



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 07:52 AM EST

PDB ID : 3GVK
Title : Crystal structure of endo-neuraminidase NF mutant
Authors : Schulz, E.C.; Dickmanns, A.; Ficner, R.
Deposited on : 2009-03-31
Resolution : 1.84 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

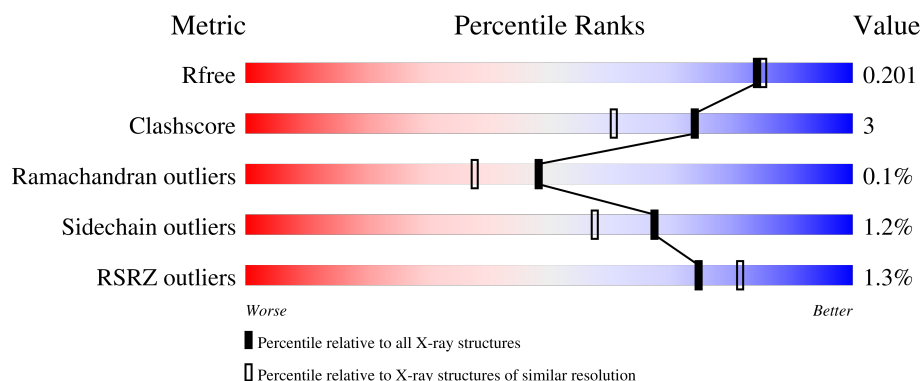
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.




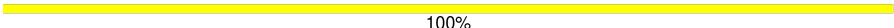

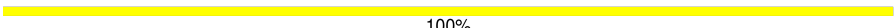
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	670	<div> <div>89%</div> <div>6%</div> <div>.</div> </div>
1	B	670	<div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	C	670	<div> <div>94%</div> <div>6%</div> <div>.</div> </div>
2	D	3	<div> <div>67%</div> <div>33%</div> </div>
2	E	3	<div> <div>100%</div> </div>

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18367 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.

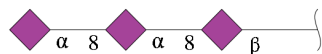
- Molecule 1 is a protein called Endo-N-acetylneuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	17	0
			5163	3266	892	985	20			
1	B	666	Total	C	N	O	S	0	14	0
			5295	3341	911	1023	20			
1	C	666	Total	C	N	O	S	0	12	0
			5287	3335	916	1016	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	VAL	-	expression tag	UNP Q858B1
A	242	PRO	-	expression tag	UNP Q858B1
A	243	ARG	-	expression tag	UNP Q858B1
A	244	GLY	-	expression tag	UNP Q858B1
A	245	SER	-	expression tag	UNP Q858B1
A	350	ALA	HIS	engineered mutation	UNP Q858B1
B	241	VAL	-	expression tag	UNP Q858B1
B	242	PRO	-	expression tag	UNP Q858B1
B	243	ARG	-	expression tag	UNP Q858B1
B	244	GLY	-	expression tag	UNP Q858B1
B	245	SER	-	expression tag	UNP Q858B1
B	350	ALA	HIS	engineered mutation	UNP Q858B1
C	241	VAL	-	expression tag	UNP Q858B1
C	242	PRO	-	expression tag	UNP Q858B1
C	243	ARG	-	expression tag	UNP Q858B1
C	244	GLY	-	expression tag	UNP Q858B1
C	245	SER	-	expression tag	UNP Q858B1
C	350	ALA	HIS	engineered mutation	UNP Q858B1

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			61	33	3	25			
2	E	3	Total	C	N	O	0	0	0
			61	33	3	25			
2	G	3	Total	C	N	O	0	0	0
			61	33	3	25			
2	H	3	Total	C	N	O	0	0	0
			61	33	3	25			
2	J	3	Total	C	N	O	0	0	0
			61	33	3	25			
2	K	3	Total	C	N	O	0	0	0
			61	33	3	25			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			41	22	2	17			
3	I	2	Total	C	N	O	0	0	0
			41	22	2	17			
3	L	2	Total	C	N	O	0	0	0
			41	22	2	17			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

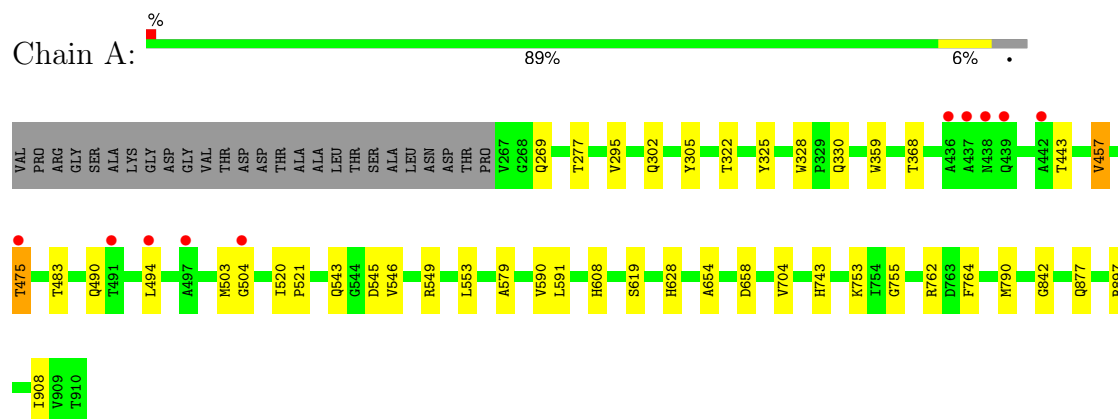
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	615	Total 615	O 615	0	0
5	B	766	Total 766	O 766	0	0
5	C	749	Total 749	O 749	0	0

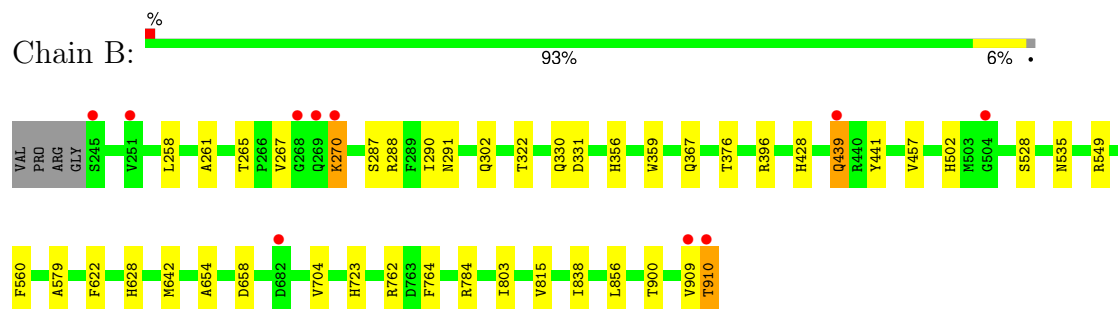
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

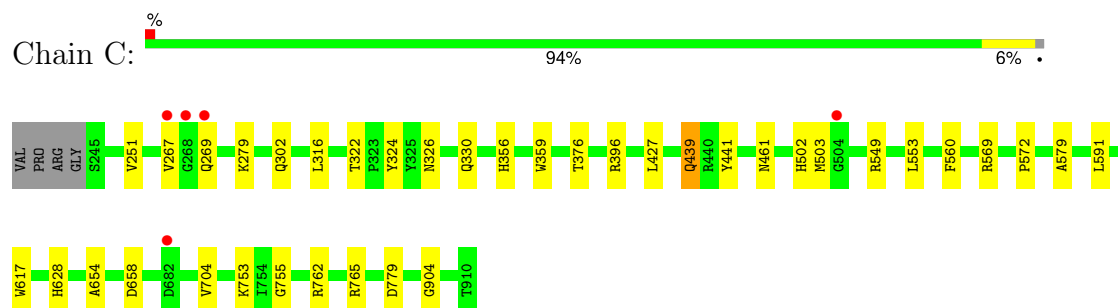
- Molecule 1: Endo-N-acetylneuraminidase



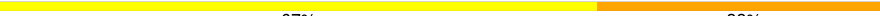
- Molecule 1: Endo-N-acetylneuraminidase



- Molecule 1: Endo-N-acetylneuraminidase



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain D:  67% 33%

SLB1
SLA2
SLA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain E:  100%

SLB1
SLA2
SLA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain G:  67% 33%

SLB1
SLA2
SLA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain H:  100%


SLB1
SLA2
SLA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain J:  33% 67%

SLB1
SLA2
SLA3

- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain K:  67% 33%

SLB1
SLA2
SLA3

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain F:  50% 50%

SLB1
SLA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain I:  50% 50%

SLB1
SLA2

- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid

Chain L:  100%

SLB1
SLA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.40Å 153.70Å 157.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.84 15.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.84) 99.7 (15.00-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.5.0039	Depositor
R, R_{free}	0.265 , 0.282 0.171 , 0.201	Depositor DCC
R_{free} test set	9487 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18367	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SLB, NA, SIA

