14,15	0.29	0	17,19,21	0.35	0
9	NAG	A	943	1	14,14,15	0.28	0	17,19,21	0.49	0
11	GLU	B	921	-	8,9,9	1.09	1 (12%)	8,11,11	1.19	1 (12%)

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
9	NAG	D	902	2	-	2/6/23/26	0/1/1/1
10	QEL	B	920	-	-	5/16/26/26	0/3/3/3
11	GLU	D	907	-	-	2/9/9/9	-
9	NAG	A	945	1	-	0/6/23/26	0/1/1/1
9	NAG	C	941	1	-	2/6/23/26	0/1/1/1
8	GLY	A	942	-	-	0/2/2/2	-
10	QEL	C	939	-	-	5/16/26/26	0/3/3/3
9	NAG	A	944	1	-	2/6/23/26	0/1/1/1
8	GLY	C	940	-	-	0/2/2/2	-
9	NAG	B	913	2	-	2/6/23/26	0/1/1/1
9	NAG	B	912	2	-	2/6/23/26	0/1/1/1
9	NAG	D	901	2	-	2/6/23/26	0/1/1/1
9	NAG	A	943	1	-	2/6/23/26	0/1/1/1
11	GLU	B	921	-	-	0/9/9/9	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	920	QEL	O1-C14	-10.60	1.22	1.42
10	C	939	QEL	O1-C14	-9.54	1.24	1.42
10	B	920	QEL	C14-C13	-3.61	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	939	QEL	C14-C13	-3.60	1.49	1.54
10	B	920	QEL	C3-C18	-3.37	1.32	1.39
10	C	939	QEL	C3-C18	-3.35	1.32	1.39
10	B	920	QEL	C24-C13	-2.81	1.47	1.52
10	C	939	QEL	C24-C13	-2.79	1.47	1.52
10	B	920	QEL	C9-C8	-2.72	1.44	1.52
10	C	939	QEL	C16-C15	-2.71	1.34	1.39
10	C	939	QEL	C9-C8	-2.69	1.44	1.52
10	B	920	QEL	C16-C15	-2.67	1.34	1.39
10	C	939	QEL	C19-C3	2.58	1.43	1.38
10	B	920	QEL	C19-C3	2.54	1.42	1.38
10	B	920	QEL	C16-C2	2.48	1.42	1.38
10	C	939	QEL	C16-C2	2.45	1.42	1.38
11	D	907	GLU	OXT-C	-2.24	1.23	1.30
11	B	921	GLU	OXT-C	-2.23	1.23	1.30
8	C	940	GLY	OXT-C	-2.19	1.23	1.30
8	A	942	GLY	OXT-C	-2.18	1.23	1.30
10	C	939	QEL	O2-C18	2.13	1.41	1.37
10	B	920	QEL	O2-C18	2.12	1.41	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	939	QEL	O1-C14-C15	5.12	122.32	111.20
10	C	939	QEL	C24-C13-C14	-4.96	104.64	111.97
10	B	920	QEL	C24-C13-C14	-4.91	104.70	111.97
10	B	920	QEL	C11-N1-C10	3.77	116.31	109.13
10	B	920	QEL	C12-C8-C7	-3.76	102.14	112.01
10	C	939	QEL	C12-C8-C7	-3.75	102.16	112.01
10	C	939	QEL	C11-N1-C10	3.74	116.26	109.13
9	D	902	NAG	C1-O5-C5	3.09	116.33	112.19
10	B	920	QEL	O1-C14-C15	2.90	117.52	111.20
11	D	907	GLU	OXT-C-O	-2.68	117.99	124.08
11	B	921	GLU	OXT-C-O	-2.66	118.05	124.08
10	B	920	QEL	O1-C14-C13	2.55	114.72	108.36
10	C	939	QEL	C19-C15-C14	-2.36	117.15	120.71
10	B	920	QEL	C4-C7-C8	2.35	118.75	114.45
10	C	939	QEL	C4-C7-C8	2.34	118.75	114.45
10	B	920	QEL	C19-C15-C14	-2.30	117.25	120.71
9	A	945	NAG	C1-O5-C5	2.12	115.03	112.19
8	C	940	GLY	OXT-C-O	-2.12	117.89	123.33
8	A	942	GLY	OXT-C-O	-2.09	117.96	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	939	QEL	C11-N1-C13	2.00	120.54	114.02

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	920	QEL	C14-C13-N1-C10
10	B	920	QEL	C24-C13-N1-C10
10	B	920	QEL	C24-C13-N1-C11
10	C	939	QEL	C14-C13-N1-C10
10	C	939	QEL	C24-C13-N1-C10
10	C	939	QEL	C24-C13-N1-C11
9	B	913	NAG	C4-C5-C6-O6
9	B	912	NAG	O5-C5-C6-O6
9	A	943	NAG	C4-C5-C6-O6
9	B	913	NAG	O5-C5-C6-O6
9	A	943	NAG	O5-C5-C6-O6
9	C	941	NAG	C4-C5-C6-O6
9	B	912	NAG	C4-C5-C6-O6
9	C	941	NAG	O5-C5-C6-O6
9	A	944	NAG	C4-C5-C6-O6
9	D	901	NAG	C4-C5-C6-O6
9	A	944	NAG	O5-C5-C6-O6
9	D	901	NAG	O5-C5-C6-O6
9	D	902	NAG	O5-C5-C6-O6
9	D	902	NAG	C3-C2-N2-C7
10	B	920	QEL	C24-C13-C14-C15
10	C	939	QEL	C24-C13-C14-C15
10	B	920	QEL	N1-C13-C14-C15
10	C	939	QEL	N1-C13-C14-C15
11	D	907	GLU	OE2-CD-CG-CB
11	D	907	GLU	OE1-CD-CG-CB

There are no ring outliers.

