



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:33 PM UTC

PDB ID : 8XC4 / pdb_00008xc4
Title : Nipah virus attachment glycoprotein head domain in complex with a broadly neutralizing antibody 1E5
Authors : Fan, P.F.; Yu, C.M.; Chen, W.
Deposited on : 2023-12-08
Resolution : 3.24 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

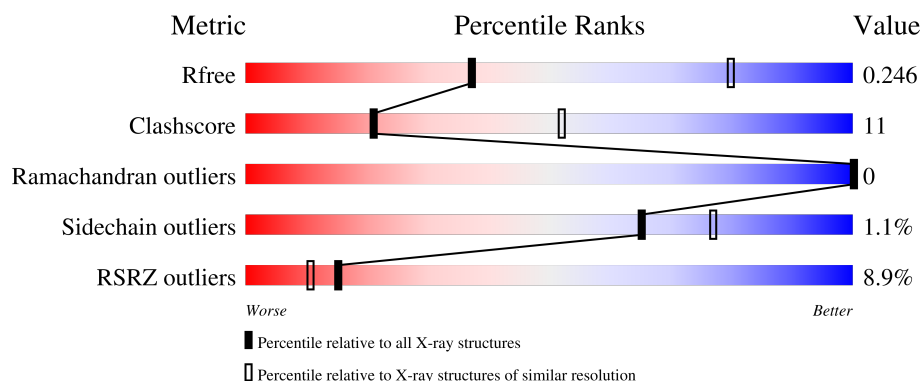
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

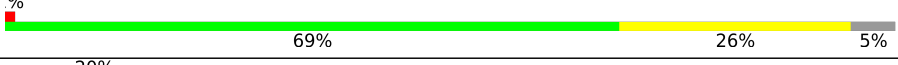
The reported resolution of this entry is 3.24 Å.

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.



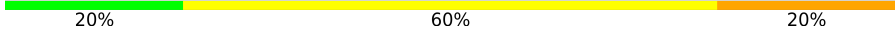
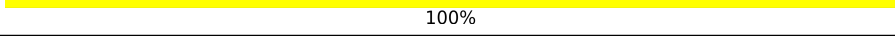
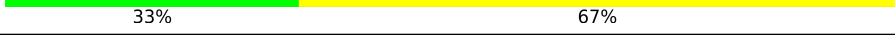
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	439	
1	B	439	
2	C	242	
2	E	242	
3	D	214	

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Mol	Chain	Length	Quality of chain
3	F	214	
4	G	4	
5	H	5	
5	K	5	
6	I	3	
6	L	3	
7	J	5	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13778 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 Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3383	2153	566	643	21			
1	B	428	Total	C	N	O	S	0	0	0
			3383	2153	566	643	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	HIS	-	expression tag	UNP Q4VCP5
A	165	HIS	-	expression tag	UNP Q4VCP5
A	166	HIS	-	expression tag	UNP Q4VCP5
A	167	HIS	-	expression tag	UNP Q4VCP5
A	168	HIS	-	expression tag	UNP Q4VCP5
A	169	HIS	-	expression tag	UNP Q4VCP5
A	170	GLY	-	expression tag	UNP Q4VCP5
A	171	SER	-	expression tag	UNP Q4VCP5
A	172	GLY	-	expression tag	UNP Q4VCP5
A	173	GLY	-	expression tag	UNP Q4VCP5
A	174	GLY	-	expression tag	UNP Q4VCP5
A	175	SER	-	expression tag	UNP Q4VCP5
B	164	HIS	-	expression tag	UNP Q4VCP5
B	165	HIS	-	expression tag	UNP Q4VCP5
B	166	HIS	-	expression tag	UNP Q4VCP5
B	167	HIS	-	expression tag	UNP Q4VCP5
B	168	HIS	-	expression tag	UNP Q4VCP5
B	169	HIS	-	expression tag	UNP Q4VCP5
B	170	GLY	-	expression tag	UNP Q4VCP5
B	171	SER	-	expression tag	UNP Q4VCP5
B	172	GLY	-	expression tag	UNP Q4VCP5
B	173	GLY	-	expression tag	UNP Q4VCP5
B	174	GLY	-	expression tag	UNP Q4VCP5
B	175	SER	-	expression tag	UNP Q4VCP5

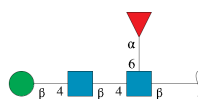
- Molecule 2 is a protein called 1E5-VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	229	Total	C	N	O	S	0	0	0
			1727	1099	281	342	5			
2	E	229	Total	C	N	O	S	0	0	0
			1727	1099	281	342	5			

- Molecule 3 is a protein called 1E5-VL.

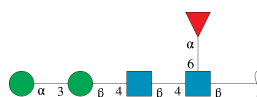
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1612	1008	268	331	5			
3	F	211	Total	C	N	O	S	0	0	0
			1612	1008	268	331	5			

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



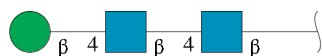
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



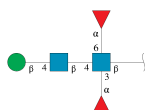
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	5	Total	C	N	O	0	0	0
			60	34	2	24			
5	K	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



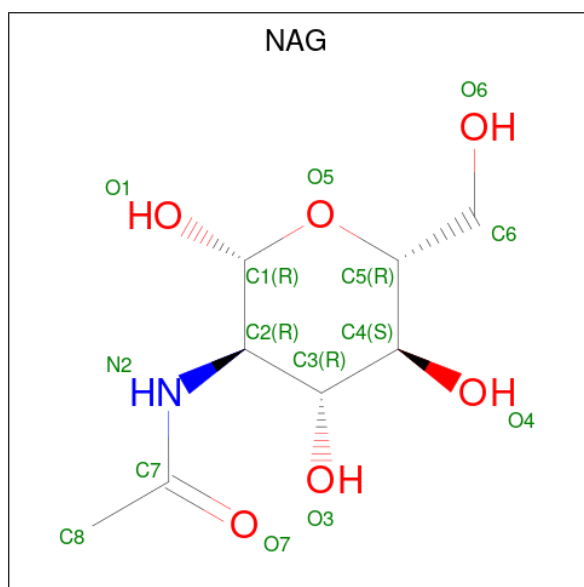
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	5	Total	C	N	O	0	0	0
			59	34	2	23			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

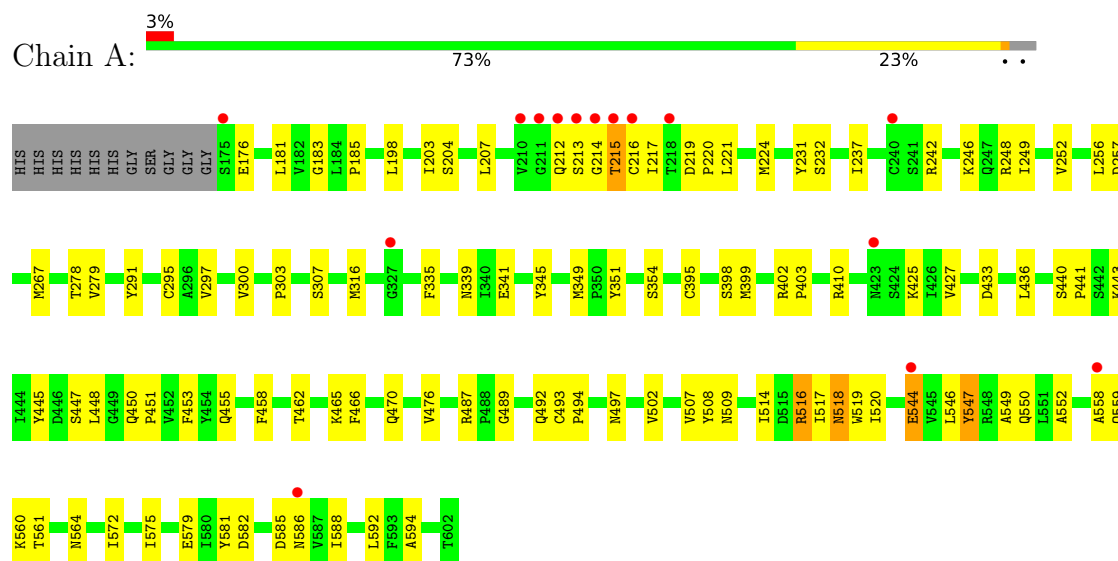


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

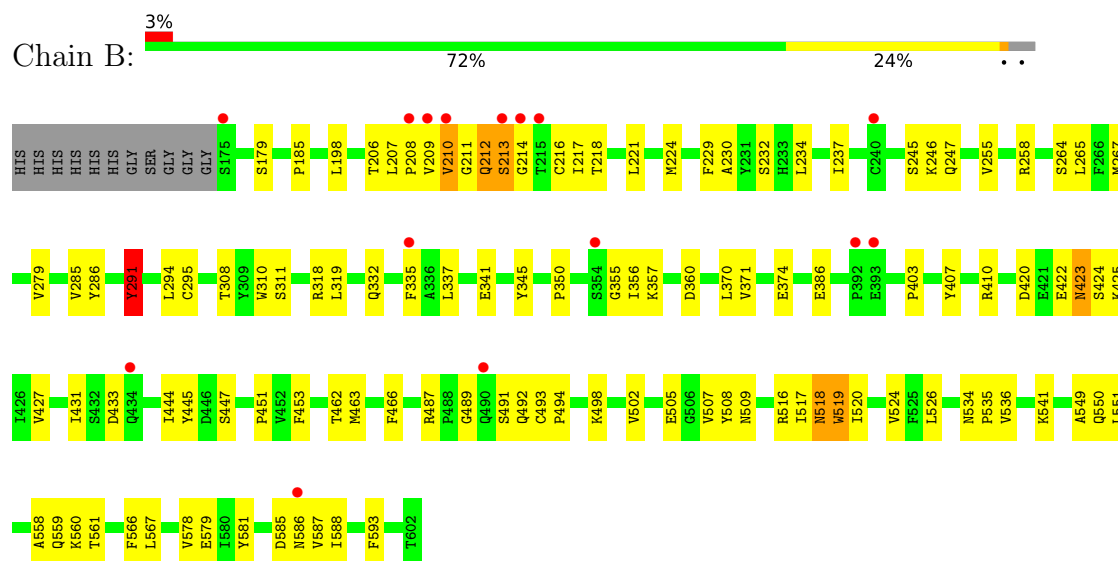
3 Residue-property plots

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.