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	0.37	0/5360	0.53	0/7301
1	B	0.38	0/5479	0.54	0/7463
1	C	0.37	0/5469	0.53	0/7450
All	All	0.37	0/16308	0.54	0/22214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5163	0	4929	31	0
1	B	5295	0	5039	38	0
1	C	5287	0	5040	27	0
2	D	61	0	48	3	0
2	E	61	0	50	0	0
2	G	61	0	50	2	0
2	H	61	0	50	0	0
2	J	61	0	49	3	0
2	K	61	0	50	1	0
3	F	41	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	41	0	34	1	0
3	L	41	0	34	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	615	0	0	3	0
5	B	766	0	0	5	0
5	C	749	0	0	3	0
All	All	18367	0	15407	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (94) 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:A:543:GLN:HE22	1:A:546:VAL:H	1.23	0.86
1:B:302:GLN:HE22	1:B:654:ALA:H	1.26	0.83
1:C:302:GLN:HE22	1:C:654:ALA:H	1.29	0.80
3:F:1:SLB:O6	3:F:1:SLB:H92	1.84	0.78
1:B:367:GLN:HE22	1:B:764:PHE:H	1.33	0.76
1:A:302:GLN:HE22	1:A:654:ALA:H	1.33	0.73
1:A:897:ARG:HH11	1:B:910[A]:THR:HG22	1.54	0.72
1:B:367:GLN:HE21	1:C:765:ARG:HH22	1.36	0.72
1:C:322:THR:HG22	1:C:324:TYR:H	1.55	0.72
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.76	0.68
1:A:475:THR:HG22	1:A:483:THR:OG1	2.02	0.58
1:B:628:HIS:HE1	1:B:658:ASP:OD1	1.87	0.58
1:B:910[A]:THR:HG23	1:C:904:GLY:HA2	1.86	0.57
1:C:396:ARG:HB3	1:C:560:PHE:CZ	2.40	0.56
1:A:330:GLN:HB3	1:A:704:VAL:O	2.04	0.56
2:D:1:SLB:H6	2:D:1:SLB:H112	1.88	0.55
1:B:302:GLN:HE22	1:B:654:ALA:N	2.01	0.54
1:C:322:THR:HB	1:C:326:ASN:OD1	2.07	0.54
1:B:723:HIS:HE1	5:B:1470:HOH:O	1.89	0.54
1:C:322:THR:HG21	5:C:1231:HOH:O	2.09	0.53
1:B:396:ARG:HB3	1:B:560:PHE:CZ	2.44	0.53
1:B:428:HIS:ND1	1:B:502:HIS:HD2	2.06	0.53
1:C:549:ARG:HD3	1:C:579:ALA:O	2.08	0.53
1:A:628:HIS:HD2	5:A:1542:HOH:O	1.92	0.52
1:A:842:GLY:HA2	1:B:838[B]:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910[A]:THR:CG2	1:C:904:GLY:HA2	2.39	0.52
1:B:356:HIS:HE1	5:B:1693:HOH:O	1.92	0.52
1:A:543:GLN:NE2	1:A:545:ASP:H	2.08	0.52
1:A:457:VAL:HA	1:A:504:GLY:O	2.09	0.51
1:C:569[A]:ARG:HH21	1:C:569[A]:ARG:HG3	1.74	0.51
1:B:367:GLN:HE21	1:C:765:ARG:NH2	2.06	0.51
1:A:443[A]:THR:HG22	1:A:483:THR:HG22	1.93	0.51
1:B:838[B]:ILE:HD11	1:B:856:LEU:HB2	1.91	0.51
1:A:764:PHE:HB3	1:C:316:LEU:HD23	1.93	0.50
1:B:549:ARG:HD3	1:B:579:ALA:O	2.12	0.50
1:C:302:GLN:HE22	1:C:654:ALA:N	2.03	0.50
1:B:622:PHE:CZ	1:B:642[B]:MET:HE1	2.48	0.49
1:A:790[B]:MET:HG2	1:B:784:ARG:HB2	1.95	0.49
1:C:628:HIS:HE1	1:C:658:ASP:OD1	1.95	0.49
1:A:842:GLY:HA2	1:B:838[B]:ILE:HD12	1.95	0.49
1:B:330:GLN:HB3	1:B:704:VAL:O	2.13	0.49
1:C:356:HIS:HE1	5:C:1692:HOH:O	1.96	0.49
1:B:261:ALA:O	1:B:265:THR:HG22	2.14	0.48
1:A:269:GLN:HE22	1:B:291:ASN:HD21	1.62	0.48
1:A:908:ILE:HD12	1:B:900:THR:HG21	1.95	0.48
1:B:356:HIS:HD2	1:B:376:THR:O	1.97	0.48
1:B:838[B]:ILE:CD1	1:B:856:LEU:HB2	2.44	0.48
5:B:1661:HOH:O	2:G:1:SLB:C1	2.61	0.48
1:A:295[A]:VAL:HG22	1:A:305:TYR:CE1	2.48	0.47
1:A:549:ARG:HD3	1:A:579:ALA:O	2.14	0.47
1:C:753:LYS:HE2	1:C:755:GLY:O	2.14	0.47
2:K:1:SLB:O6	2:K:1:SLB:H92	2.15	0.47
1:C:427:LEU:N	1:C:503:MET:O	2.27	0.46
1:B:838[B]:ILE:HD13	1:B:838[B]:ILE:H	1.80	0.46
1:A:608:HIS:HD2	1:A:619:SER:OG	1.98	0.46
1:C:356:HIS:HD2	1:C:376:THR:O	1.98	0.46
1:A:328:TRP:HD1	1:A:330:GLN:HE21	1.64	0.46
1:A:368[A]:THR:CG2	5:A:1194:HOH:O	2.63	0.46
1:A:753:LYS:HE2	1:A:755:GLY:O	2.16	0.46
1:A:302:GLN:HE22	1:A:654:ALA:N	2.06	0.46
1:A:743:HIS:HD2	5:A:1637:HOH:O	1.99	0.45
1:B:367:GLN:NE2	1:C:765:ARG:HH22	2.08	0.45
1:A:877:GLN:NE2	3:I:1:SLB:O7	2.50	0.45
1:B:909:VAL:HA	1:B:910[B]:THR:HA	1.80	0.45
1:C:330:GLN:HB3	1:C:704:VAL:O	2.16	0.44
2:J:1:SLB:O10	2:J:2:SIA:H91	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:HIS:HD2	5:B:1631:HOH:O	2.00	0.44
1:B:909:VAL:HG12	1:B:910[B]:THR:HG22	2.00	0.44
1:C:439:GLN:HE22	1:C:441:TYR:HB2	1.83	0.44
1:B:439[A]:GLN:NE2	1:B:441:TYR:H	2.15	0.43
2:J:1:SLB:H91	2:J:1:SLB:O6	2.18	0.43
1:B:439[A]:GLN:HE22	1:B:441:TYR:HB2	1.83	0.43
1:B:287:SER:OG	1:C:753:LYS:HE3	2.19	0.43
2:J:1:SLB:N5	2:J:1:SLB:O7	2.51	0.43
1:A:490:GLN:HB2	1:A:494:LEU:HD11	2.01	0.42
1:A:553:LEU:HD22	1:A:591[A]:LEU:HD21	2.00	0.42
2:D:1:SLB:H6	2:D:1:SLB:C11	2.50	0.42
5:B:1136:HOH:O	1:C:779:ASP:HB2	2.19	0.42
1:C:553:LEU:HD22	1:C:591[A]:LEU:HD21	2.01	0.42
3:F:1:SLB:O6	3:F:1:SLB:C9	2.58	0.42
1:C:572:PRO:HD3	1:C:617:TRP:CD1	2.55	0.42
2:G:1:SLB:O6	2:G:1:SLB:H92	2.20	0.42
1:B:265:THR:HG23	1:B:288:ARG:HH11	1.84	0.41
1:C:251:VAL:O	1:C:279:LYS:HD2	2.20	0.41
1:C:461:ASN:HD22	1:C:502:HIS:HD2	1.68	0.41
1:A:368[A]:THR:HG21	5:C:1111:HOH:O	2.20	0.41
1:B:331:ASP:HB3	1:B:528:SER:HA	2.01	0.41
1:A:503:MET:HG2	1:A:504:GLY:HA3	2.03	0.41
1:B:270:LYS:HB3	1:B:290:ILE:HG12	2.02	0.41
2:D:1:SLB:H112	2:D:1:SLB:C6	2.51	0.41
1:A:277:THR:HG22	1:A:295[A]:VAL:HG23	2.02	0.41
1:B:803[B]:ILE:HD13	1:B:815:VAL:CG2	2.50	0.41
1:A:520:ILE:HA	1:A:521:PRO:HD3	1.96	0.40
1:B:396:ARG:HH21	1:B:535:ASN:HD22	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	659/670 (98%)	633 (96%)	26 (4%)	0	100	100
1	B	677/670 (101%)	654 (97%)	23 (3%)	0	100	100
1	C	676/670 (101%)	650 (96%)	25 (4%)	1 (0%)	48	38
All	All	2012/2010 (100%)	1937 (96%)	74 (4%)	1 (0%)	48	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	267	VAL

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	564/566 (100%)	557 (99%)	7 (1%)	67	57
1	B	577/566 (102%)	566 (98%)	11 (2%)	52	36
1	C	575/566 (102%)	571 (99%)	4 (1%)	81	76
All	All	1716/1698 (101%)	1694 (99%)	22 (1%)	67	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	THR
1	A	325	TYR
1	A	359	TRP
1	A	457	VAL
1	A	475	THR
1	A	590	VAL
1	A	762	ARG
1	B	258	LEU
1	B	267	VAL
1	B	270	LYS
1	B	322	THR
1	B	359	TRP

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Mol	Chain	Res	Type
1	B	439[A]	GLN
1	B	439[B]	GLN
1	B	457	VAL
1	B	762	ARG
1	B	910[A]	THR
1	B	910[B]	THR
1	C	269	GLN
1	C	359	TRP
1	C	439	GLN
1	C	762	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	274	ASN
1	A	302	GLN
1	A	326	ASN
1	A	330	GLN
1	A	388	HIS
1	A	397	ASN
1	A	461	ASN
1	A	490	GLN
1	A	502	HIS
1	A	535	ASN
1	A	543	GLN
1	A	608	HIS
1	A	628	HIS
1	A	676	ASN
1	A	699	ASN
1	A	743	HIS
1	A	853	GLN
1	B	269	GLN
1	B	302	GLN
1	B	326	ASN
1	B	338	ASN
1	B	356	HIS
1	B	367	GLN
1	B	397	ASN
1	B	415	ASN
1	B	445	HIS
1	B	461	ASN

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Mol	Chain	Res	Type
1	B	502	HIS
1	B	535	ASN
1	B	570	GLN
1	B	628	HIS
1	B	676	ASN
1	B	723	HIS
1	B	853	GLN
1	C	269	GLN
1	C	302	GLN
1	C	338	ASN
1	C	356	HIS
1	C	415	ASN
1	C	438	ASN
1	C	439	GLN
1	C	461	ASN
1	C	608	HIS
1	C	628	HIS
1	C	699	ASN
1	C	853	GLN
1	C	896	ASN

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 ⓘ

24 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	SLB	D	1	2	21,21,21	1.27	4 (19%)	24,31,31	4.75	10 (41%)
2	SIA	D	2	2	20,20,21	0.68	0	21,28,31	1.28	4 (19%)
2	SIA	D	3	2	20,20,21	0.63	0	21,28,31	1.25	3 (14%)
2	SLB	E	1	2	21,21,21	0.95	1 (4%)	24,31,31	4.63	8 (33%)
2	SIA	E	2	2	20,20,21	0.60	0	21,28,31	1.38	4 (19%)
2	SIA	E	3	2	20,20,21	0.57	0	21,28,31	1.40	5 (23%)
3	SLB	F	1	3	21,21,21	0.88	1 (4%)	24,31,31	4.57	5 (20%)
3	SIA	F	2	3	20,20,21	0.72	0	21,28,31	1.19	2 (9%)
2	SLB	G	1	2	21,21,21	1.72	5 (23%)	24,31,31	4.33	8 (33%)
2	SIA	G	2	2	20,20,21	0.64	0	21,28,31	1.24	3 (14%)
2	SIA	G	3	2	20,20,21	0.52	0	21,28,31	1.25	5 (23%)
2	SLB	H	1	2	21,21,21	0.94	1 (4%)	24,31,31	4.37	8 (33%)
2	SIA	H	2	2	20,20,21	0.60	0	21,28,31	1.32	4 (19%)
2	SIA	H	3	2	20,20,21	0.60	0	21,28,31	1.24	4 (19%)
3	SLB	I	1	3	21,21,21	0.99	1 (4%)	24,31,31	4.58	7 (29%)
3	SIA	I	2	3	20,20,21	0.66	0	21,28,31	1.27	4 (19%)
2	SLB	J	1	2	21,21,21	1.66	5 (23%)	24,31,31	6.84	15 (62%)
2	SIA	J	2	2	20,20,21	0.63	0	21,28,31	1.26	4 (19%)
2	SIA	J	3	2	20,20,21	0.57	0	21,28,31	1.30	4 (19%)
2	SLB	K	1	2	21,21,21	1.07	1 (4%)	24,31,31	4.28	6 (25%)
2	SIA	K	2	2	20,20,21	0.62	0	21,28,31	1.28	4 (19%)
2	SIA	K	3	2	20,20,21	0.60	0	21,28,31	1.28	4 (19%)
3	SLB	L	1	3	21,21,21	1.07	1 (4%)	24,31,31	4.51	6 (25%)
3	SIA	L	2	3	20,20,21	0.64	0	21,28,31	1.25	3 (14%)

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	SLB	D	1	2	-	10/20/38/38	0/1/1/1
2	SIA	D	2	2	-	7/18/34/38	0/1/1/1
2	SIA	D	3	2	-	3/18/34/38	0/1/1/1
2	SLB	E	1	2	-	4/20/38/38	0/1/1/1
2	SIA	E	2	2	-	0/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	E	3	2	-	0/18/34/38	0/1/1/1
3	SLB	F	1	3	-	1/20/38/38	0/1/1/1
3	SIA	F	2	3	-	8/18/34/38	0/1/1/1
2	SLB	G	1	2	-	5/20/38/38	0/1/1/1
2	SIA	G	2	2	-	1/18/34/38	0/1/1/1
2	SIA	G	3	2	-	0/18/34/38	0/1/1/1
2	SLB	H	1	2	-	4/20/38/38	0/1/1/1
2	SIA	H	2	2	-	1/18/34/38	0/1/1/1
2	SIA	H	3	2	-	4/18/34/38	0/1/1/1
3	SLB	I	1	3	-	6/20/38/38	0/1/1/1
3	SIA	I	2	3	-	6/18/34/38	0/1/1/1
2	SLB	J	1	2	-	6/20/38/38	0/1/1/1
2	SIA	J	2	2	-	6/18/34/38	0/1/1/1
2	SIA	J	3	2	-	2/18/34/38	0/1/1/1
2	SLB	K	1	2	-	2/20/38/38	0/1/1/1
2	SIA	K	2	2	-	0/18/34/38	0/1/1/1
2	SIA	K	3	2	-	2/18/34/38	0/1/1/1
3	SLB	L	1	3	-	3/20/38/38	0/1/1/1
3	SIA	L	2	3	-	0/18/34/38	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	SLB	O6-C2	-5.06	1.38	1.43
2	K	1	SLB	O2-C2	3.58	1.44	1.39
2	J	1	SLB	O6-C6	-3.50	1.38	1.44
2	J	1	SLB	O2-C2	3.48	1.44	1.39
3	L	1	SLB	O2-C2	3.43	1.44	1.39
2	H	1	SLB	O2-C2	3.28	1.44	1.39
2	G	1	SLB	O2-C2	3.25	1.44	1.39
2	J	1	SLB	O1B-C1	-3.13	1.19	1.30
3	I	1	SLB	O2-C2	3.09	1.44	1.39
2	E	1	SLB	O2-C2	3.00	1.43	1.39
2	D	1	SLB	C2-C1	-2.90	1.49	1.53
2	D	1	SLB	O2-C2	2.84	1.43	1.39
3	F	1	SLB	O2-C2	2.81	1.43	1.39
2	G	1	SLB	O1B-C1	-2.53	1.21	1.30
2	G	1	SLB	O6-C6	-2.47	1.40	1.44
2	D	1	SLB	O6-C2	-2.27	1.40	1.43
2	G	1	SLB	C2-C1	-2.15	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	SLB	C2-C1	-2.14	1.50	1.53
2	J	1	SLB	C3-C2	2.05	1.54	1.51
2	D	1	SLB	O1B-C1	-2.03	1.23	1.30