5 monomers are involved in 18 short contacts:

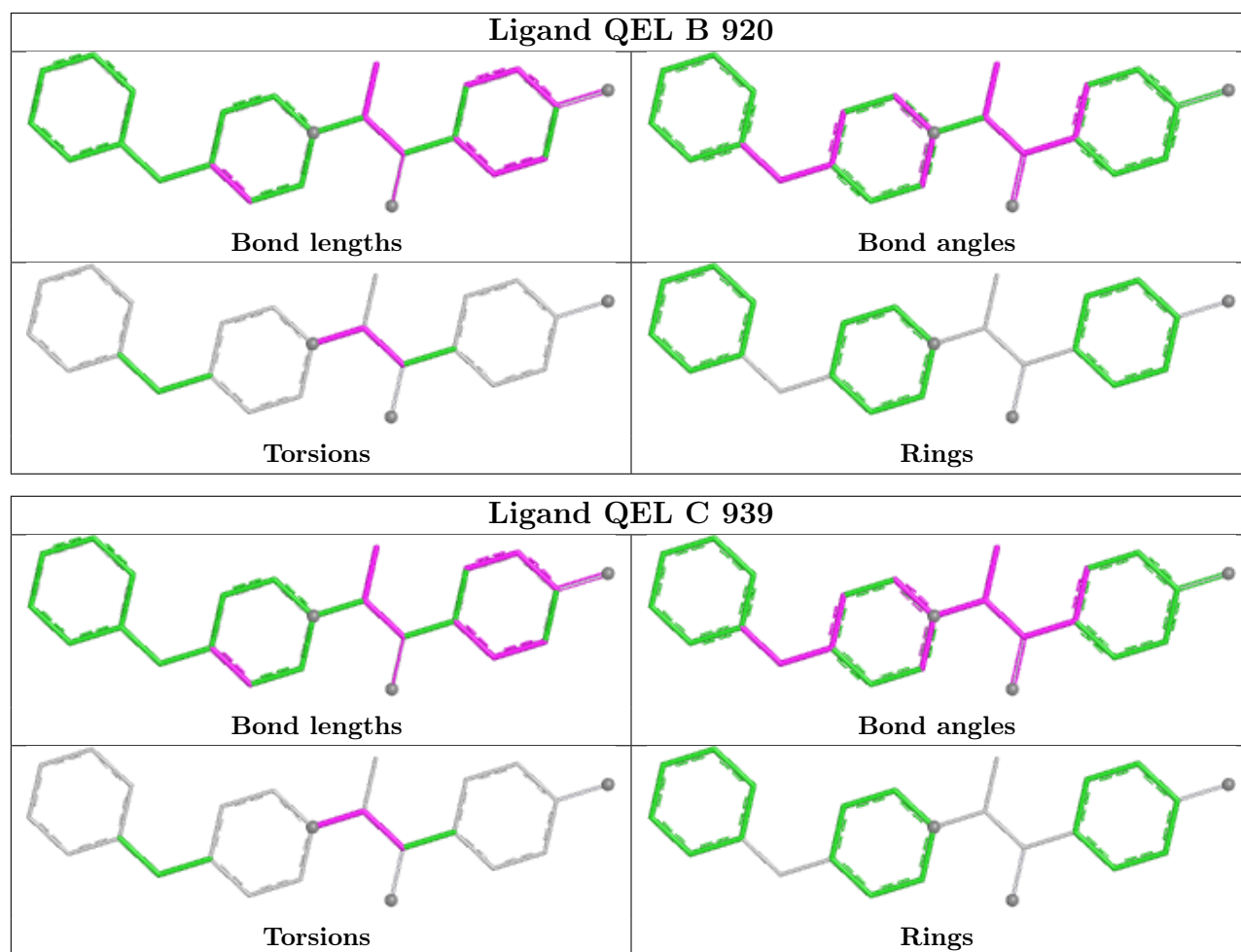
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	920	QEL	6	0
11	D	907	GLU	2	0
8	A	942	GLY	2	0
10	C	939	QEL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	921	GLU	2	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	743/825 (90%)	0.52	56 (7%) 20 19	125, 207, 315, 377	0
1	C	754/825 (91%)	0.61	67 (8%) 15 16	122, 208, 319, 371	0
2	B	720/820 (87%)	0.39	46 (6%) 25 22	107, 181, 281, 330	0
2	D	727/820 (88%)	0.49	54 (7%) 20 19	109, 188, 296, 327	0
All	All	2944/3290 (89%)	0.50	223 (7%) 20 19	107, 198, 305, 377	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	7.5
1	C	636	TRP	6.6
1	C	40	GLN	6.5
1	C	36	ARG	6.5
2	D	611	GLY	6.0
2	D	76	THR	5.5
1	A	94	HIS	5.4
1	C	634	MET	5.4
1	A	459	CYS	5.3
1	C	707	GLU	5.3
2	D	78	PRO	5.3
1	A	768	TRP	5.0
2	B	140	SER	5.0
1	A	309	VAL	4.9
2	D	481	VAL	4.8
1	C	122	THR	4.7
1	C	64	SER	4.7
2	B	800	ILE	4.7
2	D	685	THR	4.6
1	C	616	ASN	4.4
2	B	344	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	342	GLU	4.2
1	C	39	GLU	4.1
1	A	506	LEU	4.1
1	A	493	SER	4.1
2	D	213	ASP	4.0
1	A	51	LYS	4.0
2	B	534	ILE	3.9
1	C	529	PHE	3.9
2	B	539	SER	3.9
2	B	76	THR	3.8
1	A	408	PHE	3.8
1	C	661	GLU	3.8
2	B	333	ASN	3.8
1	A	396	THR	3.7
1	A	351	TYR	3.7
1	C	578	TYR	3.7
1	A	480	ALA	3.7
2	D	763	GLY	3.7
1	C	274	GLY	3.7
2	B	472	VAL	3.6
2	D	498	ILE	3.6
1	A	581	ASP	3.6
1	C	239	ASP	3.6
1	C	574	ALA	3.6
1	C	136	SER	3.5
1	A	314	ILE	3.5
2	D	630	ILE	3.5
2	B	821	VAL	3.5
1	C	554	PHE	3.4
1	A	413	PRO	3.4
2	B	256	TRP	3.4
2	B	749	VAL	3.4
2	D	360	PRO	3.3
2	B	471	SER	3.3
2	D	356	TYR	3.3
2	D	120	LEU	3.3
1	A	727	HIS	3.2
1	C	431	VAL	3.2
1	C	781	GLU	3.2
2	D	313	PHE	3.2
1	C	216	ALA	3.2
2	B	681	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	475	GLU	3.2
1	C	42	PHE	3.1
1	A	247	TRP	3.1
1	A	332	ASP	3.1
2	D	728	ALA	3.1
2	D	467	LYS	3.0
2	D	355	GLY	3.0
2	D	147	GLY	3.0
1	A	343	ASP	3.0
2	D	727	ASP	2.9
2	B	419	VAL	2.9
2	D	527	VAL	2.9
2	D	684	GLY	2.9
2	B	54	HIS	2.9
1	A	350	GLN	2.9
2	D	144	PHE	2.9
1	C	103	THR	2.8
1	C	814	ALA	2.8
1	C	79	CYS	2.8
2	D	357	GLN	2.8
2	D	79	LYS	2.8
1	C	575	VAL	2.8
2	B	497	MET	2.8
1	C	266	ILE	2.8
1	C	637	ALA	2.8
1	A	686	GLN	2.8
2	B	525	PHE	2.8
1	C	386	THR	2.8
2	B	142	MET	2.7
1	C	37	LYS	2.7
1	C	192	GLU	2.7