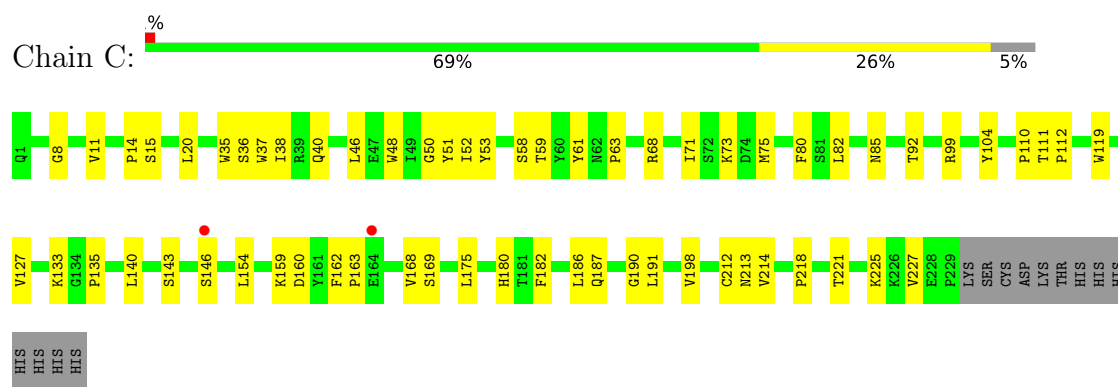
• Molecule 1: Glycoprotein



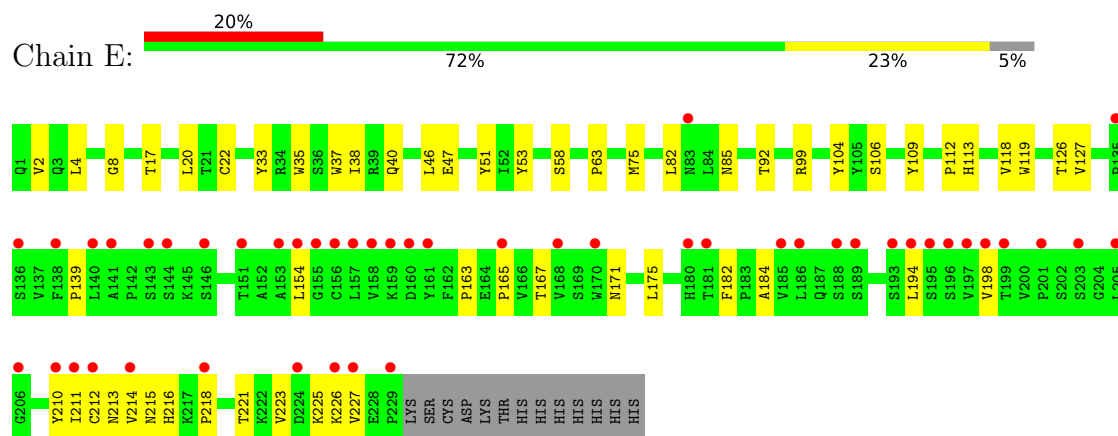
• Molecule 1: Glycoprotein



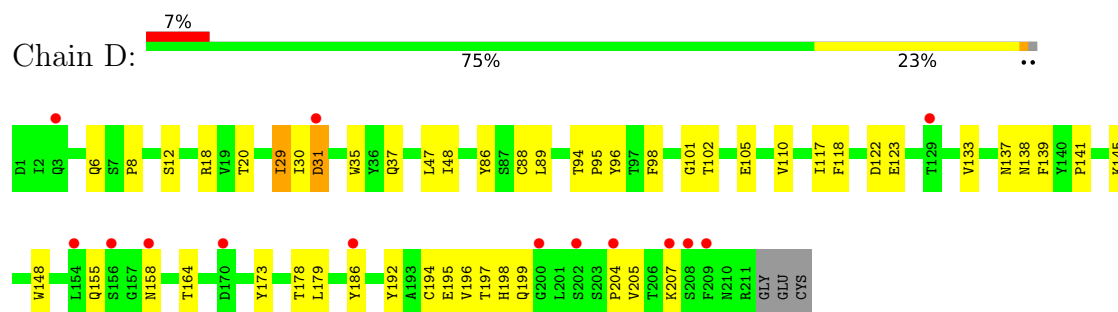
• Molecule 2: 1E5-VH



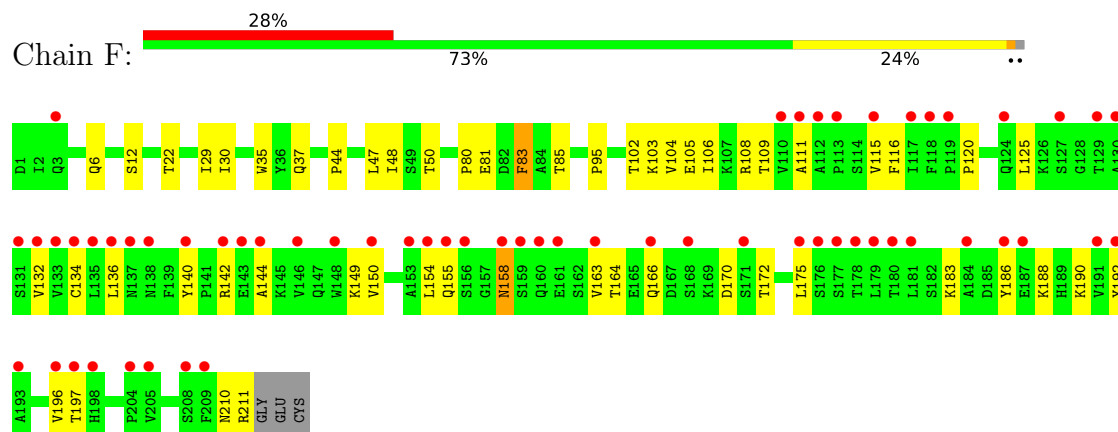
• Molecule 2: 1E5-VH



• Molecule 3: 1E5-VL



• Molecule 3: 1E5-VL



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

Chain G:  75% 25%

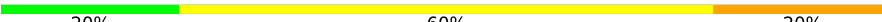


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  80% 20%

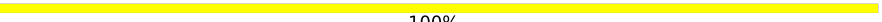


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  20% 60% 20%

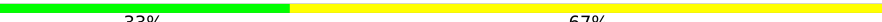


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



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

Chain L:  33% 67%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  20% 20% 60%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	193.42Å 193.42Å 198.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.69 – 3.24 33.69 – 3.24	Depositor EDS
% Data completeness (in resolution range)	95.7 (33.69-3.24) 95.6 (33.69-3.24)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.218 , 0.247 0.221 , 0.246	Depositor DCC
R_{free} test set	2004 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13778	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: NAG, FUC, MAN, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/3463	0.76	3/4708 (0.1%)
1	B	0.40	0/3463	0.82	10/4708 (0.2%)
2	C	0.31	0/1778	0.69	2/2437 (0.1%)
2	E	0.19	0/1778	0.55	0/2437
3	D	0.30	0/1645	0.72	1/2234 (0.0%)
3	F	0.34	0/1645	0.76	1/2234 (0.0%)
All	All	0.35	0/13772	0.74	17/18758 (0.1%)

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

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

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	TYR	CA-CB-CG	7.69	127.73	113.90
1	B	291	TYR	CB-CA-C	7.61	122.74	109.80
1	B	212	GLN	CB-CA-C	-6.81	108.73	116.63
1	A	517	ILE	N-CA-C	-6.65	103.84	110.62
1	B	208	PRO	N-CA-C	-6.63	98.81	112.47
2	C	162	PHE	CA-C-O	-6.51	114.19	120.64
1	A	518	ASN	N-CA-C	-6.23	98.74	108.90
1	B	209	VAL	N-CA-C	-6.13	106.76	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	158	ASN	N-CA-C	-6.02	105.52	112.92
1	B	517	ILE	N-CA-C	-5.92	104.07	110.23
3	D	29	ILE	N-CA-C	-5.80	99.28	107.75
1	B	424	SER	N-CA-C	-5.76	104.89	112.72
2	C	190	GLY	N-CA-C	-5.55	107.60	115.43
1	B	518	ASN	N-CA-C	-5.45	99.64	108.52
1	B	535	PRO	CB-CA-C	-5.40	104.50	111.46
1	A	215	THR	N-CA-C	-5.27	103.44	110.55
1	B	420	ASP	N-CA-C	-5.14	103.36	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	516	ARG	Sidechain
1	B	291	TYR	Sidechain