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	SLB	O2-C2-C3	-19.42	80.04	109.44
2	J	1	SLB	O6-C6-C5	-16.94	94.33	109.84
3	I	1	SLB	O2-C2-C3	-15.75	85.59	109.44
3	F	1	SLB	O2-C2-C3	-15.52	85.93	109.44
2	D	1	SLB	O2-C2-C3	-15.49	85.99	109.44
2	E	1	SLB	O2-C2-C3	-15.02	86.70	109.44
3	L	1	SLB	O2-C2-C3	-14.84	86.97	109.44
2	K	1	SLB	O2-C2-C3	-14.73	87.14	109.44
2	G	1	SLB	O2-C2-C3	-14.27	87.83	109.44
2	H	1	SLB	O2-C2-C3	-13.29	89.31	109.44
2	D	1	SLB	O2-C2-C1	-12.01	85.37	110.73
3	F	1	SLB	O2-C2-C1	-11.97	85.45	110.73
2	E	1	SLB	O2-C2-C1	-11.67	86.09	110.73
3	L	1	SLB	O2-C2-C1	-11.03	87.43	110.73
3	I	1	SLB	O2-C2-C1	-10.81	87.90	110.73
2	H	1	SLB	O2-C2-C1	-10.21	89.16	110.73
2	H	1	SLB	O2-C2-O6	-10.18	83.85	109.51
2	J	1	SLB	C4-C5-N5	9.87	129.89	110.44
2	K	1	SLB	O2-C2-C1	-9.75	90.13	110.73
2	E	1	SLB	O2-C2-O6	-9.72	85.02	109.51
2	J	1	SLB	O2-C2-C1	-9.70	90.23	110.73
3	L	1	SLB	O2-C2-O6	-9.45	85.70	109.51
3	I	1	SLB	O2-C2-O6	-9.42	85.77	109.51
3	F	1	SLB	O2-C2-O6	-9.21	86.29	109.51
2	J	1	SLB	C3-C4-C5	-9.14	95.61	109.72
2	K	1	SLB	O2-C2-O6	-8.72	87.54	109.51
2	G	1	SLB	O2-C2-C1	-7.70	94.46	110.73
2	G	1	SLB	O2-C2-O6	-7.54	90.51	109.51
2	G	1	SLB	O6-C6-C5	6.36	115.66	109.84
2	J	1	SLB	C3-C2-C1	6.36	124.64	112.84
2	D	1	SLB	O2-C2-O6	-6.30	93.64	109.51
2	G	1	SLB	O1A-C1-C2	-5.47	114.73	123.85
2	J	1	SLB	O2-C2-O6	-5.41	95.88	109.51
2	H	1	SLB	O6-C6-C5	5.41	114.79	109.84
2	G	1	SLB	C3-C2-C1	5.39	122.85	112.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	SLB	O1A-C1-C2	-5.10	115.34	123.85
3	L	1	SLB	O6-C6-C5	5.03	114.44	109.84
2	D	1	SLB	O6-C6-C5	-4.93	105.33	109.84
2	K	1	SLB	O6-C6-C5	4.59	114.05	109.84
2	E	1	SLB	O6-C6-C5	4.38	113.85	109.84
2	J	1	SLB	O10-C10-N5	-4.15	114.65	121.98
2	J	1	SLB	O9-C9-C8	4.02	119.60	111.16
2	K	1	SLB	C3-C2-C1	3.94	120.16	112.84
2	J	1	SLB	C5-N5-C10	3.91	132.27	123.11
3	I	1	SLB	C3-C2-C1	3.83	119.96	112.84
2	J	1	SLB	O1A-C1-C2	-3.83	117.47	123.85
3	I	1	SLB	O6-C6-C5	3.82	113.34	109.84
2	J	1	SLB	O8-C8-C9	3.77	117.60	109.03
2	E	1	SLB	C3-C2-C1	3.77	119.83	112.84
2	J	1	SLB	O4-C4-C5	3.73	118.32	109.84
2	D	1	SLB	C3-C2-C1	3.63	119.57	112.84
3	F	1	SLB	C3-C2-C1	3.50	119.33	112.84
3	L	1	SLB	C3-C2-C1	3.48	119.31	112.84
3	L	2	SIA	C6-C5-N5	-3.45	105.41	110.91
2	E	2	SIA	C6-C5-N5	-3.42	105.46	110.91
2	H	1	SLB	C6-C5-N5	-3.40	105.48	110.91
2	D	1	SLB	C5-N5-C10	3.38	131.03	123.11
2	D	1	SLB	C6-C5-N5	3.34	116.23	110.91
2	H	1	SLB	O6-C6-C7	3.33	111.86	106.65
2	K	3	SIA	C6-C5-N5	-3.18	105.83	110.91
2	H	3	SIA	C4-C5-N5	-3.13	104.27	110.44
2	E	3	SIA	C6-C5-N5	-3.10	105.95	110.91
3	F	1	SLB	O1A-C1-C2	-3.09	118.70	123.85
3	L	1	SLB	O1A-C1-C2	-3.08	118.71	123.85
2	H	2	SIA	C6-C5-N5	-3.06	106.02	110.91
3	I	2	SIA	C6-C5-N5	-3.02	106.09	110.91
2	E	2	SIA	C4-C5-N5	-3.01	104.51	110.44
3	F	2	SIA	C6-C5-N5	-2.98	106.15	110.91
2	K	2	SIA	C6-C5-N5	-2.97	106.17	110.91
2	D	1	SLB	O9-C9-C8	2.96	117.37	111.16
2	J	2	SIA	C4-C5-N5	-2.96	104.61	110.44
2	E	3	SIA	C4-C5-N5	-2.88	104.76	110.44
2	K	2	SIA	O6-C2-C1	2.87	113.13	107.72
2	G	2	SIA	C4-C5-N5	-2.85	104.82	110.44
2	H	2	SIA	C4-C5-N5	-2.84	104.84	110.44
2	D	3	SIA	C4-C5-N5	-2.83	104.85	110.44
2	E	3	SIA	O6-C2-C1	2.83	113.06	107.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	SLB	C3-C4-C5	2.80	114.05	109.72
2	J	3	SIA	C6-C5-N5	-2.76	106.50	110.91
2	D	2	SIA	C6-C5-N5	-2.76	106.50	110.91
2	E	3	SIA	O1B-C1-C2	2.67	119.65	112.71
3	I	2	SIA	O1B-C1-C2	2.66	119.62	112.71
3	I	1	SLB	O6-C6-C7	2.65	110.78	106.65
2	J	3	SIA	C4-C5-N5	-2.64	105.23	110.44
3	I	1	SLB	O1A-C1-C2	-2.57	119.56	123.85
2	E	1	SLB	O1A-C1-C2	-2.52	119.65	123.85
2	J	3	SIA	O1B-C1-C2	2.52	119.25	112.71
2	H	3	SIA	O6-C2-C1	2.50	112.44	107.72
2	J	1	SLB	O7-C7-C6	-2.49	104.05	109.44
2	G	3	SIA	C6-C5-N5	-2.49	106.93	110.91
3	L	2	SIA	O1B-C1-C2	2.47	119.14	112.71
2	E	1	SLB	C3-C4-C5	2.47	113.54	109.72
2	G	3	SIA	C4-C5-N5	-2.46	105.59	110.44
2	E	2	SIA	O6-C2-C1	2.46	112.36	107.72
2	G	3	SIA	O1B-C1-C2	2.45	119.08	112.71
3	F	2	SIA	O1B-C1-C2	2.44	119.07	112.71
2	J	1	SLB	O10-C10-C11	2.43	126.38	122.05
2	K	3	SIA	O6-C2-C1	2.41	112.26	107.72
2	K	3	SIA	O1B-C1-C2	2.37	118.88	112.71
2	H	2	SIA	O6-C2-C1	2.36	112.17	107.72
2	D	3	SIA	O1B-C1-C2	2.35	118.83	112.71
2	E	1	SLB	O6-C6-C7	2.34	110.30	106.65
2	J	2	SIA	O1B-C1-C2	2.33	118.78	112.71
2	G	1	SLB	C5-N5-C10	2.31	128.51	123.11
2	D	3	SIA	C6-C5-N5	-2.30	107.23	110.91
2	K	3	SIA	C4-C5-N5	-2.29	105.92	110.44
3	I	2	SIA	O1A-C1-C2	-2.24	118.02	122.85
3	L	2	SIA	C4-C5-N5	-2.23	106.03	110.44
2	G	2	SIA	O1B-C1-C2	2.23	118.51	112.71
2	D	2	SIA	O1B-C1-C2	2.21	118.47	112.71
2	G	3	SIA	O6-C2-C1	2.20	111.86	107.72
2	J	2	SIA	C6-C5-N5	-2.18	107.43	110.91
2	H	3	SIA	O1B-C1-C2	2.16	118.34	112.71
2	H	2	SIA	C9-C8-C7	2.15	116.56	112.17
2	J	3	SIA	O1A-C1-C2	-2.13	118.24	122.85
2	D	2	SIA	C4-C5-N5	-2.13	106.24	110.44
2	E	3	SIA	O1A-C1-C2	-2.13	118.26	122.85
2	K	2	SIA	C9-C8-C7	2.12	116.50	112.17
2	H	1	SLB	O1A-C1-C2	-2.12	120.31	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	SLB	C3-C2-C1	2.11	116.76	112.84
2	K	2	SIA	C4-C5-N5	-2.09	106.32	110.44
2	E	2	SIA	O1B-C1-C2	2.09	118.15	112.71
2	H	3	SIA	C6-C5-N5	-2.09	107.58	110.91
2	D	1	SLB	O8-C8-C9	2.09	113.77	109.03
2	G	2	SIA	C6-C5-N5	-2.08	107.59	110.91
3	I	2	SIA	C4-C5-N5	-2.08	106.35	110.44
2	D	2	SIA	O6-C2-C1	2.07	111.63	107.72
2	K	1	SLB	C3-C4-C5	2.06	112.91	109.72
2	G	3	SIA	O1A-C1-C2	-2.06	118.40	122.85
2	J	2	SIA	O6-C2-C1	2.01	111.51	107.72