1	C	140	THR	2.7
2	B	206	ASP	2.7
2	D	248	GLY	2.7
2	D	644	ALA	2.7
2	B	431	ARG	2.7
2	D	324	THR	2.7
2	D	477	ASP	2.7
1	C	305	PRO	2.7
1	C	420	CYS	2.7
2	D	323	ASN	2.7
1	C	555	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	526	SER	2.7
1	A	358	ASN	2.7
1	A	405	GLN	2.7
2	B	282	TYR	2.7
2	B	65	VAL	2.6
1	A	103	THR	2.6
2	D	525	PHE	2.6
2	D	800	ILE	2.6
1	C	142	PRO	2.6
1	A	545	GLU	2.6
1	A	781	GLU	2.6
1	C	343	ASP	2.6
2	D	123	ILE	2.6
1	A	688	SER	2.6
2	D	81	ILE	2.6
2	D	245	ASN	2.6
1	C	161	ASN	2.5
1	A	430	PRO	2.5
2	B	694	ASN	2.5
2	D	354	ASP	2.5
1	C	348	PHE	2.5
2	D	206	ASP	2.5
1	C	62	ALA	2.5
1	A	830	LEU	2.5
1	A	122	THR	2.5
1	C	94	HIS	2.4
2	B	608	LEU	2.4
1	C	34	SER	2.4
2	D	426	SER	2.4
1	C	223	ALA	2.4
2	B	95	GLN	2.4
2	B	739	MET	2.4
2	D	250	THR	2.4
2	B	156	VAL	2.4
2	D	77	ASP	2.4
2	B	498	ILE	2.4
2	D	220	LEU	2.4
2	D	127	HIS	2.4
1	A	462	LEU	2.4
2	B	75	GLU	2.4
2	B	521	GLU	2.3
2	D	235	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	812	ASN	2.3
2	B	670	LYS	2.3
2	D	327	LYS	2.3
1	A	380	ILE	2.3
1	A	793	VAL	2.3
1	A	52	ARG	2.3
1	A	562	LEU	2.3
2	B	672	GLN	2.3
1	A	628	SER	2.3
2	B	832	SER	2.3
1	C	822	GLY	2.3
1	C	380	ILE	2.3
1	C	480	ALA	2.3
2	B	106	GLU	2.3
1	A	514	VAL	2.3
1	C	297	GLU	2.3
1	A	759	GLY	2.3
2	B	475	THR	2.2
2	D	146	PHE	2.2
2	B	59	PHE	2.2
1	C	193	LYS	2.2
1	C	251	GLU	2.2
1	A	633	GLY	2.2
1	C	793	VAL	2.2
1	A	680	ILE	2.2
2	B	250	THR	2.2
1	A	264	ASP	2.2
2	B	829	MET	2.2
1	A	395	SER	2.2
2	B	208	SER	2.2
1	C	194	VAL	2.2
1	C	38	HIS	2.2
2	B	758	ALA	2.2
1	C	384	GLY	2.2
2	D	351	PHE	2.2
2	B	93	LYS	2.2
1	C	821	ALA	2.1
2	D	566	LEU	2.2
1	A	756	SER	2.1
2	D	659	TYR	2.1
2	D	821	VAL	2.1
1	A	458	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	124	ARG	2.1
1	A	160	TRP	2.1
1	C	433	LYS	2.1
2	D	100	ALA	2.1
1	A	509	GLN	2.1
1	A	404	HIS	2.1
1	C	78	VAL	2.1
1	A	305	PRO	2.1
2	B	244	ALA	2.1
1	A	189	SER	2.1
1	A	530	SER	2.1
2	B	133	ILE	2.1
1	C	754	PHE	2.1
1	A	315	TRP	2.1
1	C	88	TYR	2.1
1	C	734	ALA	2.1
1	C	231	VAL	2.1
1	A	702	MET	2.1
1	A	611	TRP	2.1
2	B	786	ASP	2.1
2	D	528	PRO	2.1
1	C	268	GLY	2.0
2	B	117	ALA	2.0
1	A	693	PHE	2.0
2	D	536	VAL	2.0
2	D	799	GLY	2.0
1	C	114	TYR	2.0
1	A	518	THR	2.0
2	B	249	LEU	2.0
1	C	83	ILE	2.0
2	D	610	TRP	2.0
1	A	632	LEU	2.0
1	C	577	LEU	2.0
2	D	158	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