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	3383	0	3309	70	3
1	B	3383	0	3309	79	3
2	C	1727	0	1672	43	0
2	E	1727	0	1672	46	0
3	D	1612	0	1576	38	0
3	F	1612	0	1576	45	0
4	G	49	0	43	0	0
5	H	60	0	52	0	0
5	K	60	0	52	1	0
6	I	39	0	34	1	0
6	L	39	0	34	0	0
7	J	59	0	52	2	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
All	All	13778	0	13407	299	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (299) 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)
2:C:92:THR:HG22	2:C:127:VAL:H	1.25	1.00
3:F:150:VAL:HG23	3:F:155:GLN:HG3	1.52	0.91
1:B:207:LEU:HD11	1:B:267:MET:HE3	1.54	0.88
3:F:190:LYS:HG3	3:F:210:ASN:HB3	1.58	0.86
1:A:207:LEU:HD11	1:A:267:MET:HE3	1.61	0.83
1:A:586:ASN:ND2	3:F:30:ILE:O	2.14	0.81
2:C:63:PRO:HD2	3:D:95:PRO:HG3	1.64	0.79
3:F:150:VAL:CG2	3:F:155:GLN:HG3	2.12	0.78
1:B:403:PRO:HG3	1:B:502:VAL:HG11	1.66	0.76
2:C:38:ILE:HD11	2:C:119:TRP:CZ3	2.22	0.75
1:B:423:ASN:HD22	1:B:423:ASN:H	1.35	0.74
3:D:148:TRP:HB2	3:D:155:GLN:HB3	1.70	0.73
2:C:8:GLY:HA3	2:C:20:LEU:HD23	1.69	0.73
2:C:11:VAL:HG23	2:C:163:PRO:HG3	1.70	0.73
3:F:111:ALA:HB3	3:F:140:TYR:H	1.54	0.71
3:F:106:ILE:O	3:F:166:GLN:NE2	2.23	0.70
2:E:38:ILE:HD11	2:E:119:TRP:CZ3	2.26	0.70
1:A:403:PRO:HG3	1:A:502:VAL:HG11	1.74	0.69
1:B:211:GLY:HA3	1:B:217:ILE:HD11	1.73	0.69
3:F:85:THR:HG22	3:F:103:LYS:HG2	1.73	0.69
1:A:470:GLN:HB3	1:A:476:VAL:HG13	1.74	0.68
3:F:136:LEU:HD21	3:F:196:VAL:HG11	1.74	0.68
1:B:319:LEU:HD23	1:B:332:GLN:HB3	1.74	0.68
3:D:133:VAL:HG22	3:D:178:THR:HG22	1.76	0.68
2:C:187:GLN:HG2	2:C:191:LEU:O	1.92	0.68
1:A:224:MET:HE3	1:A:564:ASN:HB2	1.74	0.67
1:B:585:ASP:HB2	1:B:587:VAL:HG22	1.76	0.67
1:B:286:TYR:O	1:B:357:LYS:HD3	1.93	0.67
1:B:234:LEU:HD11	1:B:245:SER:HB3	1.74	0.66
2:C:52:ILE:HD12	2:C:59:THR:HG22	1.76	0.66
1:B:371:VAL:HB	1:B:374:GLU:HG2	1.78	0.66
1:A:579:GLU:HB3	1:A:588:ILE:HD11	1.78	0.65
3:D:195:GLU:HG3	3:D:205:VAL:HG22	1.77	0.65
3:F:125:LEU:O	3:F:183:LYS:HD3	1.97	0.64
1:A:224:MET:HE1	1:A:575:ILE:HB	1.80	0.64
2:E:211:ILE:HG12	2:E:226:LYS:HG2	1.79	0.64
2:E:214:VAL:HB	2:E:223:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:O	1:A:425:LYS:HA	1.98	0.64
1:B:519:TRP:O	1:B:541:LYS:HG2	1.97	0.63
1:B:507:VAL:HG21	1:B:559:GLN:O	1.99	0.62
3:F:108:ARG:HG2	3:F:109:THR:H	1.65	0.62
3:F:83:PHE:HB2	3:F:106:ILE:CD1	2.31	0.61
1:A:492:GLN:O	1:A:493:CYS:SG	2.58	0.61
1:B:505:GLU:HA	2:C:110:PRO:HB2	1.82	0.61
3:D:145:LYS:HB3	3:D:197:THR:HB	1.83	0.61
1:B:230:ALA:HB2	1:B:291:TYR:CE2	2.36	0.61
1:B:536:VAL:HG22	1:B:550:GLN:HG3	1.82	0.60
2:E:215:ASN:HA	2:E:221:THR:O	2.02	0.60
2:C:38:ILE:HD11	2:C:119:TRP:CH2	2.37	0.59
2:E:8:GLY:HA3	2:E:20:LEU:HD23	1.84	0.59
3:F:142:ARG:NH2	3:F:163:VAL:HG11	2.17	0.59
2:E:40:GLN:HB2	2:E:46:LEU:HD23	1.84	0.59
3:F:83:PHE:HD1	3:F:104:VAL:O	1.86	0.59
3:F:35:TRP:HB2	3:F:48:ILE:HB	1.85	0.58
3:D:186:TYR:HA	3:D:192:TYR:OH	2.03	0.58
1:A:440:SER:HB2	1:A:455:GLN:HG3	1.86	0.58
3:F:108:ARG:CZ	3:F:111:ALA:HB2	2.33	0.58
1:B:286:TYR:HB2	1:B:291:TYR:CD1	2.39	0.57
7:J:1:NAG:H62	7:J:2:NAG:C1	2.33	0.57
1:A:213:SER:HB3	1:B:214:GLY:O	2.03	0.57
2:C:35:TRP:CE3	2:C:99:ARG:HB3	2.40	0.57
2:C:135:PRO:HD2	2:C:221:THR:HG21	1.86	0.57
1:B:559:GLN:HE22	2:C:111:THR:HG21	1.70	0.56
1:A:354:SER:HB2	1:A:443:LYS:HG3	1.88	0.56
2:C:133:LYS:HE2	2:C:160:ASP:O	2.06	0.56
3:F:108:ARG:NH2	3:F:111:ALA:HB2	2.21	0.56
1:A:448:LEU:HD11	1:A:514:ILE:O	2.05	0.56
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.88	0.56
1:A:176:GLU:HA	1:A:257:ASP:HB3	1.87	0.55
2:C:168:VAL:HG12	2:C:214:VAL:HG22	1.88	0.55
1:B:487:ARG:NH1	1:B:489:GLY:HA3	2.22	0.55
2:C:92:THR:HG22	2:C:127:VAL:N	2.09	0.55
1:B:286:TYR:HA	1:B:291:TYR:HD1	1.69	0.55
1:B:185:PRO:HB3	1:B:567:LEU:HD21	1.88	0.55
2:C:169:SER:O	2:C:213:ASN:HB2	2.06	0.55
2:E:175:LEU:HD21	2:E:198:VAL:HG21	1.89	0.55
2:C:37:TRP:CG	2:C:82:LEU:HD12	2.42	0.55
1:A:351:TYR:CE2	1:A:441:PRO:HD3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:O	1:B:332:GLN:HA	2.07	0.54
1:A:402:ARG:HD2	2:E:33:TYR:CD1	2.42	0.54
3:F:29:ILE:O	3:F:29:ILE:HG13	2.07	0.54
3:F:155:GLN:HB3	3:F:158:ASN:ND2	2.23	0.54
1:B:229:PHE:C	1:B:291:TYR:HE2	2.16	0.54
1:A:219:ASP:N	1:A:220:PRO:HD3	2.23	0.54
1:B:216:CYS:SG	1:B:218:THR:HG23	2.48	0.54
2:E:35:TRP:CZ3	2:E:99:ARG:HB3	2.43	0.53
1:B:286:TYR:HB2	1:B:291:TYR:CE1	2.43	0.53
1:A:212:GLN:HG3	1:A:217:ILE:HD11	1.90	0.53
1:A:441:PRO:HD2	1:A:458:PHE:CE2	2.43	0.53
2:C:180:HIS:CE1	3:D:138:ASN:HD21	2.26	0.53
1:A:546:LEU:HB3	1:A:547:TYR:CD2	2.44	0.53
2:E:4:LEU:HD21	2:E:35:TRP:HZ3	1.74	0.53
1:A:183:GLY:O	1:A:185:PRO:HD3	2.09	0.53
2:C:175:LEU:HD21	2:C:198:VAL:HG21	1.90	0.52
2:E:92:THR:HG22	2:E:126:THR:HA	1.89	0.52
2:C:212:CYS:HB2	2:C:225:LYS:H	1.74	0.52
1:B:423:ASN:H	1:B:423:ASN:ND2	2.05	0.52
2:E:35:TRP:CE3	2:E:99:ARG:HB3	2.45	0.52
1:A:279:VAL:HG13	1:A:295:CYS:SG	2.50	0.52
1:B:206:THR:HG21	1:B:264:SER:CB	2.40	0.52
2:C:154:LEU:HD12	2:C:227:VAL:HB	1.92	0.52
2:E:225:LYS:HD3	2:E:226:LYS:H	1.73	0.52
3:D:86:TYR:O	3:D:101:GLY:HA2	2.10	0.52
3:F:108:ARG:HG2	3:F:109:THR:N	2.24	0.52
2:E:92:THR:HG22	2:E:127:VAL:H	1.74	0.52
1:A:550:GLN:HG2	1:A:552:ALA:O	2.10	0.52
3:D:122:ASP:OD1	3:D:123:GLU:N	2.40	0.52
3:D:198:HIS:CG	3:D:199:GLN:H	2.27	0.52
1:B:508:TYR:HB3	1:B:560:LYS:HG3	1.92	0.51
1:A:237:ILE:HG12	1:A:246:LYS:HB2	1.91	0.51
1:A:256:LEU:HD11	3:D:18:ARG:HB3	1.92	0.51
3:D:30:ILE:HD12	3:D:30:ILE:H	1.72	0.51
1:A:221:LEU:HB3	1:A:232:SER:HB3	1.92	0.51
1:B:524:VAL:HB	1:B:561:THR:HG21	1.92	0.51
3:F:190:LYS:HD2	3:F:211:ARG:HH21	1.75	0.51
1:A:487:ARG:HD2	1:A:487:ARG:O	2.11	0.51
1:B:410:ARG:NH1	1:B:431:ILE:O	2.43	0.51
3:F:30:ILE:H	3:F:30:ILE:HD12	1.76	0.51
1:A:487:ARG:HD2	1:A:487:ARG:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:TYR:O	1:B:451:PRO:HA	2.12	0.50
2:E:37:TRP:CG	2:E:82:LEU:HD12	2.46	0.50
1:A:507:VAL:HG21	1:A:559:GLN:O	2.10	0.50
3:D:31:ASP:OD1	3:D:31:ASP:N	2.42	0.50
1:B:487:ARG:HH22	1:B:493:CYS:HB3	1.77	0.50
3:D:35:TRP:HB2	3:D:48:ILE:HB	1.93	0.50
1:A:204:SER:HB3	1:A:592:LEU:HB2	1.93	0.50
1:B:586:ASN:ND2	3:D:30:ILE:O	2.45	0.50
1:A:216:CYS:SG	1:A:588:ILE:HG22	2.52	0.49
1:B:487:ARG:HH12	1:B:489:GLY:HA3	1.76	0.49
1:B:279:VAL:HG13	1:B:295:CYS:SG	2.51	0.49
1:B:294:LEU:HG	1:B:350:PRO:HG3	1.93	0.49
3:F:170:ASP:OD2	3:F:172:THR:OG1	2.23	0.49
3:D:195:GLU:CG	3:D:205:VAL:HG22	2.41	0.49
1:A:181:LEU:HD21	1:A:572:ILE:HG12	1.95	0.49
3:D:6:GLN:NE2	3:D:102:THR:HG23	2.28	0.49
1:A:214:GLY:HA3	1:B:210:VAL:HG13	1.94	0.49
2:E:154:LEU:HD11	2:E:210:TYR:HD2	1.78	0.49
1:B:286:TYR:CA	1:B:291:TYR:HD1	2.26	0.49
2:E:63:PRO:HD2	3:F:95:PRO:HG3	1.94	0.49
3:F:108:ARG:HG2	3:F:108:ARG:NH2	2.27	0.49
3:F:144:ALA:HA	3:F:197:THR:O	2.13	0.49
1:B:487:ARG:HD2	1:B:487:ARG:O	2.12	0.49
2:E:99:ARG:CG	2:E:118:VAL:HB	2.43	0.49
2:E:17:THR:HG22	2:E:85:ASN:HA	1.95	0.48
2:C:73:LYS:HA	2:C:80:PHE:HA	1.94	0.48
3:F:115:VAL:HG22	3:F:136:LEU:CD2	2.43	0.48
1:B:462:THR:HG21	1:B:494:PRO:O	2.13	0.48
2:C:48:TRP:HZ2	2:C:51:TYR:HD2	1.61	0.48
2:E:212:CYS:N	2:E:225:LYS:O	2.36	0.48
1:B:258:ARG:O	3:F:22:THR:HB	2.13	0.48
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.95	0.48
2:E:184:ALA:HB2	2:E:194:LEU:HD23	1.95	0.48
1:A:198:LEU:HB2	1:A:549:ALA:HB2	1.95	0.47
1:B:524:VAL:HB	1:B:561:THR:CG2	2.43	0.47
1:B:558:ALA:HB1	1:B:579:GLU:O	2.13	0.47
2:C:8:GLY:HA3	2:C:20:LEU:CD2	2.43	0.47
1:A:450:GLN:H	1:A:516:ARG:HH22	1.63	0.47
2:C:61:TYR:HE1	2:C:71:ILE:HG13	1.80	0.47
1:B:579:GLU:HB3	1:B:588:ILE:HD11	1.97	0.47
3:F:120:PRO:HG3	3:F:132:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:THR:HG21	1:A:494:PRO:O	2.15	0.47
1:A:514:ILE:HG12	1:A:520:ILE:O	2.15	0.47
3:D:29:ILE:HG13	3:D:29:ILE:O	2.14	0.47
1:A:203:ILE:HD13	1:A:594:ALA:HB2	1.97	0.47
1:A:558:ALA:HB1	1:A:579:GLU:O	2.15	0.47
1:B:487:ARG:NH1	1:B:493:CYS:O	2.44	0.47
2:C:143:SER:HB2	2:C:146:SER:HB3	1.96	0.47
3:D:198:HIS:CG	3:D:199:GLN:N	2.83	0.47
3:F:85:THR:HA	3:F:102:THR:O	2.15	0.47
1:A:224:MET:CE	1:A:564:ASN:HB2	2.42	0.47
1:A:445:TYR:O	1:A:451:PRO:HA	2.15	0.47
1:A:433:ASP:N	1:A:433:ASP:OD1	2.48	0.46
1:A:447:SER:O	1:A:516:ARG:NH2	2.48	0.46
1:A:487:ARG:HH12	1:A:489:GLY:HA3	1.80	0.46
2:E:171:ASN:OD1	2:E:210:TYR:HA	2.15	0.46
1:A:351:TYR:CZ	1:A:441:PRO:HD3	2.50	0.46
1:B:308:THR:HA	1:B:407:TYR:HE2	1.81	0.46
1:B:551:LEU:HD13	1:B:593:PHE:CD2	2.50	0.46
2:C:140:LEU:HB3	3:D:118:PHE:CD1	2.51	0.46
3:F:136:LEU:HD13	3:F:144:ALA:HB3	1.97	0.46
3:F:12:SER:HA	3:F:105:GLU:O	2.15	0.46
3:F:149:LYS:HG3	3:F:154:LEU:HD13	1.97	0.46
1:B:221:LEU:HB3	1:B:232:SER:HB3	1.96	0.46
2:E:92:THR:CG2	2:E:127:VAL:H	2.29	0.46
3:F:136:LEU:HD13	3:F:144:ALA:CB	2.45	0.46
1:B:341:GLU:HG3	1:B:427:VAL:HG22	1.98	0.45
2:C:36:SER:HB2	2:C:50:GLY:O	2.16	0.45
2:C:40:GLN:HB2	2:C:46:LEU:HD23	1.97	0.45
2:E:2:VAL:HG11	2:E:99:ARG:NH1	2.31	0.45
2:C:186:LEU:HD23	2:C:187:GLN:O	2.16	0.45
3:D:205:VAL:HG11	3:D:207:LYS:HE2	1.99	0.45
1:A:453:PHE:O	1:A:466:PHE:HA	2.16	0.45
1:A:345:TYR:OH	1:A:410:ARG:HD3	2.16	0.45
1:A:462:THR:CG2	1:A:497:ASN:HB3	2.46	0.45
1:B:224:MET:HE2	1:B:265:LEU:HD21	1.99	0.45
3:D:117:ILE:HD11	3:D:194:CYS:H	1.82	0.45
2:E:119:TRP:CE3	3:F:44:PRO:HD2	2.51	0.45
1:A:212:GLN:OE1	1:B:213:SER:HA	2.16	0.45
3:D:8:PRO:O	3:D:102:THR:HG22	2.16	0.45
2:E:38:ILE:HB	2:E:47:GLU:O	2.17	0.45
1:A:492:GLN:HG2	2:E:51:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ARG:HD2	1:B:487:ARG:C	2.42	0.45
2:E:213:ASN:HA	2:E:223:VAL:O	2.17	0.45
2:C:14:PRO:O	2:C:15:SER:OG	2.28	0.45
2:E:22:CYS:HB2	2:E:37:TRP:CH2	2.51	0.45
1:B:355:GLY:HA2	1:B:444:ILE:HG22	1.97	0.45
1:A:351:TYR:O	1:A:441:PRO:HA	2.17	0.45
1:B:206:THR:OG1	1:B:264:SER:HB3	2.17	0.45
1:B:255:VAL:HG22	1:B:265:LEU:HD22	1.99	0.45
1:B:285:VAL:HG22	1:B:355:GLY:HA3	1.99	0.45
1:B:310:TRP:CD1	1:B:311:SER:N	2.85	0.45
1:B:198:LEU:HB2	1:B:549:ALA:HB2	1.99	0.44
1:A:248:ARG:HD2	1:A:248:ARG:HA	1.74	0.44
1:A:508:TYR:HB3	1:A:560:LYS:HG3	2.00	0.44
1:A:581:TYR:CE2	1:A:588:ILE:HD12	2.53	0.44
2:E:221:THR:HG22	2:E:223:VAL:HG23	2.00	0.44
1:B:345:TYR:CE1	1:B:370:LEU:HB2	2.53	0.44
1:A:252:VAL:HG11	1:A:291:TYR:HB2	1.99	0.44
2:C:159:LYS:HB3	2:C:159:LYS:HE2	1.68	0.44
3:F:188:LYS:HB3	3:F:188:LYS:HE2	1.75	0.44
3:D:138:ASN:HA	3:D:173:TYR:O	2.16	0.44
1:B:453:PHE:O	1:B:466:PHE:HA	2.17	0.44
2:C:175:LEU:CD2	2:C:198:VAL:HG21	2.48	0.43
2:E:139:PRO:HB3	2:E:227:VAL:HG22	2.00	0.43
2:E:215:ASN:OD1	2:E:216:HIS:N	2.50	0.43
1:B:207:LEU:HD11	1:B:267:MET:HB2	2.00	0.43
1:B:462:THR:HG22	1:B:487:ARG:NH2	2.32	0.43
1:B:509:ASN:HD21	1:B:526:LEU:HG	1.83	0.43
2:E:38:ILE:HD11	2:E:119:TRP:CH2	2.53	0.43
3:F:190:LYS:HA	3:F:210:ASN:HB2	2.01	0.43
1:B:492:GLN:NE2	2:C:59:THR:O	2.51	0.43
2:E:53:TYR:CD1	2:E:58:SER:HB2	2.52	0.43
1:A:242:ARG:HD2	3:F:50:THR:OG1	2.18	0.43
1:A:278:THR:O	1:A:297:VAL:HA	2.17	0.43
1:B:237:ILE:HG13	1:B:246:LYS:HB2	2.01	0.43
1:B:491:SER:HB3	3:D:94:THR:OG1	2.17	0.43
2:E:106:SER:HB3	2:E:109:TYR:HD2	1.83	0.43
2:E:113:HIS:CD2	3:F:50:THR:HG22	2.54	0.43
5:K:2:NAG:H3	5:K:5:FUC:H63	2.01	0.43
1:B:423:ASN:C	1:B:425:LYS:H	2.26	0.43
2:C:182:PHE:CE1	3:D:164:THR:HG23	2.54	0.43
3:F:116:PHE:O	3:F:134:CYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:SER:HA	1:A:249:ILE:O	2.18	0.43
1:A:300:VAL:HG12	6:I:1:NAG:H61	2.01	0.43
1:A:316:MET:HB3	1:A:335:PHE:HB2	2.00	0.43
2:C:68:ARG:HD2	2:C:85:ASN:O	2.18	0.43
1:B:360:ASP:H	7:J:4:FUC:H2	1.84	0.43
2:E:75:MET:HE3	2:E:75:MET:HB3	1.82	0.43
1:A:221:LEU:O	1:A:231:TYR:HA	2.19	0.43
1:A:509:ASN:HA	1:A:561:THR:OG1	2.19	0.43
2:E:154:LEU:HD11	2:E:210:TYR:CD2	2.53	0.43
3:F:136:LEU:HD12	3:F:175:LEU:HD22	2.00	0.43
1:B:462:THR:HG22	1:B:487:ARG:CZ	2.49	0.42
2:C:52:ILE:CD1	2:C:59:THR:HG22	2.46	0.42
2:E:167:THR:HB	2:E:215:ASN:HB3	2.01	0.42
1:B:210:VAL:HG13	1:B:212:GLN:H	1.84	0.42
1:B:520:ILE:HG12	1:B:541:LYS:HG3	2.01	0.42
1:B:447:SER:O	1:B:516:ARG:NH2	2.53	0.42
3:D:110:VAL:HG23	3:D:141:PRO:HD3	2.02	0.42
2:E:163:PRO:HG2	2:E:165:PRO:HD2	2.00	0.42
1:A:303:PRO:O	1:A:307:SER:HA	2.20	0.42
1:B:356:ILE:HG23	1:B:444:ILE:HG23	2.02	0.42
2:C:104:TYR:CZ	2:C:112:PRO:HB3	2.54	0.42
3:D:145:LYS:O	3:D:196:VAL:HA	2.20	0.42
2:C:38:ILE:HD13	2:C:38:ILE:HG21	1.75	0.41
2:C:75:MET:HE3	2:C:75:MET:HB3	1.78	0.41
1:B:491:SER:O	1:B:492:GLN:HB2	2.19	0.41
1:B:581:TYR:CE1	3:D:30:ILE:HG21	2.55	0.41
2:C:163:PRO:HG2	2:C:218:PRO:HG2	2.01	0.41
1:A:487:ARG:HH22	1:A:493:CYS:HB3	1.86	0.41
2:E:104:TYR:CZ	2:E:112:PRO:HB3	2.55	0.41
2:E:182:PHE:CD1	3:F:164:THR:HG23	2.55	0.41
1:B:534:ASN:O	1:B:536:VAL:HG23	2.20	0.41
3:D:12:SER:HA	3:D:105:GLU:O	2.21	0.41
2:E:8:GLY:HA3	2:E:20:LEU:CD2	2.47	0.41
1:A:341:GLU:HB2	1:A:427:VAL:HG13	2.01	0.41
1:A:395:CYS:HA	1:A:398:SER:OG	2.20	0.41
1:B:463:MET:CG	1:B:498:LYS:HD2	2.50	0.41
2:E:92:THR:HG22	2:E:127:VAL:N	2.34	0.41
3:F:80:PRO:HD2	3:F:81:GLU:OE1	2.20	0.41
1:A:257:ASP:O	3:D:20:THR:OG1	2.38	0.41
2:E:216:HIS:CD2	2:E:218:PRO:HD2	2.55	0.41
2:C:48:TRP:CH2	2:C:50:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:TYR:CD1	2:C:58:SER:HB2	2.56	0.41
3:F:186:TYR:HA	3:F:192:TYR:OH	2.21	0.41
1:A:399:MET:HE1	1:A:436:LEU:HG	2.02	0.41
1:A:582:ASP:HB2	1:A:585:ASP:HB2	2.02	0.41
3:D:88:CYS:O	3:D:98:PHE:HA	2.21	0.41
3:D:89:LEU:HD11	3:D:96:TYR:HB3	2.02	0.41
1:B:551:LEU:HD12	1:B:578:VAL:HG21	2.02	0.40
1:A:349:MET:HE2	1:A:349:MET:HB3	1.83	0.40
3:D:8:PRO:O	3:D:102:THR:CG2	2.68	0.40
3:F:6:GLN:NE2	3:F:102:THR:HG23	2.35	0.40
1:B:234:LEU:HD12	1:B:247:GLN:O	2.22	0.40
3:D:137:ASN:O	3:D:139:PHE:HD2	2.05	0.40
3:D:158:ASN:HB2	3:D:179:LEU:HD12	2.04	0.40
3:D:196:VAL:O	3:D:204:PRO:HD2	2.22	0.40
1:B:179:SER:O	1:B:566:PHE:HB2	2.22	0.40
2:E:99:ARG:HG2	2:E:118:VAL:HB	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:OE1	1:B:386:GLU:OE2[4_554]	1.62	0.58
1:A:544:GLU:OE1	1:B:386:GLU:CD[4_554]	2.03	0.17
1:A:544:GLU:OE1	1:B:386:GLU:OE1[4_554]	2.05	0.15