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	SLB	C6-C5-N5-C10
2	D	1	SLB	O6-C6-C7-O7
2	D	2	SIA	C7-C8-C9-O9
2	D	3	SIA	C7-C8-C9-O9
2	E	1	SLB	C6-C7-C8-C9
2	E	1	SLB	C6-C7-C8-O8
2	E	1	SLB	O7-C7-C8-C9
2	H	1	SLB	O1B-C1-C2-O6
2	J	1	SLB	C7-C8-C9-O9
2	J	1	SLB	O8-C8-C9-O9
2	K	1	SLB	O1B-C1-C2-O2
2	K	1	SLB	O1B-C1-C2-O6
2	K	3	SIA	C7-C8-C9-O9
2	K	3	SIA	O8-C8-C9-O9
3	F	2	SIA	O1A-C1-C2-O6
3	F	2	SIA	C5-C6-C7-O7
3	F	2	SIA	O6-C6-C7-O7
3	I	1	SLB	O1A-C1-C2-O2
3	I	2	SIA	O8-C8-C9-O9
3	L	1	SLB	O1A-C1-C2-O6
2	D	2	SIA	O8-C8-C9-O9
2	D	3	SIA	O8-C8-C9-O9
3	I	2	SIA	C7-C8-C9-O9
2	E	1	SLB	O7-C7-C8-O8
3	I	2	SIA	C6-C7-C8-O8
3	I	2	SIA	O7-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	D	1	SLB	C11-C10-N5-C5
2	D	1	SLB	O10-C10-N5-C5
2	D	2	SIA	C11-C10-N5-C5
2	D	2	SIA	O10-C10-N5-C5
2	G	1	SLB	C11-C10-N5-C5
2	G	1	SLB	O10-C10-N5-C5
2	J	1	SLB	C11-C10-N5-C5
2	J	1	SLB	O10-C10-N5-C5
2	J	2	SIA	C11-C10-N5-C5
2	J	2	SIA	O10-C10-N5-C5
3	I	2	SIA	O7-C7-C8-C9
3	I	2	SIA	C6-C7-C8-C9
2	H	3	SIA	C6-C7-C8-O8
2	J	1	SLB	C4-C5-N5-C10
2	H	3	SIA	O7-C7-C8-C9
2	D	2	SIA	C6-C7-C8-O8
2	J	2	SIA	C6-C7-C8-O8
2	D	2	SIA	C6-C7-C8-C9
2	H	3	SIA	O7-C7-C8-O8
2	G	1	SLB	C6-C7-C8-O8
2	H	3	SIA	C6-C7-C8-C9
2	J	2	SIA	C6-C7-C8-C9
3	I	1	SLB	C6-C7-C8-C9
3	I	1	SLB	C6-C7-C8-O8
3	F	2	SIA	O1A-C1-C2-C3
3	F	2	SIA	O1B-C1-C2-C3
2	D	1	SLB	O7-C7-C8-O8
2	H	1	SLB	O1B-C1-C2-C3
3	I	1	SLB	O8-C8-C9-O9
3	F	2	SIA	O6-C6-C7-C8
2	D	1	SLB	O1A-C1-C2-O6
3	F	2	SIA	C5-C6-C7-C8
2	D	3	SIA	O1A-C1-C2-O6
2	J	2	SIA	O1A-C1-C2-O6
2	J	3	SIA	O1A-C1-C2-O6
3	I	1	SLB	C7-C8-C9-O9
2	D	1	SLB	C6-C7-C8-O8
3	F	2	SIA	C6-C7-C8-C9
2	H	1	SLB	C6-C7-C8-O8
2	G	1	SLB	O7-C7-C8-O8
2	H	2	SIA	C6-C7-C8-C9
3	L	1	SLB	C6-C7-C8-O8

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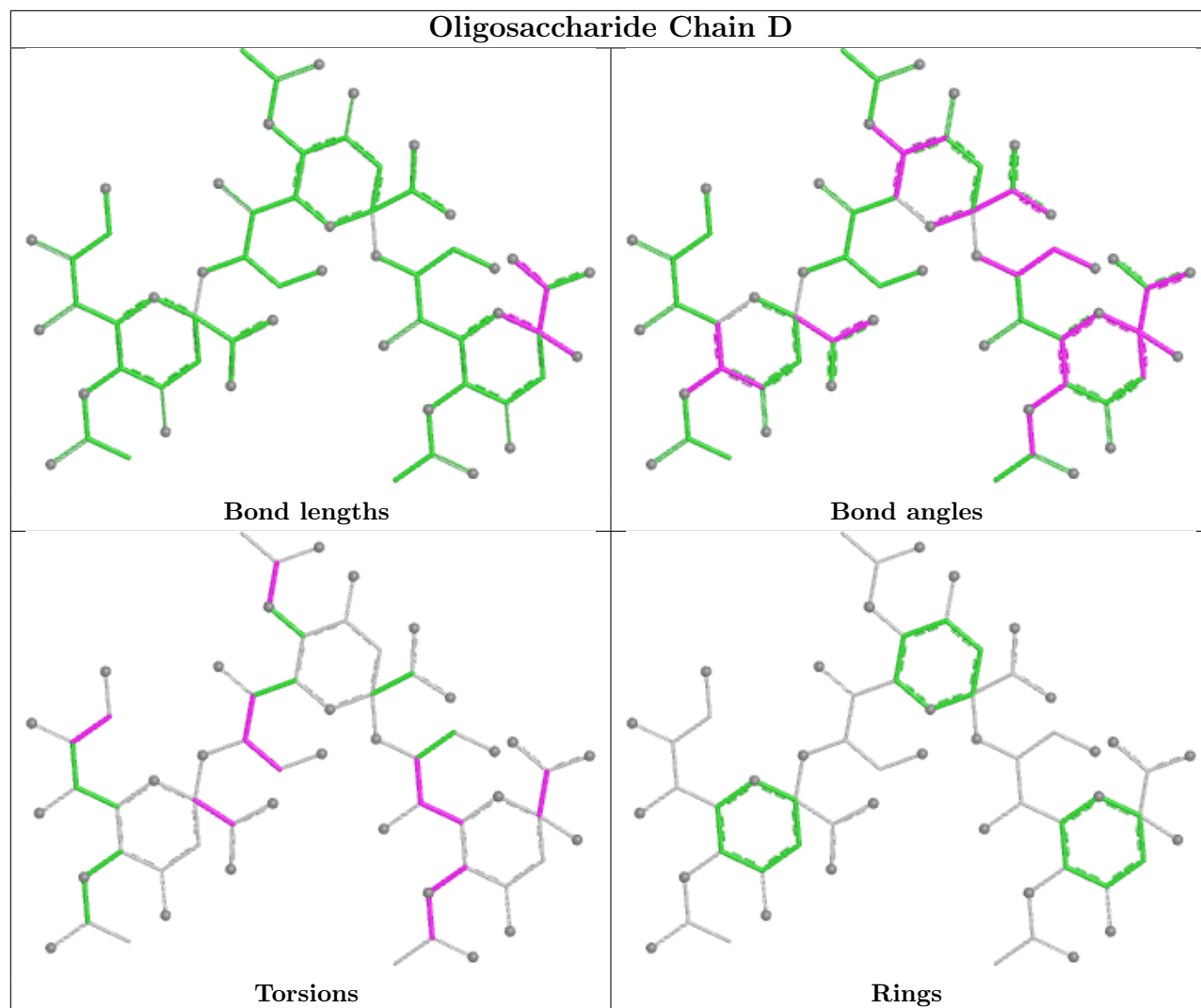
Mol	Chain	Res	Type	Atoms
2	D	2	SIA	O7-C7-C8-O8
2	D	1	SLB	O1B-C1-C2-O2
2	G	1	SLB	O1B-C1-C2-O2
2	J	1	SLB	O1B-C1-C2-O2
3	F	1	SLB	O1B-C1-C2-O2
3	I	1	SLB	O1B-C1-C2-O2
3	L	1	SLB	O1B-C1-C2-O2
2	G	2	SIA	C6-C7-C8-O8
2	J	3	SIA	O1A-C1-C2-C3
2	J	2	SIA	O7-C7-C8-O8
2	D	1	SLB	O1B-C1-C2-C3
2	H	1	SLB	O1A-C1-C2-C3
2	D	1	SLB	C4-C5-N5-C10

There are no ring outliers.

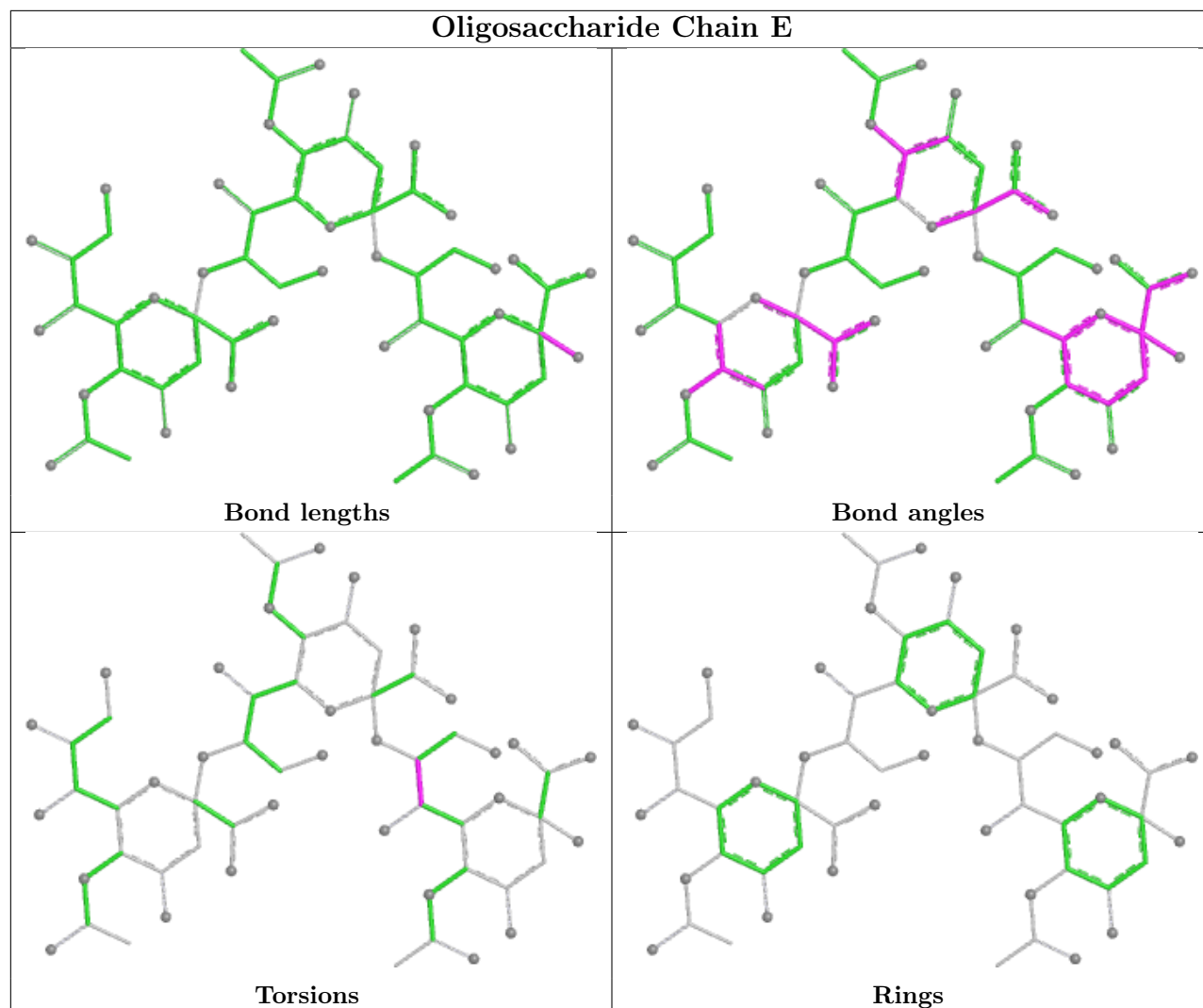
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	SLB	2	0
2	D	1	SLB	3	0
3	I	1	SLB	1	0
2	J	2	SIA	1	0
2	G	1	SLB	2	0
2	J	1	SLB	3	0
2	K	1	SLB	1	0