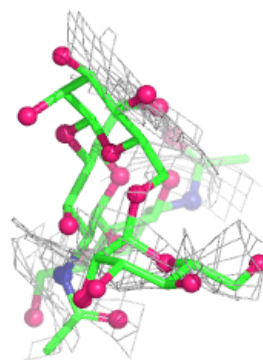
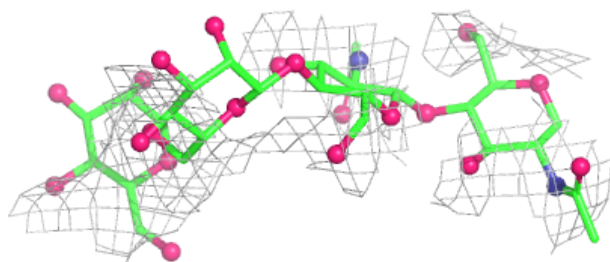
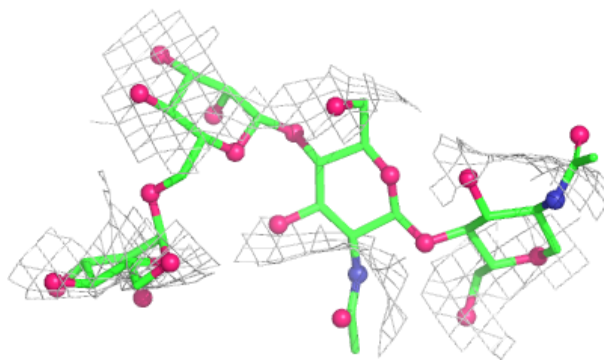
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	4	11/12	-0.23	0.14	350,359,369,372	0
3	NAG	I	2	14/15	-0.06	0.13	340,349,351,352	0
3	BMA	J	3	11/12	0.24	0.11	339,348,354,356	0
4	MAN	F	6	11/12	0.26	0.18	328,350,358,360	0
5	MAN	G	6	11/12	0.27	0.14	334,337,358,366	0
4	NAG	F	2	14/15	0.30	0.12	333,348,360,363	0
5	MAN	G	4	11/12	0.33	0.10	341,359,367,368	0
5	MAN	G	5	11/12	0.35	0.16	352,356,361,365	0
3	MAN	I	4	11/12	0.38	0.10	351,356,359,359	0
4	MAN	F	5	11/12	0.42	0.10	348,357,368,370	0
5	BMA	G	3	11/12	0.43	0.09	352,360,364,366	0
3	BMA	I	3	11/12	0.46	0.09	329,341,349,357	0
6	NAG	H	2	14/15	0.48	0.12	261,293,304,310	0
3	NAG	J	2	14/15	0.51	0.19	326,333,354,356	0
4	BMA	F	3	11/12	0.52	0.09	359,362,364,364	0
3	BMA	E	3	11/12	0.59	0.10	344,347,352,356	0
3	NAG	E	2	14/15	0.63	0.13	332,342,355,358	0
3	NAG	I	1	14/15	0.64	0.12	328,347,354,358	0
3	MAN	J	4	11/12	0.66	0.14	337,350,357,358	0
4	MAN	F	4	11/12	0.70	0.10	332,362,370,371	0
3	NAG	E	1	14/15	0.76	0.14	315,315,334,335	0
5	NAG	G	2	14/15	0.79	0.10	338,346,358,359	0
3	NAG	J	1	14/15	0.82	0.18	315,318,332,336	0
6	NAG	H	1	14/15	0.84	0.10	250,262,281,288	0
4	NAG	F	1	14/15	0.86	0.15	326,338,347,348	0
5	NAG	G	1	14/15	0.90	0.15	315,322,327,332	0