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	426/439 (97%)	403 (95%)	23 (5%)	0	100	100
1	B	426/439 (97%)	397 (93%)	29 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	227/242 (94%)	217 (96%)	10 (4%)	0	100	100
2	E	227/242 (94%)	218 (96%)	9 (4%)	0	100	100
3	D	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
3	F	209/214 (98%)	198 (95%)	11 (5%)	0	100	100
All	All	1724/1790 (96%)	1634 (95%)	90 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	385/392 (98%)	379 (98%)	6 (2%)	55	72
1	B	385/392 (98%)	376 (98%)	9 (2%)	44	68
2	C	197/210 (94%)	197 (100%)	0	100	100
2	E	197/210 (94%)	197 (100%)	0	100	100
3	D	186/188 (99%)	185 (100%)	1 (0%)	81	84
3	F	186/188 (99%)	185 (100%)	1 (0%)	81	84
All	All	1536/1580 (97%)	1519 (99%)	17 (1%)	65	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	465	LYS
1	A	518	ASN
1	A	519	TRP
1	A	544	GLU
1	A	547	TYR
1	B	210	VAL
1	B	213	SER
1	B	335	PHE

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Mol	Chain	Res	Type
1	B	337	LEU
1	B	422	GLU
1	B	423	ASN
1	B	433	ASP
1	B	518	ASN
1	B	519	TRP
3	D	31	ASP
3	F	83	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	ASN
1	A	277	ASN
1	A	333	HIS
1	A	406	HIS
1	A	509	ASN
1	A	543	ASN
1	B	195	ASN
1	B	277	ASN
1	B	559	GLN
1	B	564	ASN
2	C	208	GLN
3	D	53	ASN
3	D	137	ASN
3	D	138	ASN
3	D	189	HIS
2	E	85	ASN
3	F	53	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 ⓘ