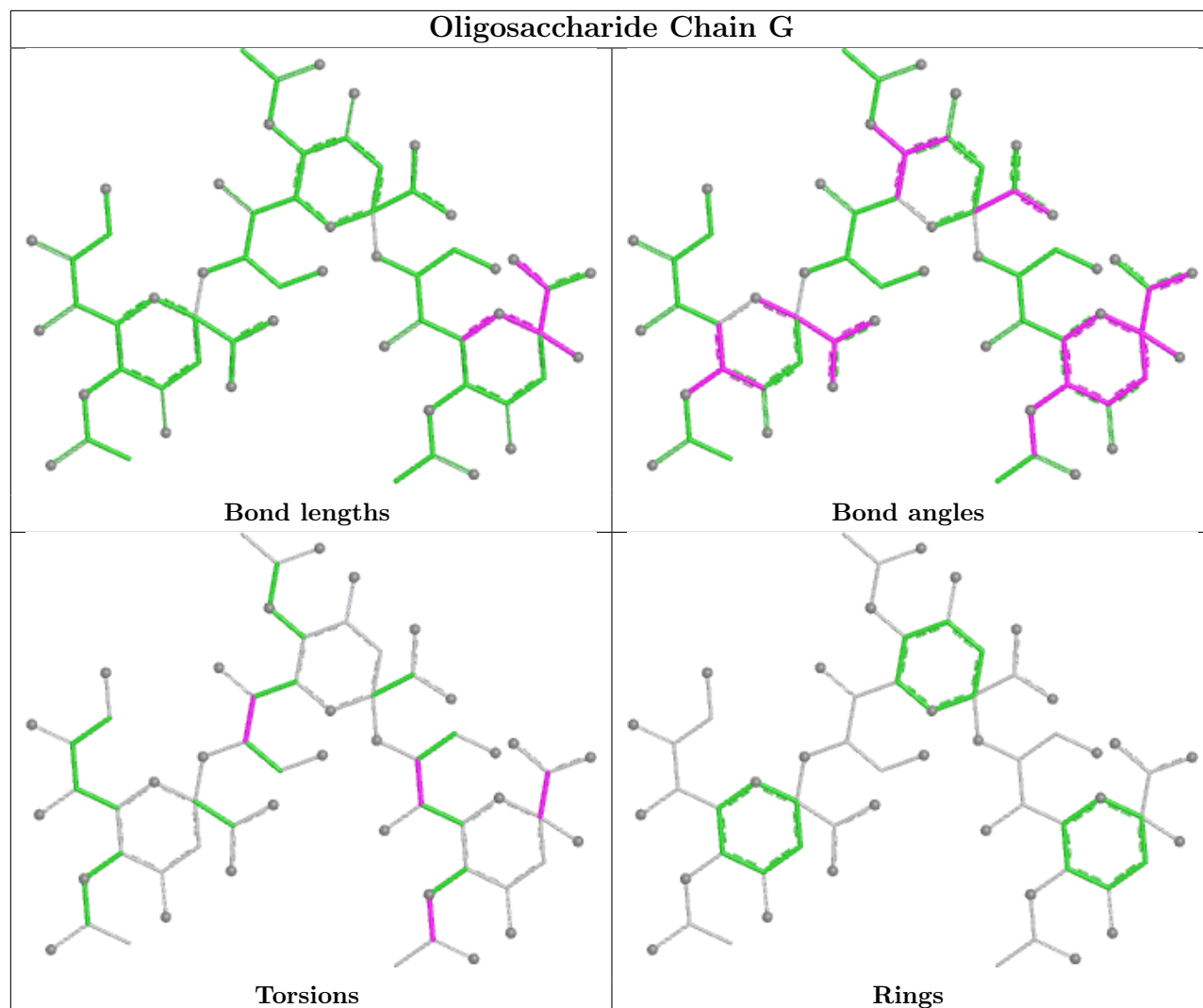
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