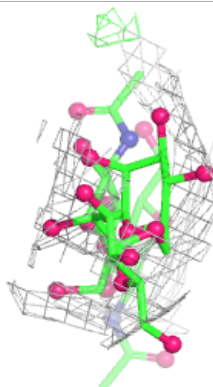
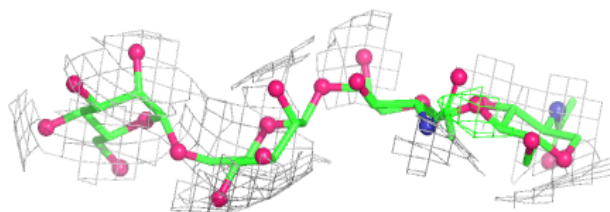
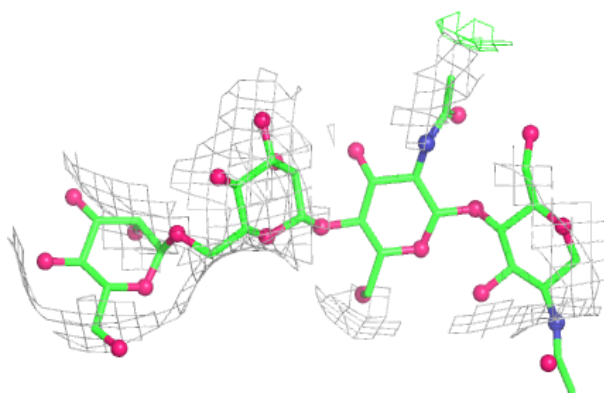
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

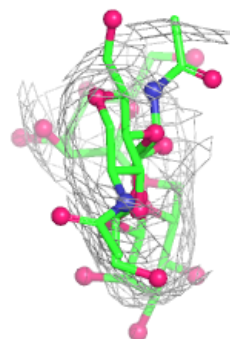
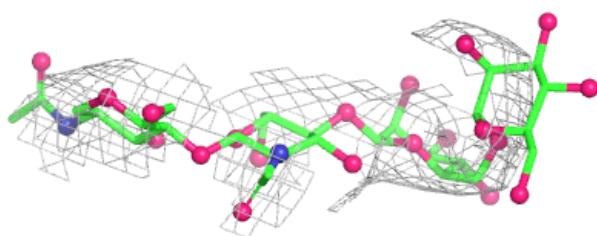
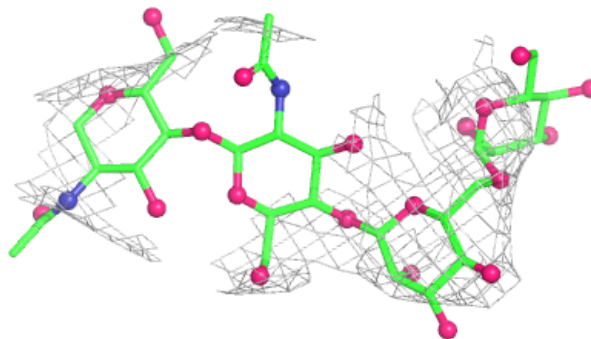
**Electron density around Chain I:**

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

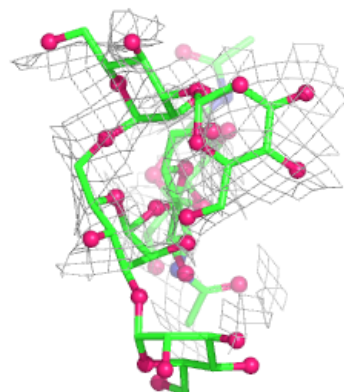
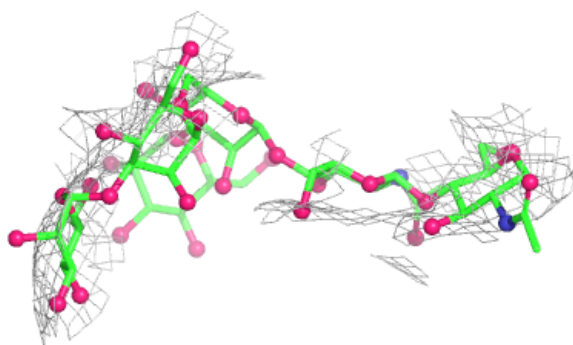
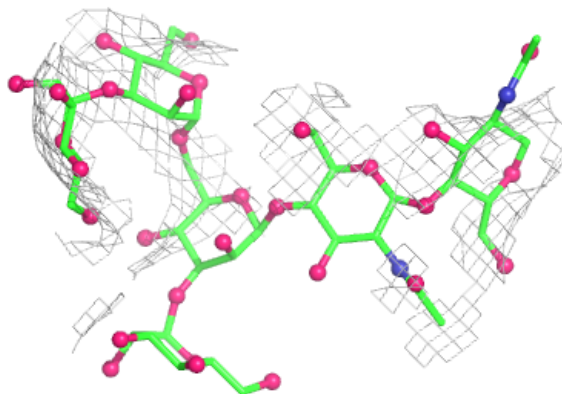