25 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	1	4,1	14,14,15	0.49	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.36	0	17,19,21	0.51	0
4	BMA	G	3	4	11,11,12	0.77	0	15,15,17	0.78	0
4	FUC	G	4	4	10,10,11	1.48	3 (30%)	14,14,16	2.17	4 (28%)
5	NAG	H	1	5,1	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	H	2	5	14,14,15	0.32	0	17,19,21	0.38	0
5	BMA	H	3	5	11,11,12	0.49	0	15,15,17	0.75	0
5	MAN	H	4	5	11,11,12	0.85	0	15,15,17	0.90	0
5	FUC	H	5	5	10,10,11	1.18	2 (20%)	14,14,16	1.00	1 (7%)
6	NAG	I	1	6,1	14,14,15	0.31	0	17,19,21	0.68	0
6	NAG	I	2	6	14,14,15	0.71	1 (7%)	17,19,21	1.18	1 (5%)
6	BMA	I	3	6	11,11,12	0.61	0	15,15,17	1.39	1 (6%)
7	NAG	J	1	7,1	14,14,15	0.90	1 (7%)	17,19,21	1.79	5 (29%)
7	NAG	J	2	7	14,14,15	0.27	0	17,19,21	0.96	2 (11%)
7	BMA	J	3	7	11,11,12	0.84	0	15,15,17	0.97	1 (6%)
7	FUC	J	4	7	10,10,11	1.02	0	14,14,16	0.95	1 (7%)
7	FUC	J	5	7	10,10,11	0.71	0	14,14,16	0.81	0
5	NAG	K	1	5,1	14,14,15	1.58	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	K	2	5	14,14,15	0.47	0	17,19,21	0.48	0
5	BMA	K	3	5	11,11,12	0.76	0	15,15,17	0.82	0
5	MAN	K	4	5	11,11,12	0.77	0	15,15,17	1.02	1 (6%)
5	FUC	K	5	5	10,10,11	1.42	2 (20%)	14,14,16	0.97	1 (7%)
6	NAG	L	1	6,1	14,14,15	0.82	1 (7%)	17,19,21	1.16	1 (5%)
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.51	0
6	BMA	L	3	6	11,11,12	0.89	1 (9%)	15,15,17	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	FUC	H	5	5	-	-	0/1/1/1
6	NAG	I	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	FUC	J	4	7	-	-	0/1/1/1
7	FUC	J	5	7	-	-	0/1/1/1
5	NAG	K	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	FUC	K	5	5	-	-	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1	NAG	O5-C1	-5.69	1.34	1.43
4	G	4	FUC	C4-C5	2.74	1.58	1.52
5	K	5	FUC	C1-C2	2.59	1.58	1.52
5	H	5	FUC	C1-C2	2.44	1.58	1.52
5	K	5	FUC	C4-C5	2.37	1.58	1.52
6	L	1	NAG	O5-C1	-2.36	1.39	1.43
6	I	2	NAG	O5-C1	2.32	1.47	1.43
4	G	4	FUC	O5-C5	2.30	1.48	1.43
7	J	1	NAG	O5-C1	-2.16	1.40	1.43
5	H	5	FUC	O5-C5	2.12	1.47	1.43
4	G	4	FUC	C4-C3	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	3	BMA	C1-C2	2.10	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	4	FUC	O5-C5-C4	5.04	118.63	109.55
4	G	4	FUC	C3-C4-C5	4.19	116.18	109.81
7	J	1	NAG	O3-C3-C2	4.01	117.74	109.40
6	I	3	BMA	C1-O5-C5	3.89	117.40	112.19
6	L	1	NAG	C1-O5-C5	3.51	116.89	112.19
4	G	4	FUC	C1-O5-C5	3.45	121.10	112.97
6	I	2	NAG	C1-O5-C5	3.19	116.47	112.19
7	J	1	NAG	O3-C3-C4	3.15	117.79	110.38
5	K	4	MAN	C1-O5-C5	2.97	116.17	112.19
7	J	1	NAG	C1-C2-N2	2.61	114.54	110.43
7	J	3	BMA	C1-C2-C3	-2.32	106.26	109.64
7	J	2	NAG	C3-C4-C5	2.16	114.15	110.23
7	J	2	NAG	C1-O5-C5	-2.16	109.30	112.19
7	J	1	NAG	C4-C3-C2	-2.13	107.90	111.02
5	K	1	NAG	C3-C4-C5	2.13	114.09	110.23
7	J	1	NAG	O4-C4-C5	2.12	114.55	109.32
5	K	5	FUC	O2-C2-C1	2.11	114.06	109.22
4	G	4	FUC	O2-C2-C1	2.08	113.99	109.22
5	H	5	FUC	O2-C2-C1	2.07	113.96	109.22
7	J	4	FUC	C1-O5-C5	2.05	117.80	112.97

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2

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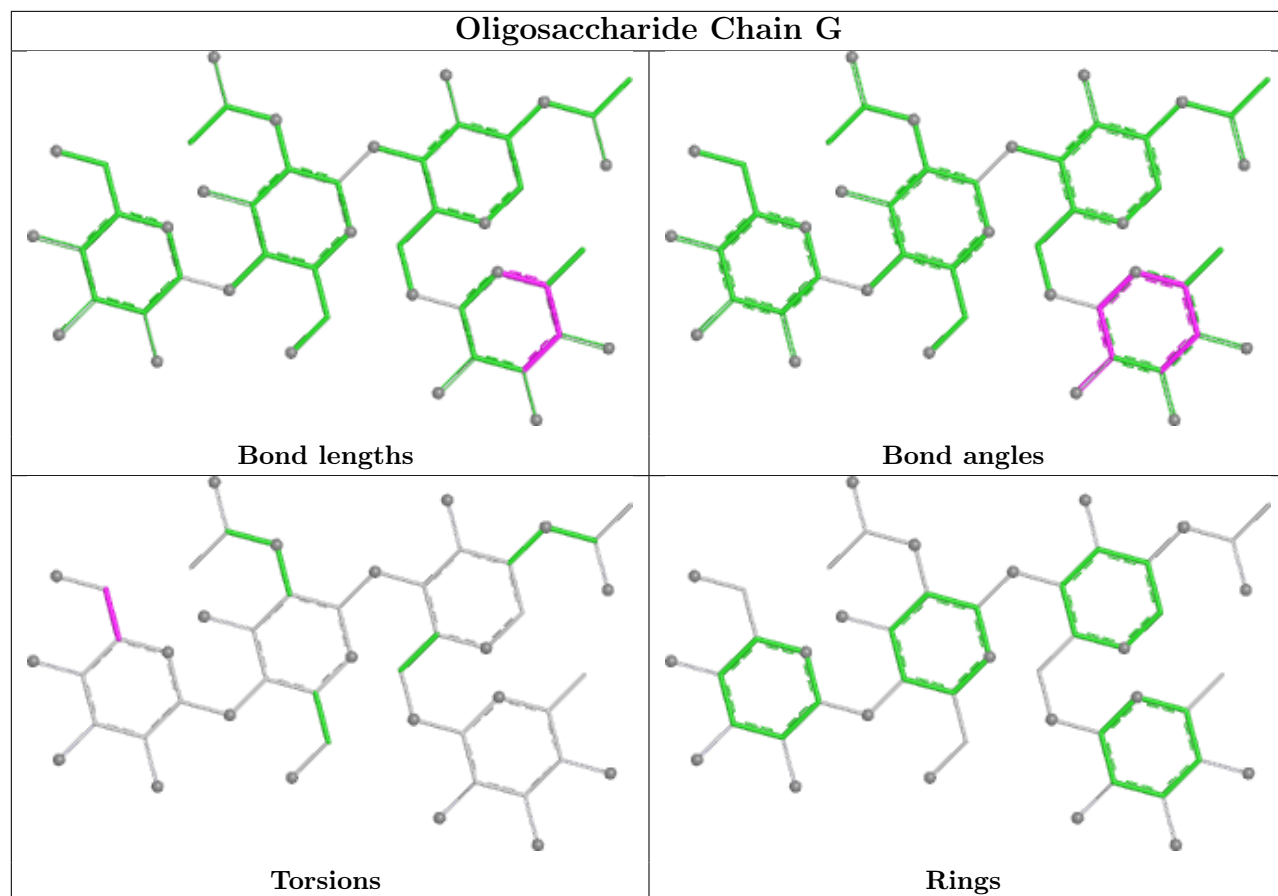
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C3-C2-N2-C7
5	K	2	NAG	O5-C5-C6-O6
5	K	1	NAG	C1-C2-N2-C7

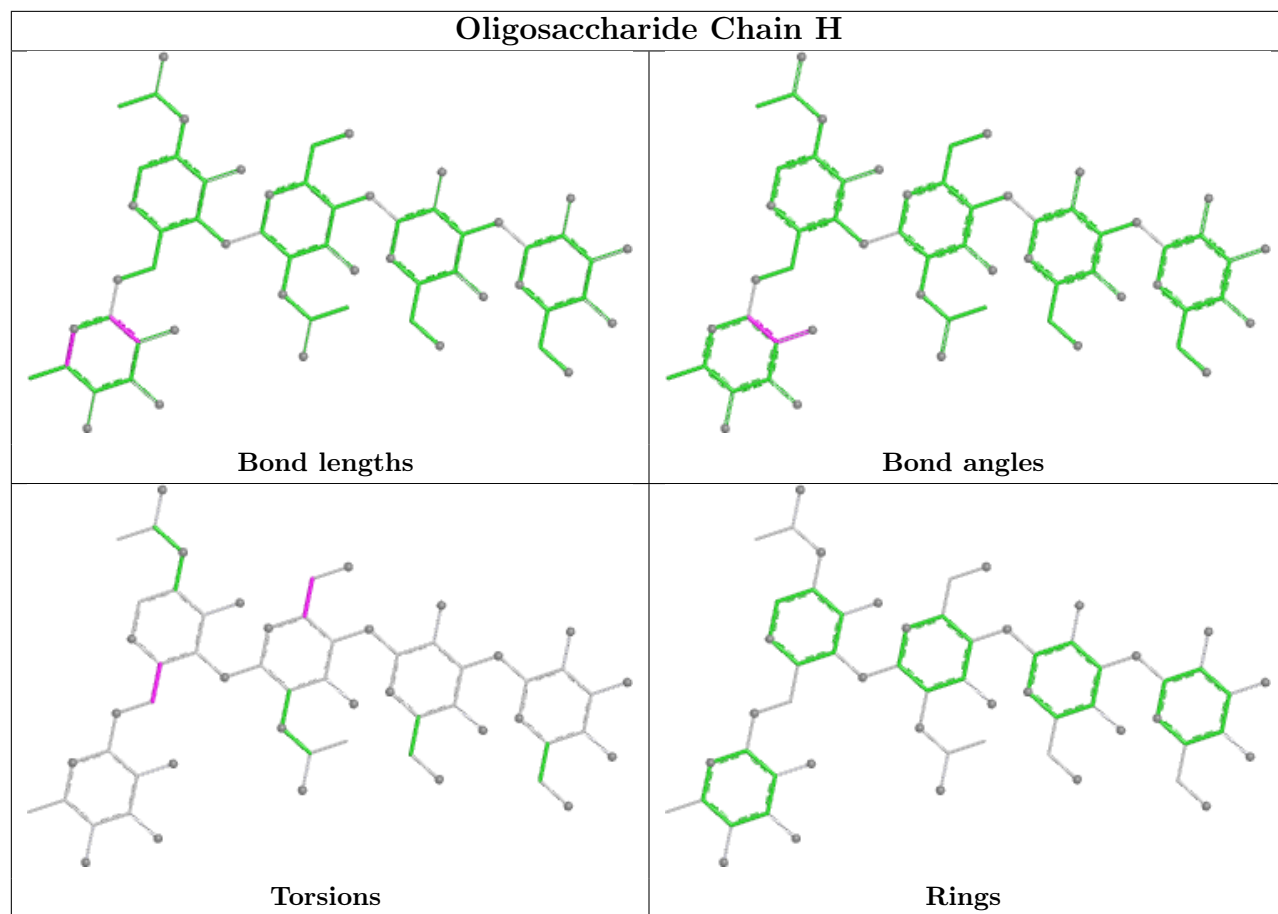
There are no ring outliers.