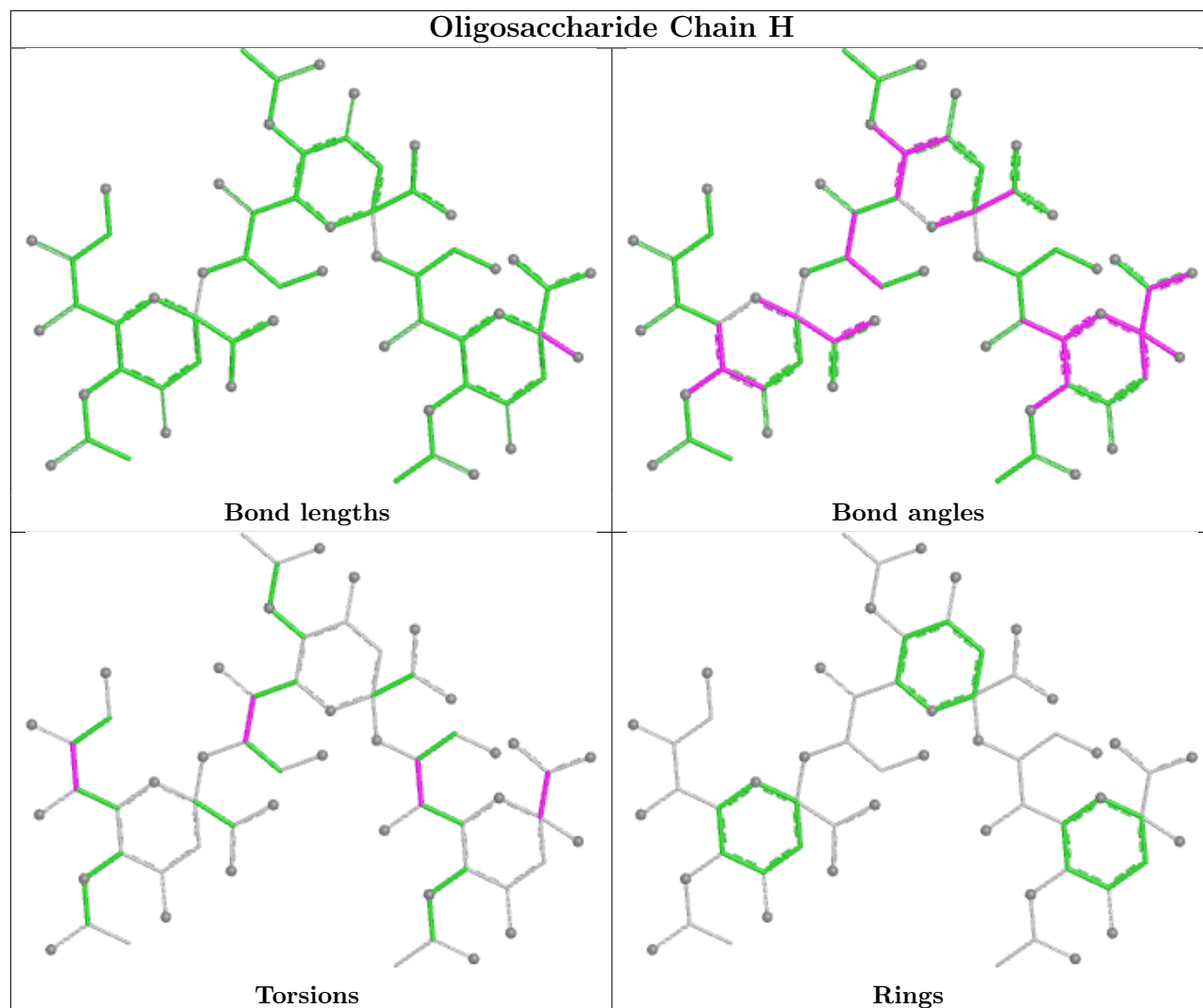
Oligosaccharide Chain E



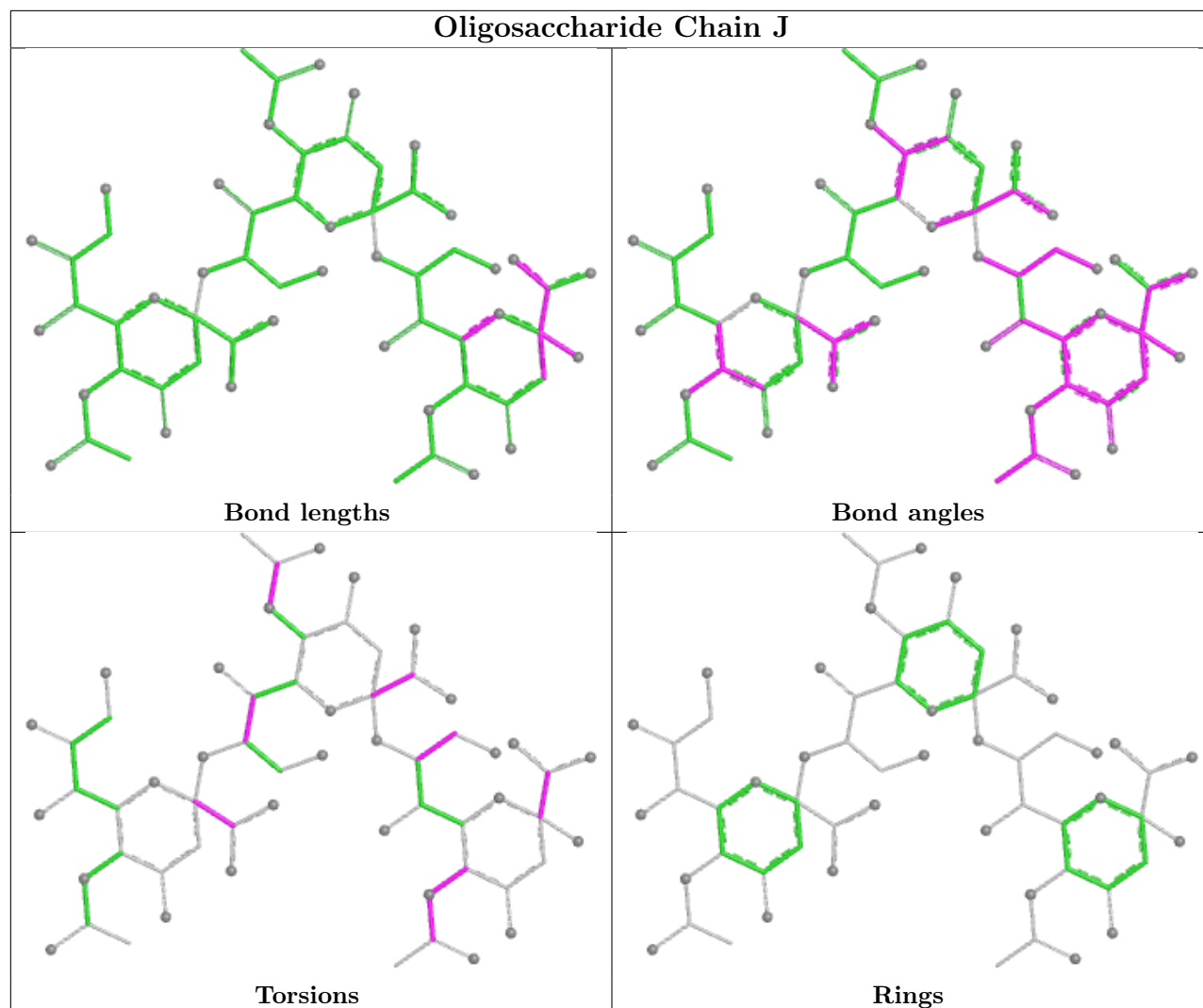
Oligosaccharide Chain G

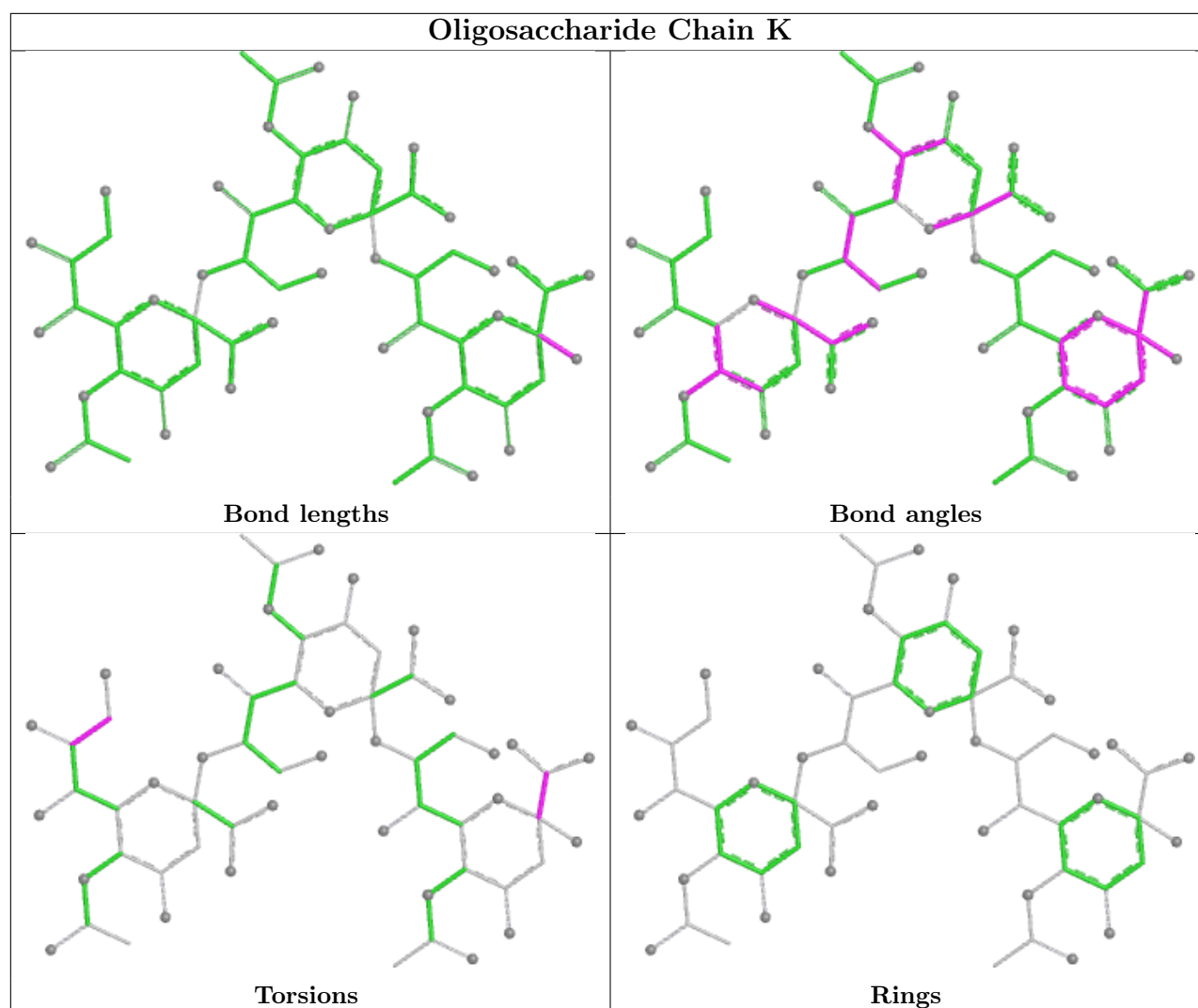


Oligosaccharide Chain H

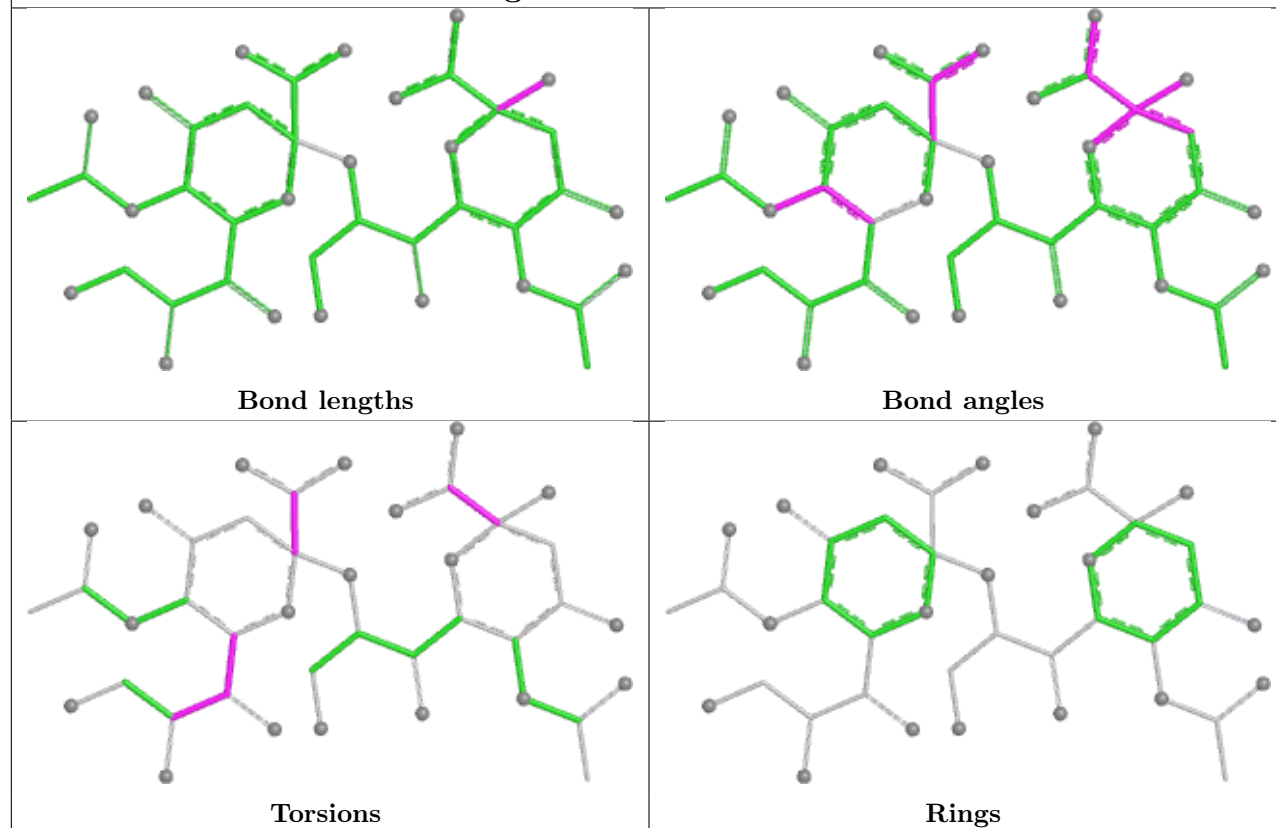


Oligosaccharide Chain J

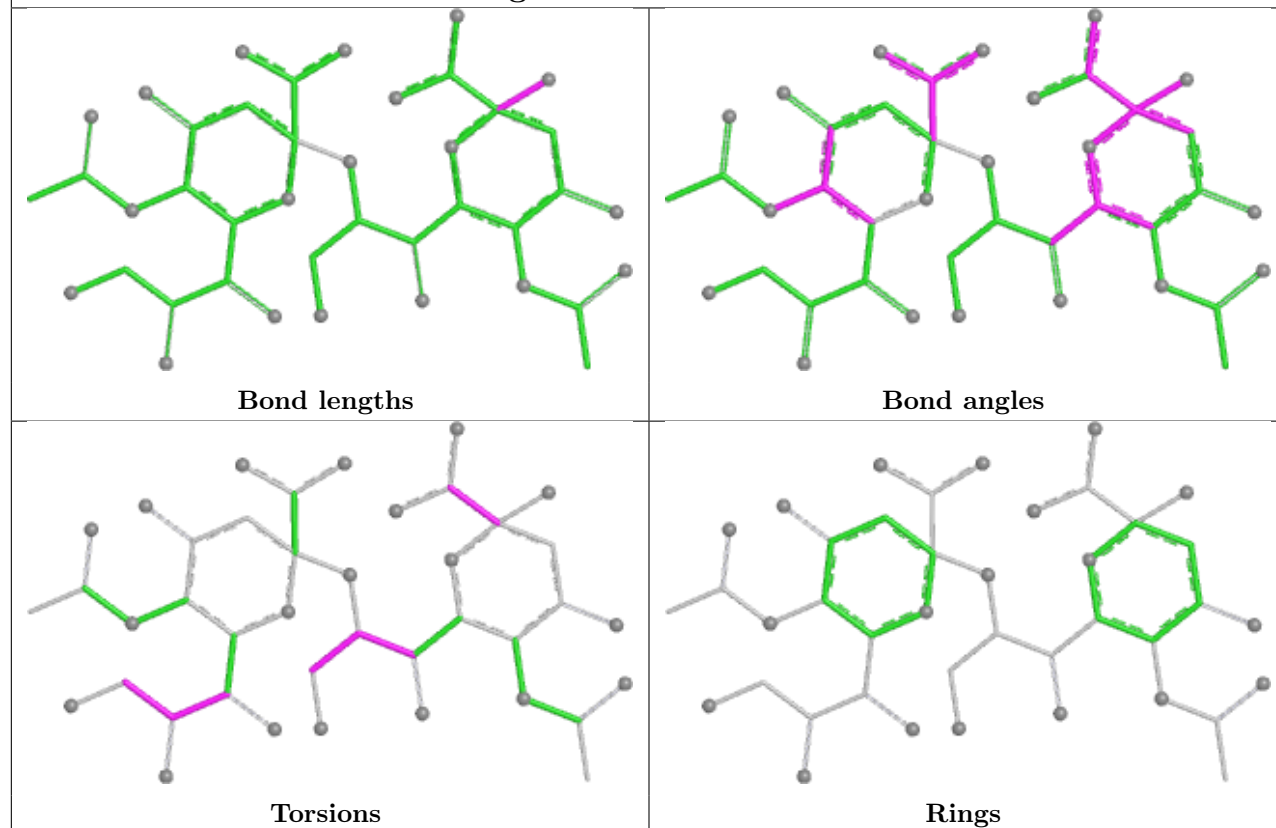


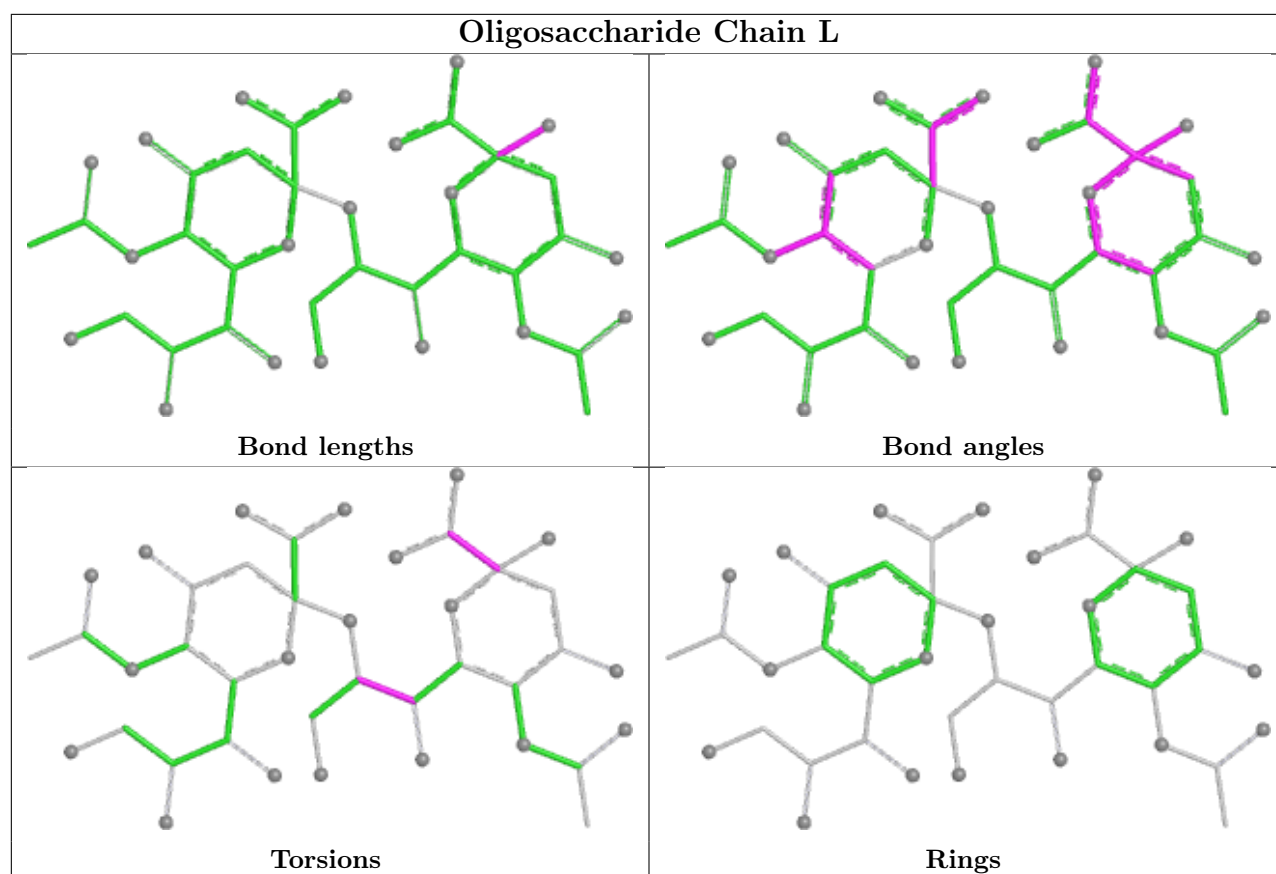


Oligosaccharide Chain F



Oligosaccharide Chain I





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	644/670 (96%)	-0.35	10 (1%) 70 77	8, 19, 41, 53	17 (2%)
1	B	666/670 (99%)	-0.55	10 (1%) 71 79	8, 18, 31, 44	14 (2%)
1	C	666/670 (99%)	-0.51	5 (0%) 82 89	10, 19, 34, 49	12 (1%)
All	All	1976/2010 (98%)	-0.47	25 (1%) 74 81	8, 18, 38, 53	43 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	910[A]	THR	5.7
1	C	269	GLN	3.7
1	B	682	ASP	3.6
1	A	494	LEU	3.5
1	A	437	ALA	3.4
1	A	436	ALA	3.3
1	C	267	VAL	3.3
1	A	475	THR	2.9
1	C	682	ASP	2.9
1	B	439[A]	GLN	2.9
1	C	504	GLY	2.6
1	A	439	GLN	2.5
1	B	268	GLY	2.5
1	B	269	GLN	2.4
1	A	491	THR	2.4
1	B	504	GLY	2.3
1	C	268	GLY	2.3
1	A	438	ASN	2.3
1	A	504	GLY	2.2
1	B	909	VAL	2.1
1	B	270	LYS	2.1
1	B	251	VAL	2.1
1	A	442	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	245	SER	2.1
1	A	497	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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

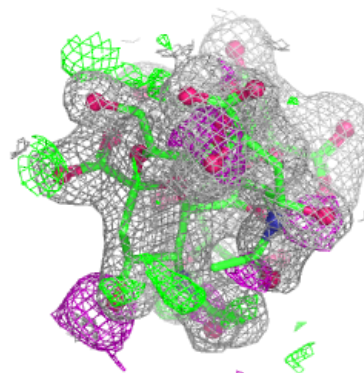
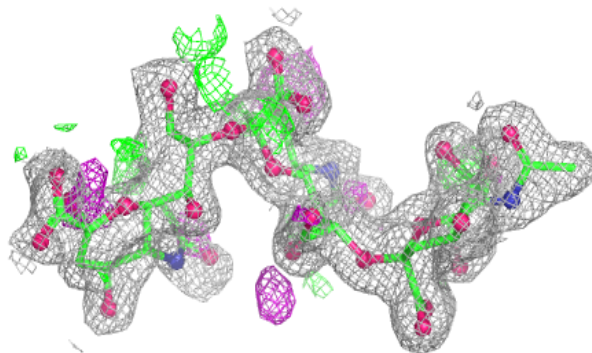
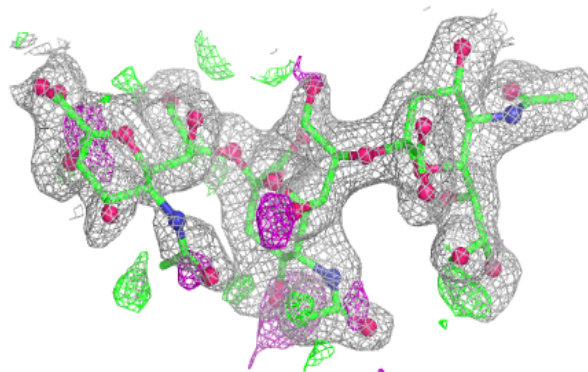
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SLB	F	1	21/21	0.50	0.21	29,33,34,34	21
2	SLB	E	1	21/21	0.68	0.14	51,53,55,56	0