Electron density around Chain J:

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

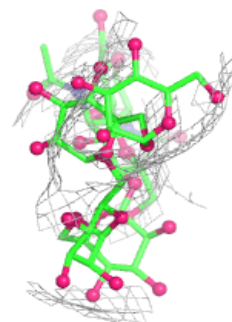
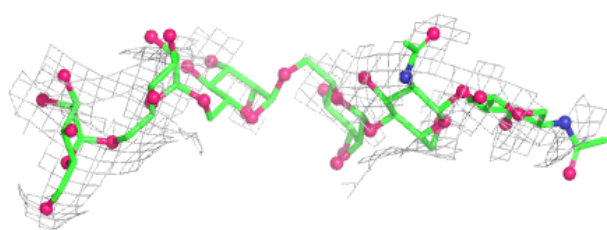
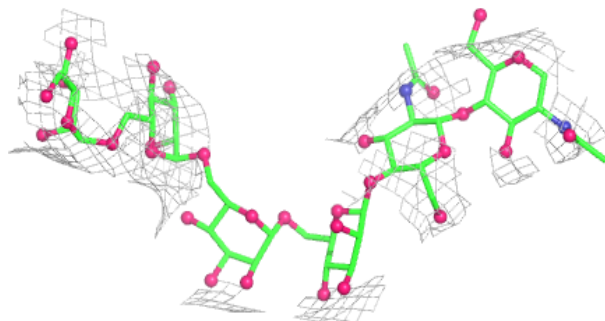
**Electron density around Chain F:**