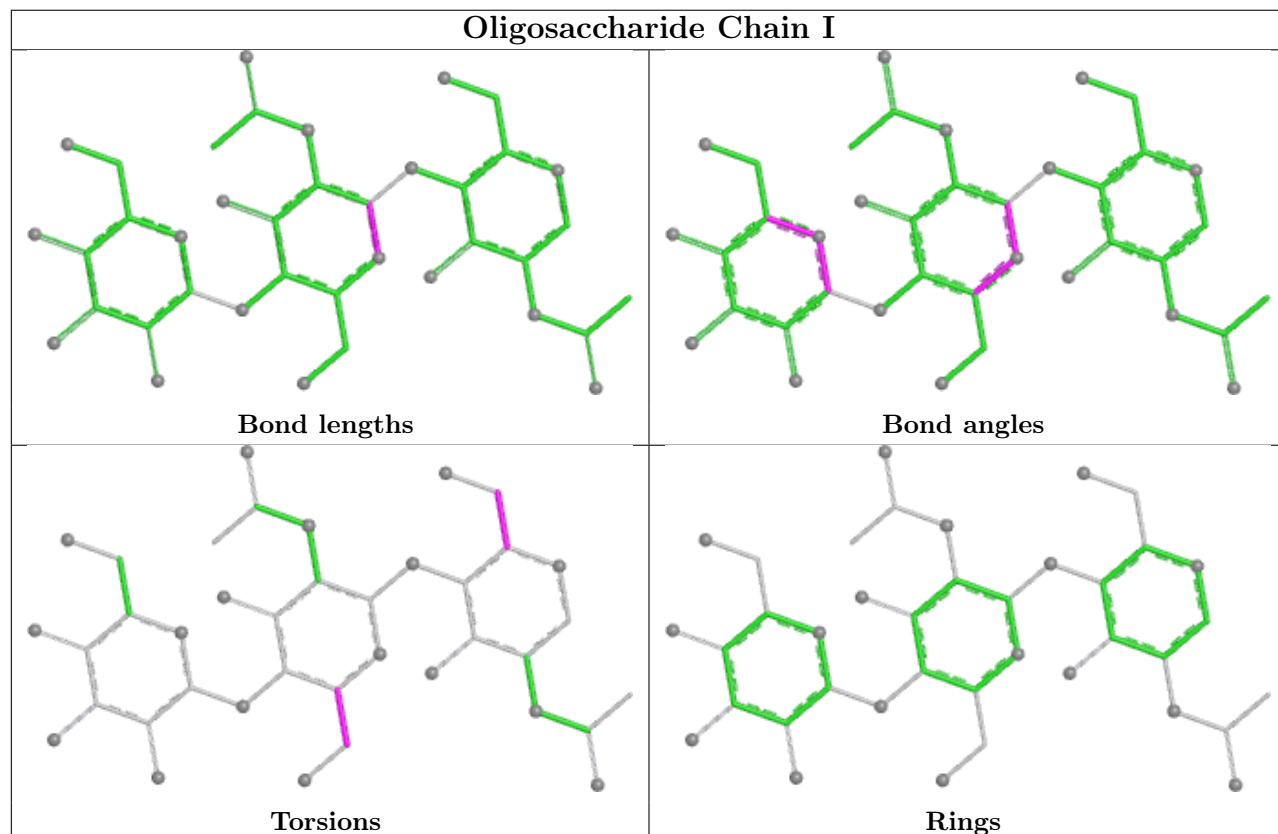
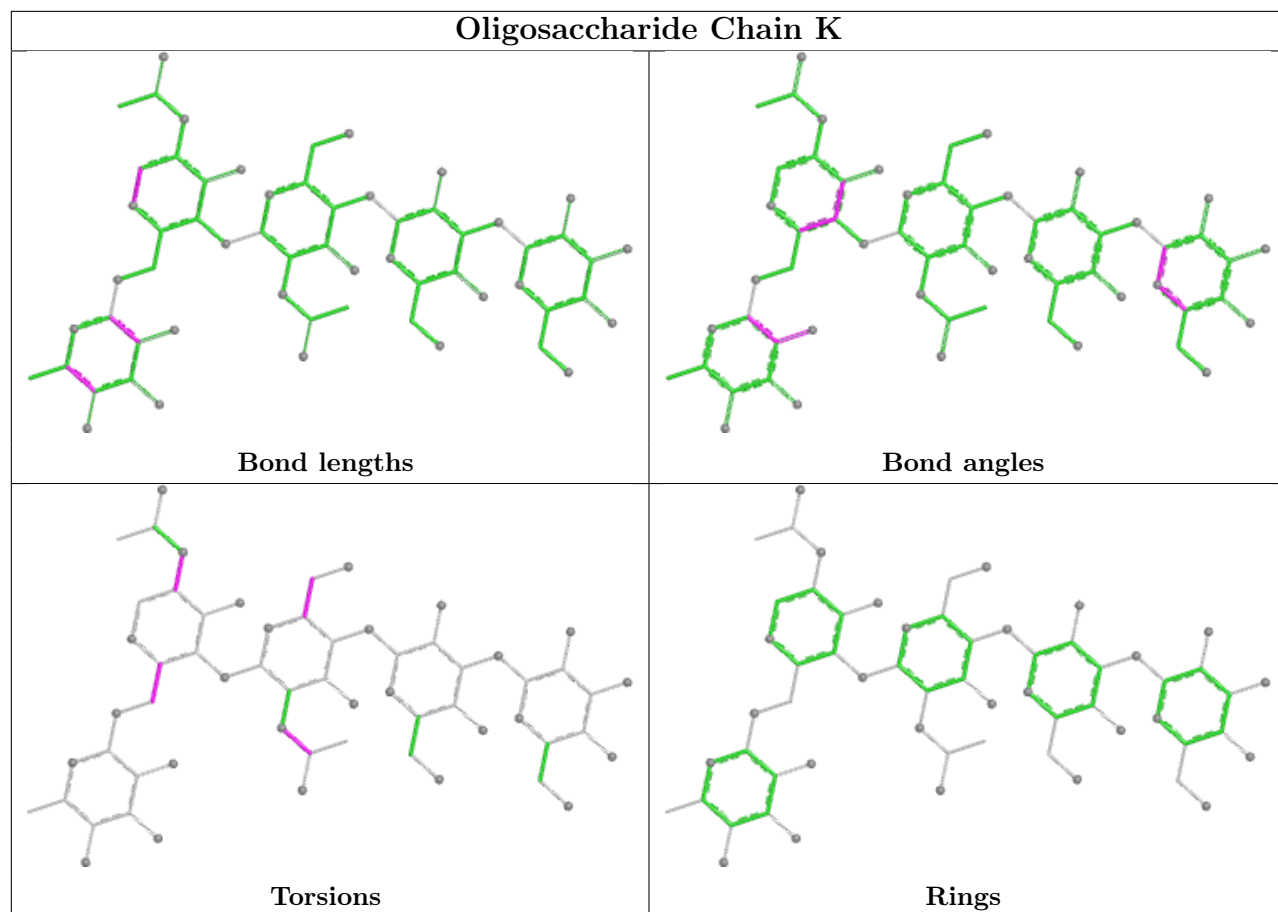
6 monomers are involved in 4 short contacts:

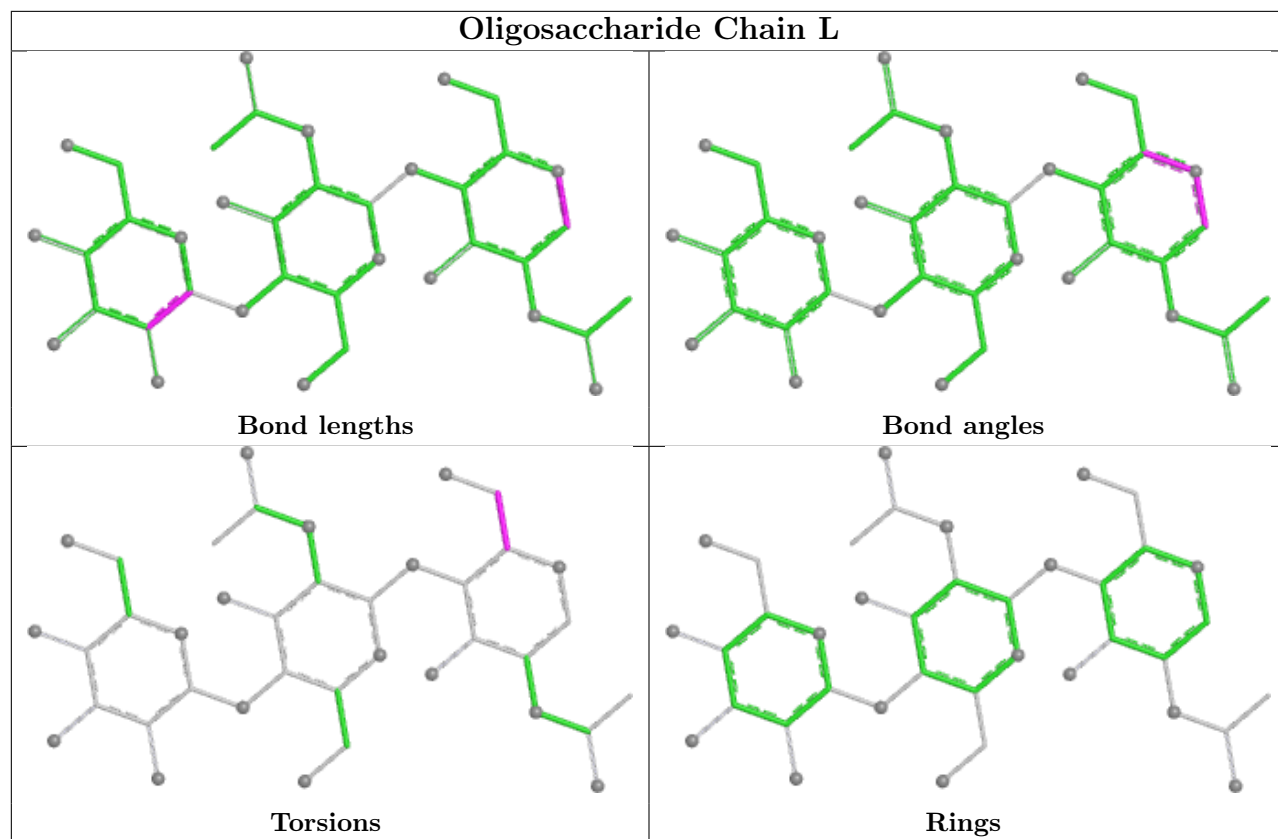
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	4	FUC	1	0
6	I	1	NAG	1	0
7	J	1	NAG	1	0
5	K	2	NAG	1	0
5	K	5	FUC	1	0
7	J	2	NAG	1	0

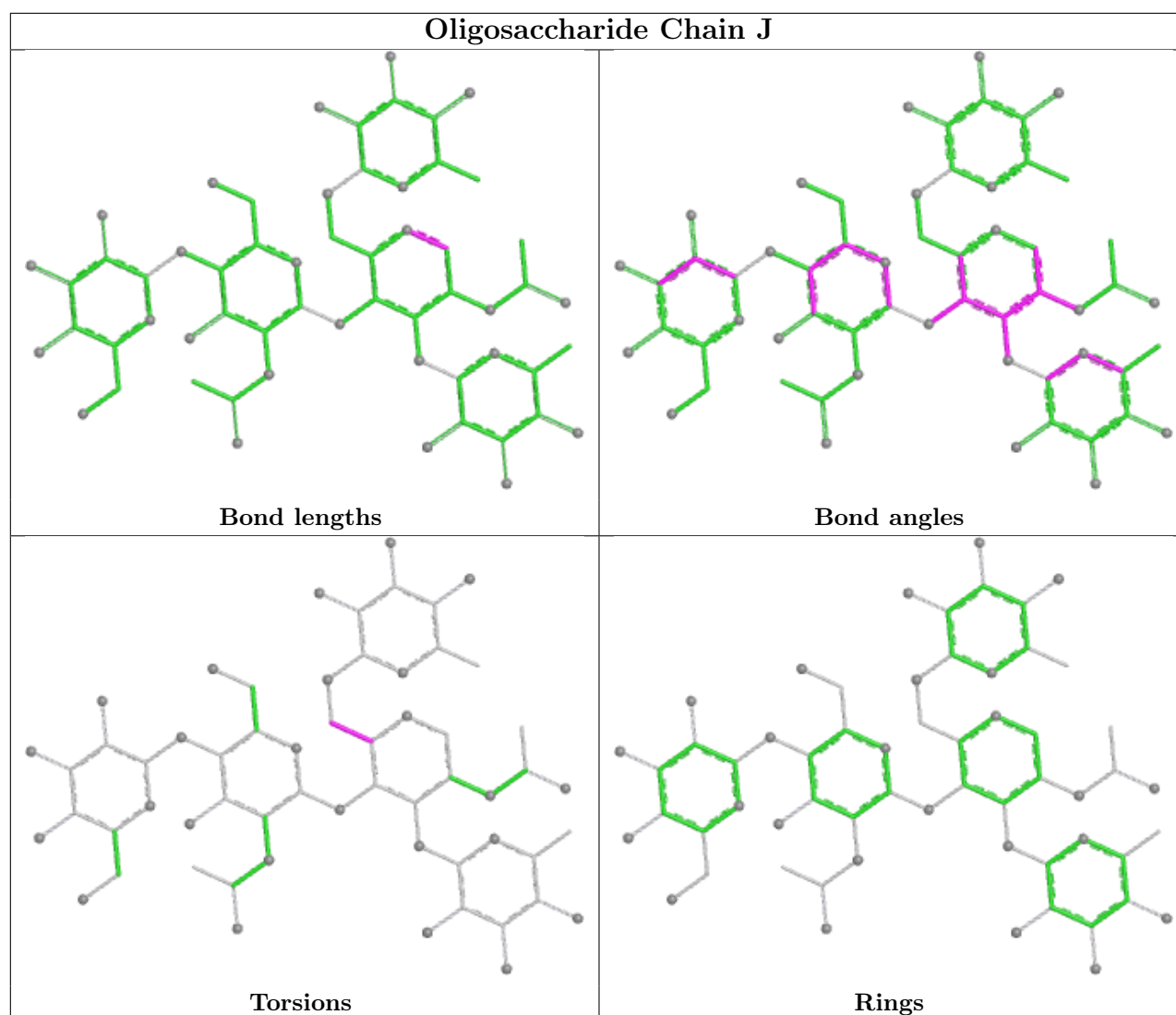
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
8	NAG	A	701	1	14,14,15	0.42	0	17,19,21	0.49	0
8	NAG	B	701	1	14,14,15	0.20	0	17,19,21	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
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