2	SIA	E	3	20/21	0.70	0.12	56,58,59,59	0
2	SLB	J	1	21/21	0.71	0.14	39,48,50,51	0
2	SLB	D	1	21/21	0.77	0.12	38,46,48,49	1
2	SIA	K	3	20/21	0.77	0.11	38,41,43,44	0
2	SLB	G	1	21/21	0.77	0.12	30,39,40,42	0
3	SLB	I	1	21/21	0.77	0.13	29,35,39,40	2
2	SIA	D	2	20/21	0.79	0.11	30,33,35,35	0
3	SLB	L	1	21/21	0.80	0.11	24,29,35,38	0
2	SIA	H	3	20/21	0.84	0.09	38,41,43,44	0
2	SIA	E	2	20/21	0.84	0.12	46,48,51,52	0
2	SIA	J	2	20/21	0.85	0.10	30,32,34,35	0
2	SLB	H	1	21/21	0.86	0.10	26,29,32,32	0
2	SIA	J	3	20/21	0.87	0.09	28,30,32,33	0
3	SIA	F	2	20/21	0.87	0.10	22,27,33,34	0
2	SIA	D	3	20/21	0.89	0.08	26,29,33,35	0
3	SIA	I	2	20/21	0.91	0.07	17,22,29,31	0
2	SIA	H	2	20/21	0.92	0.07	24,26,32,33	0
2	SIA	G	2	20/21	0.93	0.07	24,25,25,27	0
2	SLB	K	1	21/21	0.93	0.06	19,22,25,27	0
2	SIA	K	2	20/21	0.93	0.07	19,20,31,31	0
2	SIA	G	3	20/21	0.94	0.06	21,24,27,28	0
3	SIA	L	2	20/21	0.95	0.06	15,17,22,25	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

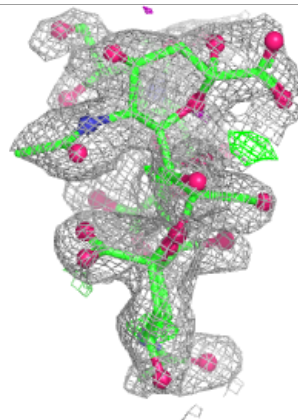
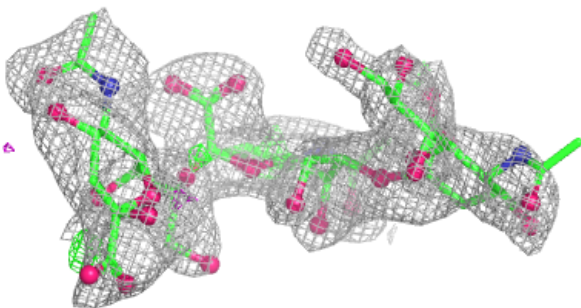
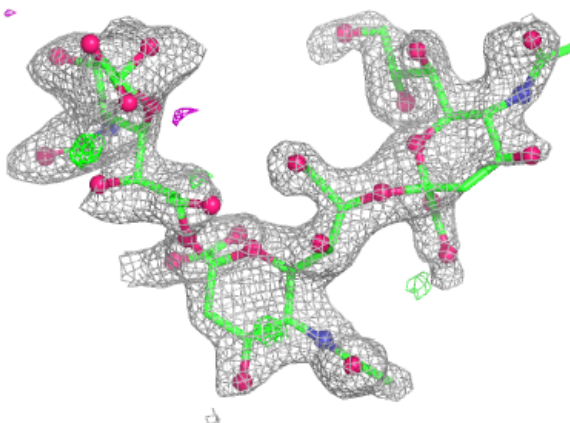
Electron density around Chain D:

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



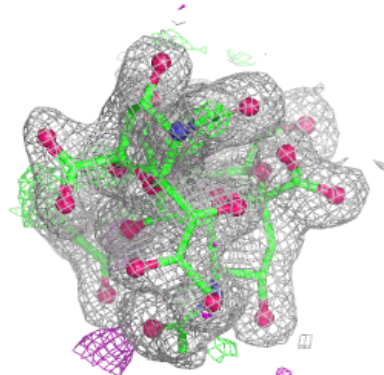
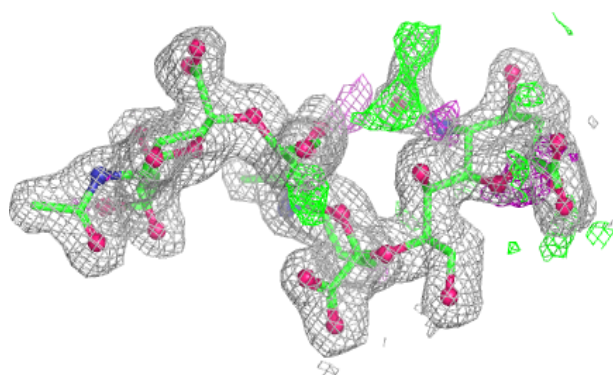
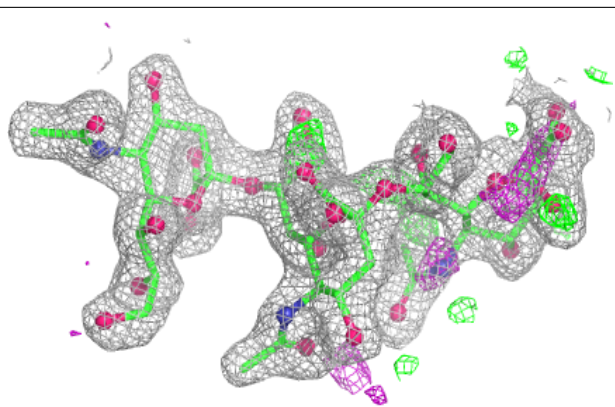
Electron density around Chain E:

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



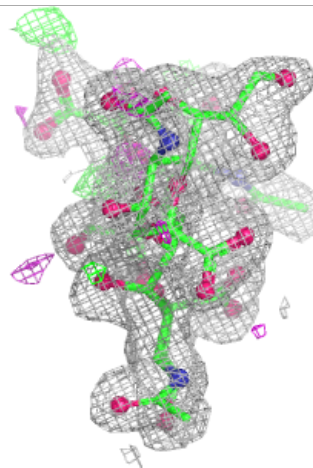
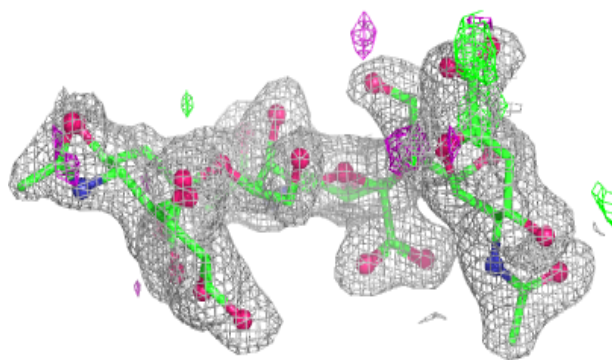
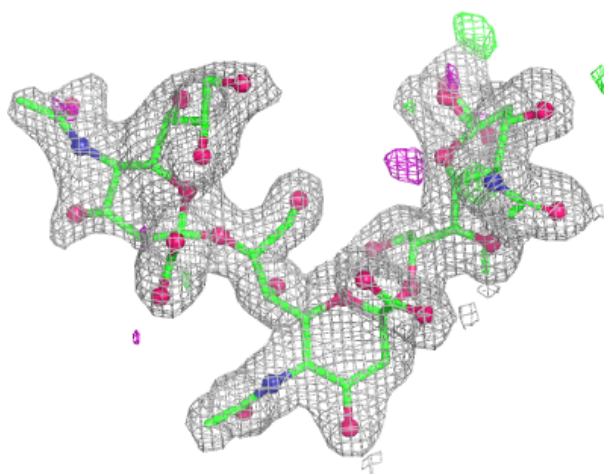
Electron density around Chain G:

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



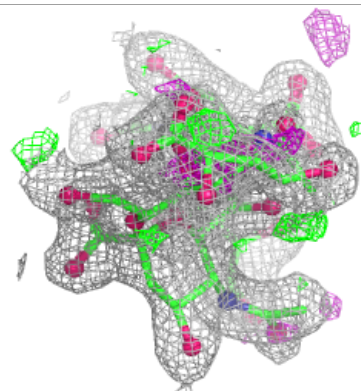
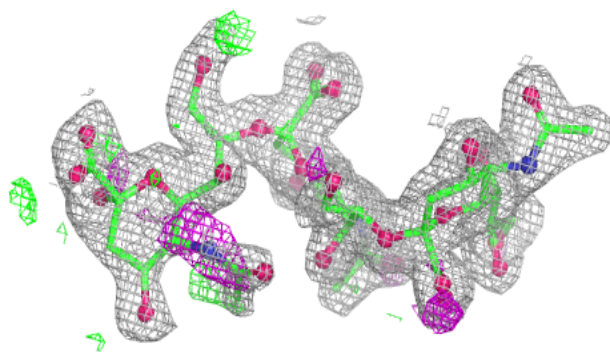
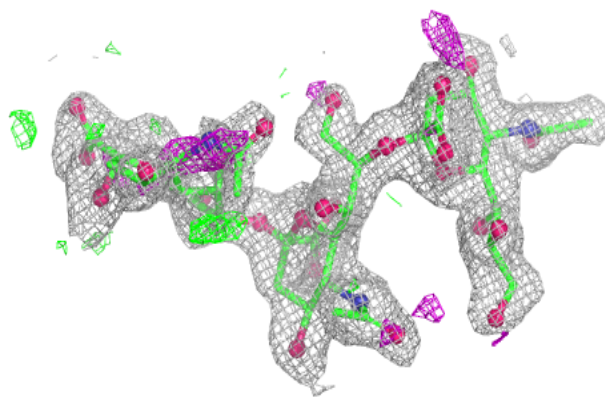
Electron density around Chain H:

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

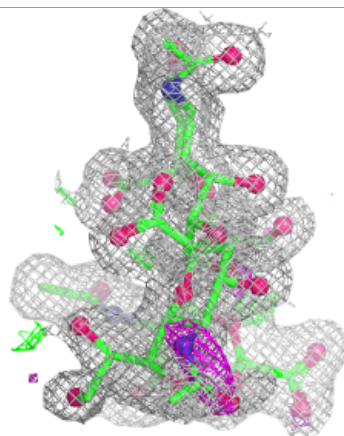
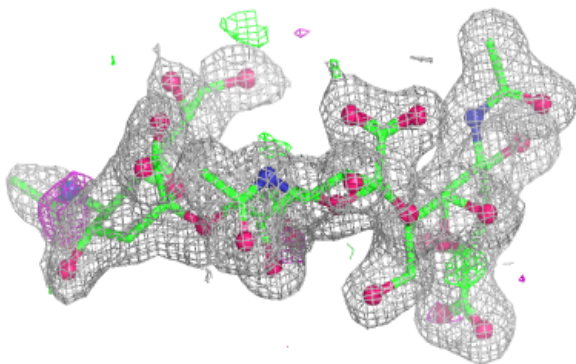
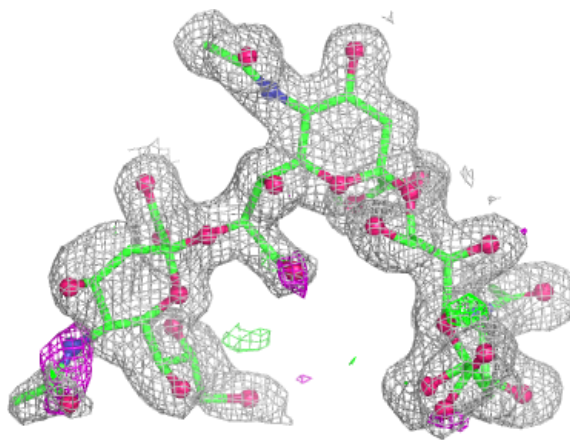


Electron density around Chain J:

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

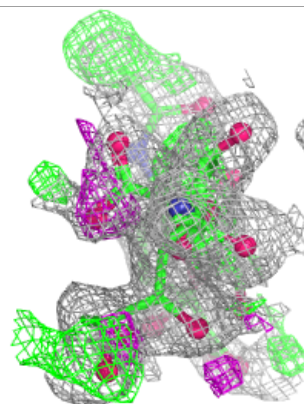
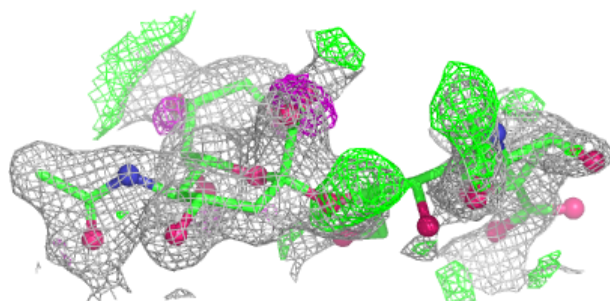
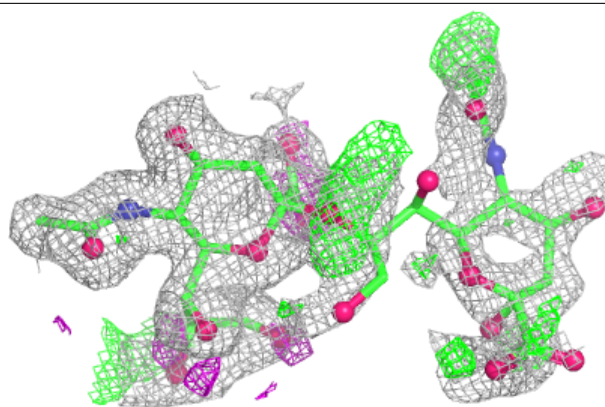
**Electron density around Chain K:**

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

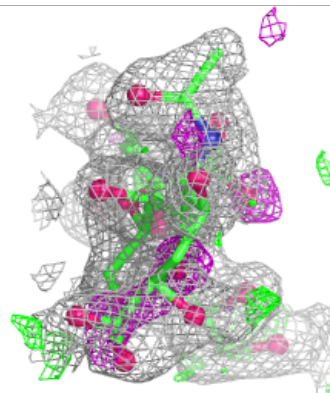
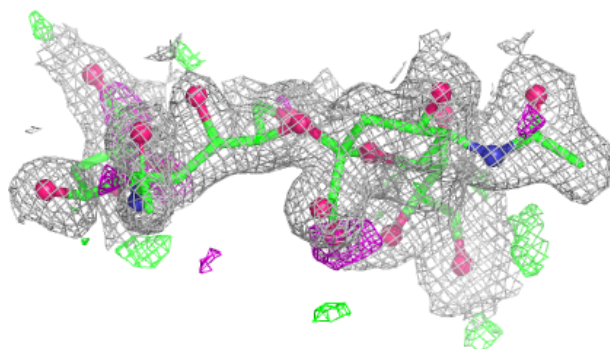
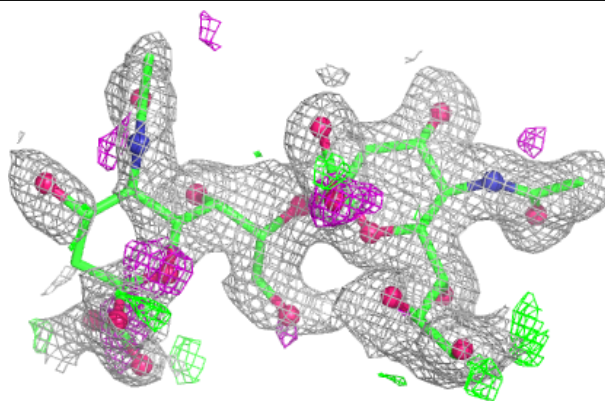


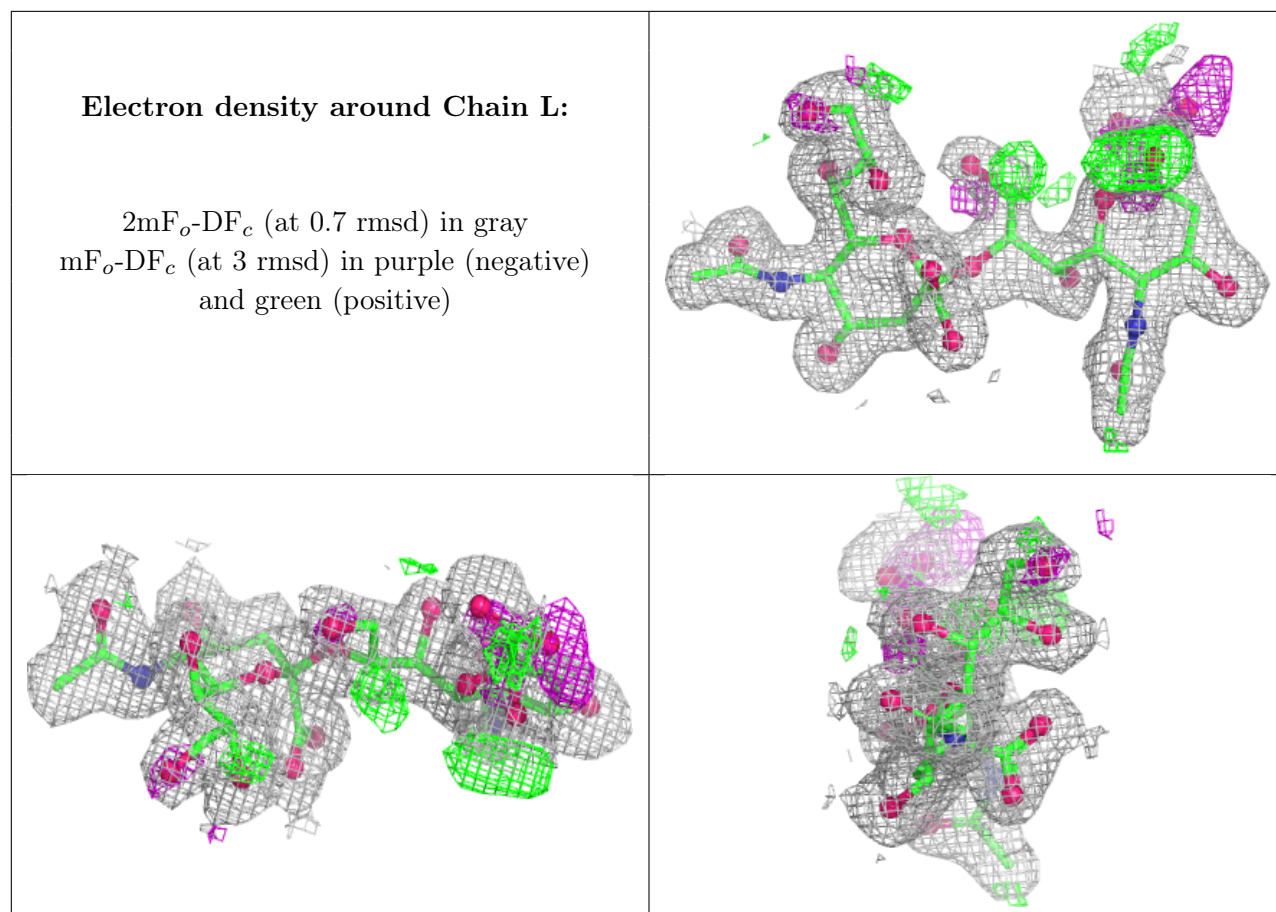
Electron density around Chain F:

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

**Electron density around Chain I:**

$2mF_o - DF_c$ (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(\AA^2)	Q<0.9
4	NA	C	1001	1/1	0.98	0.03	17,17,17,17	0
4	NA	B	1001	1/1	0.99	0.02	14,14,14,14	0
4	NA	A	1001	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.