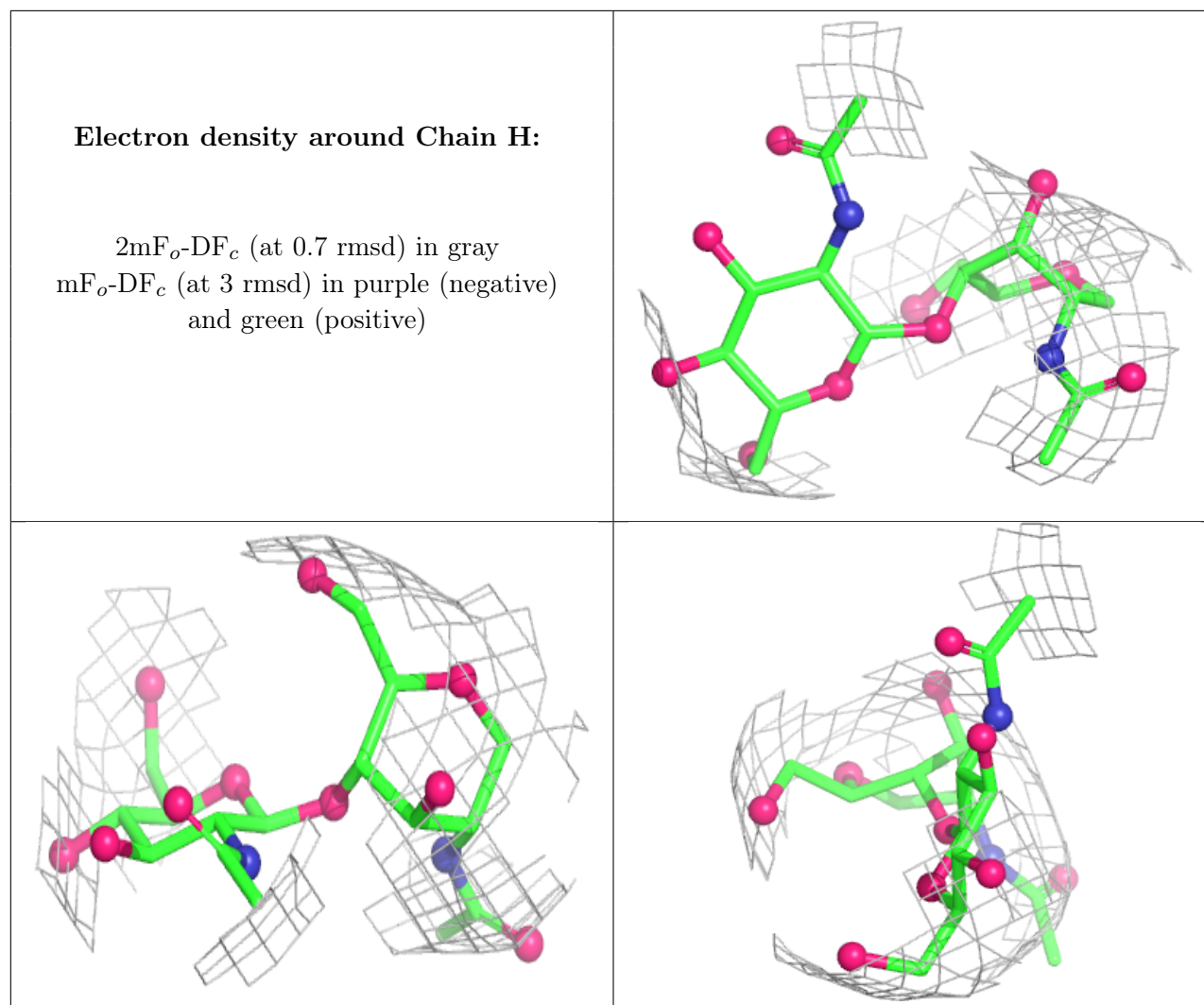
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	W	C	907	1/1	-0.23	0.17	537,537,537,537	1
7	W	C	903	1/1	0.20	0.14	516,516,516,516	1
9	NAG	C	941	14/15	0.20	0.11	281,293,309,312	0
7	W	C	911	1/1	0.22	0.09	550,550,550,550	1
9	NAG	A	945	14/15	0.31	0.17	293,330,339,339	0
7	W	B	906	1/1	0.36	0.15	550,550,550,550	1
7	W	C	902	1/1	0.39	0.10	525,525,525,525	1
7	W	C	905	1/1	0.43	0.07	550,550,550,550	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	W	A	913	1/1	0.47	0.18	509,509,509,509	1
9	NAG	A	944	14/15	0.50	0.13	270,308,315,318	0
7	W	C	926	1/1	0.52	0.20	449,449,449,449	1
7	W	C	908	1/1	0.53	0.10	550,550,550,550	1
9	NAG	B	912	14/15	0.59	0.11	224,261,273,280	0
7	W	C	934	1/1	0.59	0.16	466,466,466,466	1
9	NAG	D	901	14/15	0.62	0.11	220,253,260,261	0
7	W	C	909	1/1	0.67	0.08	550,550,550,550	1
7	W	B	905	1/1	0.68	0.15	398,398,398,398	1
7	W	C	904	1/1	0.68	0.06	533,533,533,533	1
9	NAG	B	913	14/15	0.69	0.14	197,221,231,235	0
7	W	A	901	1/1	0.70	0.19	337,337,337,337	1
7	W	A	937	1/1	0.70	0.17	408,408,408,408	1
7	W	A	923	1/1	0.75	0.20	515,515,515,515	1
7	W	A	917	1/1	0.75	0.11	523,523,523,523	1
7	W	C	915	1/1	0.76	0.11	496,496,496,496	1
7	W	A	924	1/1	0.77	0.13	526,526,526,526	1
7	W	B	908	1/1	0.77	0.09	511,511,511,511	1
7	W	B	909	1/1	0.77	0.09	550,550,550,550	1
7	W	A	925	1/1	0.77	0.16	463,463,463,463	1
9	NAG	D	902	14/15	0.78	0.12	210,244,253,265	0
7	W	C	912	1/1	0.81	0.07	549,549,549,549	1
7	W	C	910	1/1	0.81	0.10	447,447,447,447	1
7	W	C	917	1/1	0.81	0.10	433,433,433,433	1
7	W	A	916	1/1	0.81	0.11	542,542,542,542	1
7	W	A	914	1/1	0.82	0.10	514,514,514,514	1
7	W	B	902	1/1	0.82	0.14	404,404,404,404	1
7	W	C	901	1/1	0.82	0.08	489,489,489,489	1
7	W	B	907	1/1	0.83	0.07	550,550,550,550	1
7	W	A	931	1/1	0.83	0.14	456,456,456,456	1
7	W	C	922	1/1	0.83	0.07	378,378,378,378	1
7	W	C	919	1/1	0.84	0.06	467,467,467,467	1
7	W	A	929	1/1	0.84	0.11	492,492,492,492	1
7	W	C	925	1/1	0.84	0.13	475,475,475,475	1
7	W	C	913	1/1	0.85	0.09	366,366,366,366	1
7	W	C	914	1/1	0.85	0.06	484,484,484,484	1
7	W	B	911	1/1	0.85	0.11	489,489,489,489	1
7	W	C	933	1/1	0.85	0.09	529,529,529,529	1
7	W	A	926	1/1	0.85	0.13	443,443,443,443	1
7	W	A	918	1/1	0.85	0.10	549,549,549,549	1
7	W	A	915	1/1	0.86	0.10	550,550,550,550	1
9	NAG	A	943	14/15	0.86	0.12	229,244,260,264	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	W	A	903	1/1	0.86	0.14	336,336,336,336	1
10	QEL	C	939	24/24	0.86	0.23	107,135,151,160	0
7	W	C	931	1/1	0.87	0.13	475,475,475,475	1
7	W	C	920	1/1	0.87	0.07	473,473,473,473	1
7	W	A	907	1/1	0.87	0.16	212,212,212,212	1
7	W	A	909	1/1	0.88	0.17	312,312,312,312	1
7	W	C	916	1/1	0.88	0.13	456,456,456,456	1
7	W	A	927	1/1	0.89	0.11	491,491,491,491	1
7	W	A	930	1/1	0.89	0.13	450,450,450,450	1
10	QEL	B	920	24/24	0.89	0.17	100,133,155,170	0
7	W	C	927	1/1	0.89	0.10	494,494,494,494	1
11	GLU	D	907	10/10	0.89	0.09	196,208,232,234	0
7	W	C	929	1/1	0.90	0.11	426,426,426,426	1
7	W	A	920	1/1	0.90	0.11	549,549,549,549	1
7	W	A	935	1/1	0.90	0.13	495,495,495,495	1
7	W	C	936	1/1	0.91	0.13	478,478,478,478	1
7	W	A	922	1/1	0.91	0.11	542,542,542,542	1
7	W	A	932	1/1	0.91	0.12	473,473,473,473	1
7	W	C	906	1/1	0.91	0.07	550,550,550,550	1
8	GLY	A	942	5/5	0.92	0.12	166,169,185,190	0
7	W	B	910	1/1	0.92	0.10	520,520,520,520	1
7	W	C	918	1/1	0.93	0.07	398,398,398,398	1
7	W	A	933	1/1	0.93	0.10	486,486,486,486	1
7	W	B	901	1/1	0.93	0.08	312,312,312,312	1
7	W	C	921	1/1	0.93	0.06	386,386,386,386	1
7	W	A	928	1/1	0.93	0.11	426,426,426,426	1
8	GLY	C	940	5/5	0.94	0.08	180,183,189,194	0
7	W	C	935	1/1	0.94	0.11	479,479,479,479	1
7	W	A	934	1/1	0.94	0.11	394,394,394,394	1
7	W	C	932	1/1	0.94	0.10	540,540,540,540	1
7	W	A	906	1/1	0.95	0.13	213,213,213,213	1
7	W	A	921	1/1	0.95	0.11	550,550,550,550	1
7	W	A	911	1/1	0.95	0.13	251,251,251,251	1
7	W	A	919	1/1	0.95	0.11	522,522,522,522	1
11	GLU	B	921	10/10	0.95	0.07	183,200,227,229	0
7	W	A	936	1/1	0.95	0.09	473,473,473,473	1
7	W	C	928	1/1	0.96	0.09	441,441,441,441	1
7	W	A	910	1/1	0.96	0.11	171,171,171,171	1
7	W	C	923	1/1	0.97	0.07	320,320,320,320	1
7	W	B	904	1/1	0.97	0.09	417,417,417,417	1
7	W	A	912	1/1	0.97	0.09	196,196,196,196	1
7	W	C	930	1/1	0.97	0.11	465,465,465,465	1