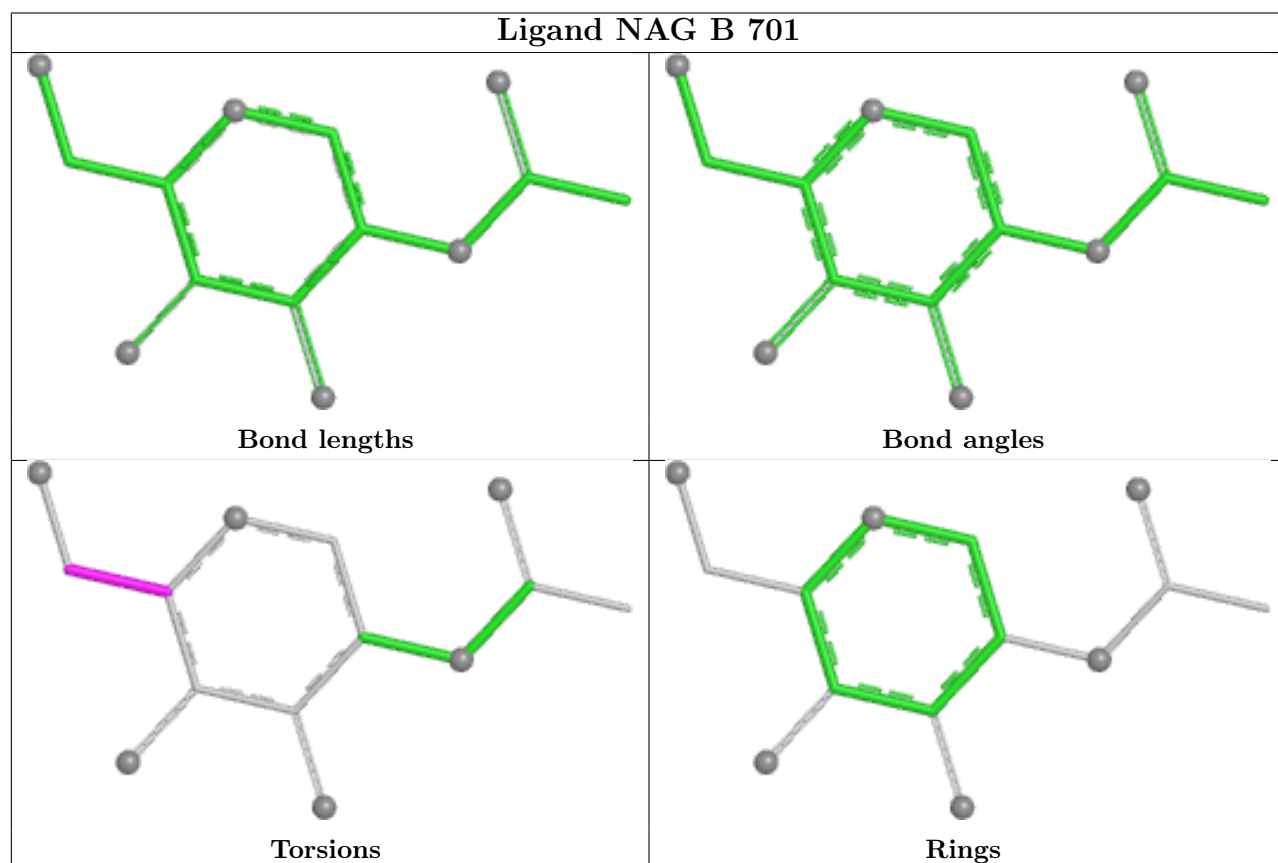
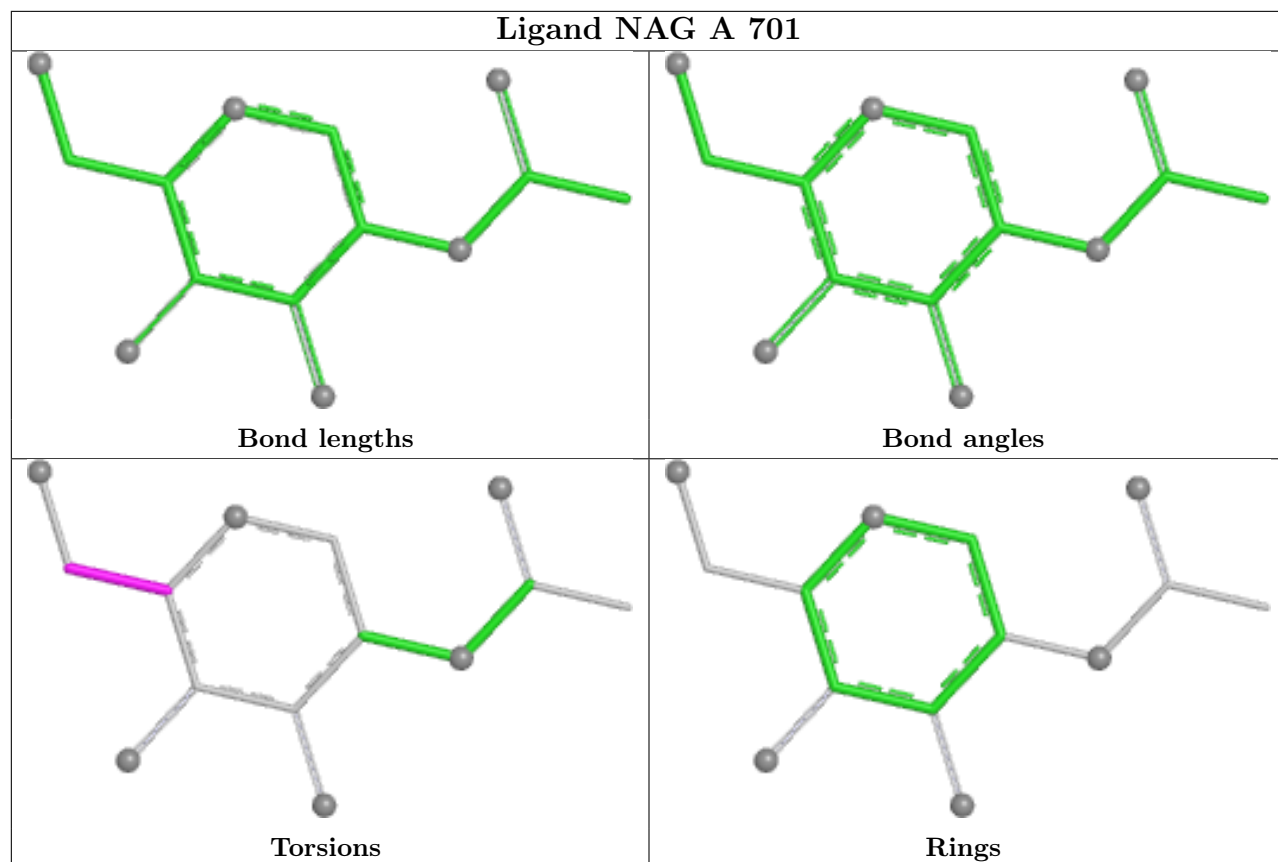
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C4-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	428/439 (97%)	0.15	15 (3%)	47 30	56, 76, 117, 238	0
1	B	428/439 (97%)	0.16	15 (3%)	47 30	60, 80, 135, 209	0
2	C	229/242 (94%)	0.14	2 (0%)	81 64	61, 88, 149, 257	0
2	E	229/242 (94%)	1.07	48 (20%)	2 2	72, 123, 344, 420	0
3	D	211/214 (98%)	0.35	14 (6%)	24 16	59, 86, 154, 185	0
3	F	211/214 (98%)	1.31	60 (28%)	1 1	71, 146, 306, 416	0
All	All	1736/1790 (96%)	0.44	154 (8%)	15 11	56, 87, 278, 420	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	177	SER	10.5
2	E	158	VAL	10.3
2	E	196	SER	7.2
3	F	178	THR	7.1
2	E	195	SER	6.4
3	F	181	LEU	6.4
3	F	129	THR	6.2
3	F	192	TYR	6.0
2	E	197	VAL	5.9
3	F	135	LEU	5.8
2	E	194	LEU	5.7
3	F	134	CYS	5.1
2	E	214	VAL	4.9
3	F	150	VAL	4.7
2	E	157	LEU	4.7
1	A	211	GLY	4.6
2	E	205	LEU	4.5
3	F	113	PRO	4.4
2	E	159	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	4.2
3	F	156	SER	4.1
3	F	115	VAL	4.1
1	A	210	VAL	4.1
1	B	335	PHE	4.0
3	D	3	GLN	4.0
2	E	186	LEU	4.0
3	F	133	VAL	3.9
3	D	31	ASP	3.9
1	B	209	VAL	3.9
3	F	175	LEU	3.9
3	F	205	VAL	3.8
3	F	168	SER	3.8
3	F	118	PHE	3.8
3	F	136	LEU	3.7
3	F	131	SER	3.7
1	A	212	GLN	3.7
2	E	227	VAL	3.7
3	F	179	LEU	3.7
3	F	163	VAL	3.6
3	F	119	PRO	3.6
1	A	213	SER	3.6
1	A	215	THR	3.6
3	F	155	GLN	3.5
3	F	142	ARG	3.5
1	A	240	CYS	3.4
3	F	112	ALA	3.4
3	F	197	THR	3.2
3	F	127	SER	3.2
1	B	210	VAL	3.2
2	E	180	HIS	3.2
2	E	168	VAL	3.2
2	E	160	ASP	3.2
2	E	181	THR	3.2
3	F	3	GLN	3.2
2	E	212	CYS	3.1
2	E	140	LEU	3.1
2	E	161	TYR	3.1
3	F	193	ALA	3.1
3	F	160	GLN	3.1
1	B	215	THR	3.1
1	B	213	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	159	SER	3.1
3	F	176	SER	3.1
2	E	189	SER	3.0
2	E	151	THR	3.0
3	F	148	TRP	3.0
3	F	196	VAL	3.0
3	F	198	HIS	3.0
1	B	175	SER	2.9
2	E	229	PRO	2.9
2	E	144	SER	2.9
2	E	193	SER	2.9
2	E	154	LEU	2.9
1	B	354	SER	2.9
2	E	165	PRO	2.9
2	E	185	VAL	2.9
1	B	490	GLN	2.8
1	B	240	CYS	2.8
3	F	154	LEU	2.8
2	E	188	SER	2.8
3	D	208	SER	2.8
1	A	586	ASN	2.7
1	A	544	GLU	2.7
1	A	218	THR	2.7
3	F	180	THR	2.7
1	B	586	ASN	2.7
3	F	138	ASN	2.7
2	E	146	SER	2.6
2	E	153	ALA	2.6
3	F	140	TYR	2.6
2	E	206	GLY	2.6
2	E	156	CYS	2.6
3	F	166	GLN	2.5
2	E	224	ASP	2.5
3	D	200	GLY	2.5
1	A	558	ALA	2.5
3	F	153	ALA	2.5
1	B	208	PRO	2.5
1	B	393	GLU	2.5
2	E	218	PRO	2.5
3	D	204	PRO	2.5
3	F	191	VAL	2.5
3	D	156	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	211	ILE	2.4
3	F	117	ILE	2.4
2	E	135	PRO	2.4
3	F	143	GLU	2.4
3	F	161	GLU	2.4
1	A	175	SER	2.4
3	F	204	PRO	2.4
2	E	210	TYR	2.4
3	F	171	SER	2.4
3	F	158	ASN	2.4
3	D	202	SER	2.4
3	D	209	PHE	2.3
1	A	216	CYS	2.3
3	F	124	GLN	2.3
2	E	141	ALA	2.3
3	F	111	ALA	2.3
3	F	186	TYR	2.3
3	D	158	ASN	2.3
2	C	164	GLU	2.2
3	D	129	THR	2.2
2	E	198	VAL	2.2
3	F	132	VAL	2.2
3	F	110	VAL	2.2
3	F	130	ALA	2.2
3	D	186	TYR	2.2
1	A	423	ASN	2.2
3	D	207	LYS	2.2
2	E	138	PHE	2.2
3	F	209	PHE	2.2
3	D	154	LEU	2.2
2	E	83	ASN	2.2
3	F	137	ASN	2.2
2	C	146	SER	2.1
2	E	136	SER	2.1
3	F	144	ALA	2.1
3	D	170	ASP	2.1
2	E	226	LYS	2.1
1	B	214	GLY	2.1
1	B	392	PRO	2.1
3	F	208	SER	2.1
2	E	155	GLY	2.1
2	E	201	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	143	SER	2.1
2	E	203	SER	2.1
2	E	170	TRP	2.1
3	F	184	ALA	2.1
2	E	199	THR	2.0
1	A	327	GLY	2.0
1	B	434	GLN	2.0
3	F	187	GLU	2.0
3	F	146	VAL	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.