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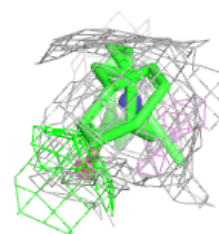
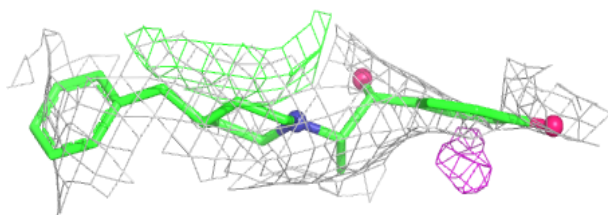
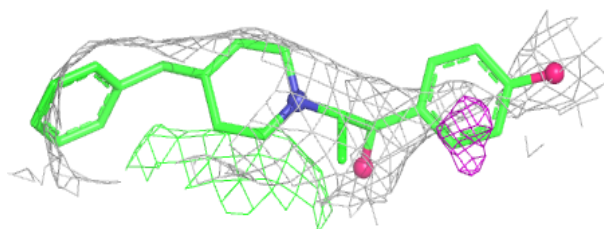
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	W	C	924	1/1	0.98	0.06	465,465,465,465	1
7	W	B	903	1/1	0.98	0.11	438,438,438,438	1
7	W	A	904	1/1	0.98	0.09	214,214,214,214	1
7	W	A	902	1/1	0.99	0.09	205,205,205,205	1
7	W	A	905	1/1	0.99	0.08	209,209,209,209	1
7	W	A	908	1/1	0.99	0.09	260,260,260,260	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.

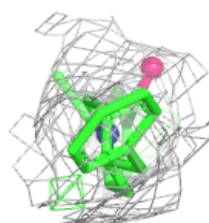
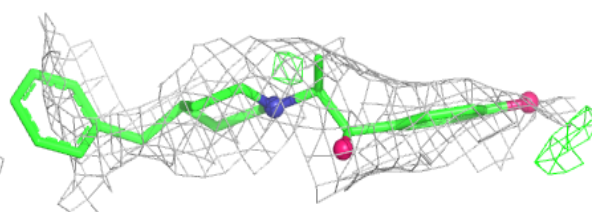
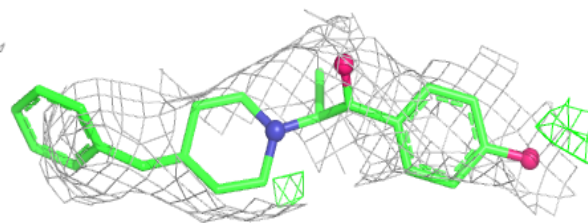
Electron density around QEL C 939:

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 QEL B 920:

$2mF_o-DF_c$ (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.