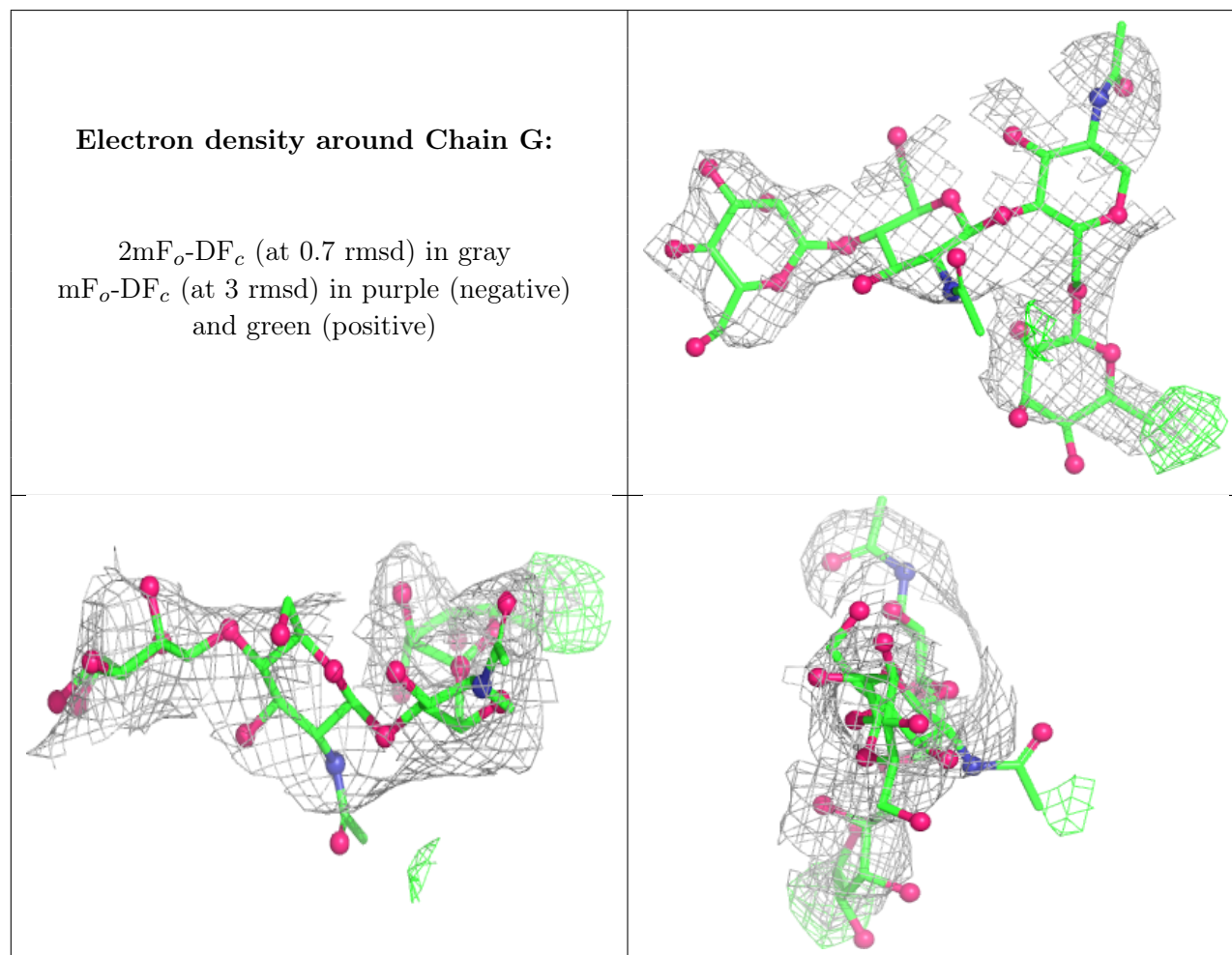
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	I	3	11/12	0.37	0.12	154,168,170,173	0
4	FUC	G	4	10/11	0.39	0.21	144,162,164,164	0
7	BMA	J	3	11/12	0.40	0.10	156,161,165,166	0
4	BMA	G	3	11/12	0.42	0.13	184,187,195,196	0
6	BMA	L	3	11/12	0.45	0.17	148,162,168,172	0
5	FUC	K	5	10/11	0.47	0.20	119,134,139,147	0
5	MAN	H	4	11/12	0.55	0.12	172,179,183,186	0
7	FUC	J	5	10/11	0.56	0.15	220,224,227,227	0
5	BMA	H	3	11/12	0.57	0.11	175,179,187,188	0
5	BMA	K	3	11/12	0.63	0.08	145,159,169,175	0
5	MAN	K	4	11/12	0.67	0.09	175,183,185,186	0
4	NAG	G	2	14/15	0.68	0.16	159,166,171,179	0
7	NAG	J	2	14/15	0.71	0.17	167,172,177,184	0
7	FUC	J	4	10/11	0.73	0.22	180,192,195,198	0
5	NAG	K	1	14/15	0.73	0.16	98,106,122,124	0
6	NAG	I	2	14/15	0.78	0.14	145,152,160,167	0
5	FUC	H	5	10/11	0.83	0.15	100,110,114,119	0
5	NAG	K	2	14/15	0.84	0.11	110,127,141,150	0
5	NAG	H	1	14/15	0.86	0.10	94,103,110,111	0

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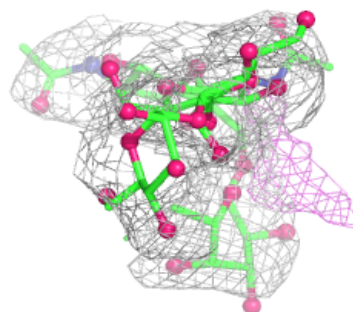
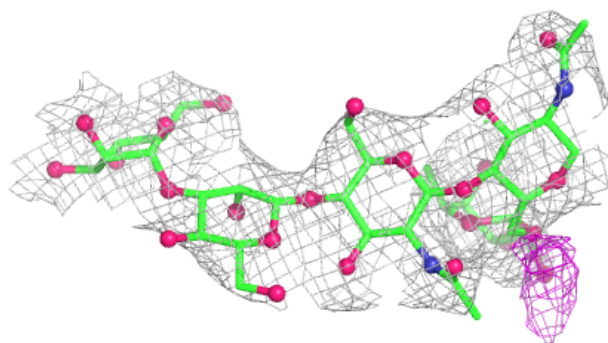
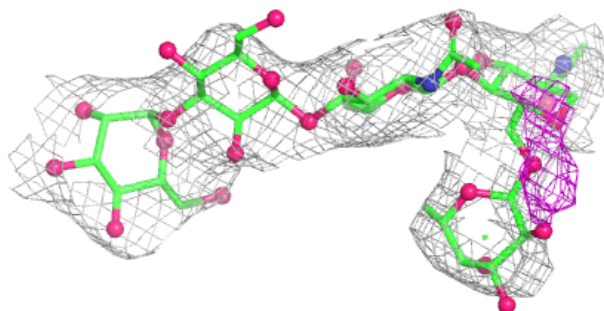
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	J	1	14/15	0.86	0.14	144,160,179,190	0
6	NAG	I	1	14/15	0.87	0.10	114,122,134,140	0
5	NAG	H	2	14/15	0.88	0.10	97,128,142,162	0
6	NAG	L	2	14/15	0.89	0.15	112,135,151,163	0
6	NAG	L	1	14/15	0.91	0.12	114,117,128,136	0
4	NAG	G	1	14/15	0.92	0.12	101,116,147,150	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.

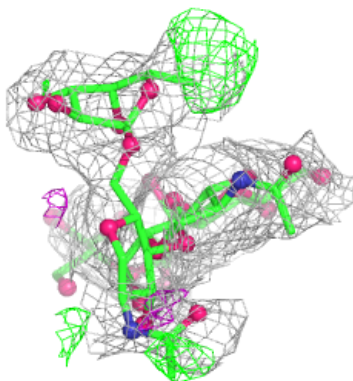
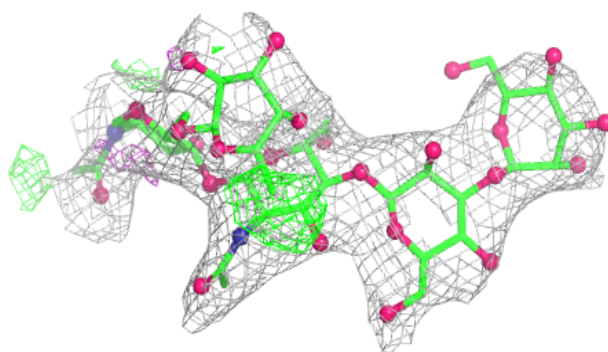
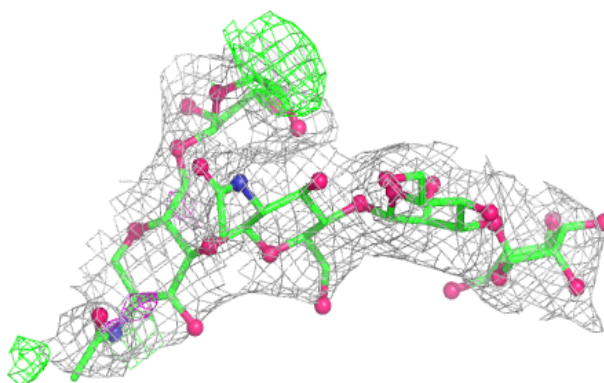


Electron density around Chain H:

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

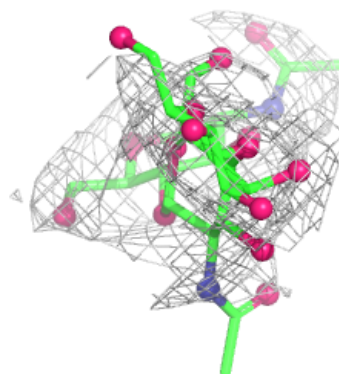
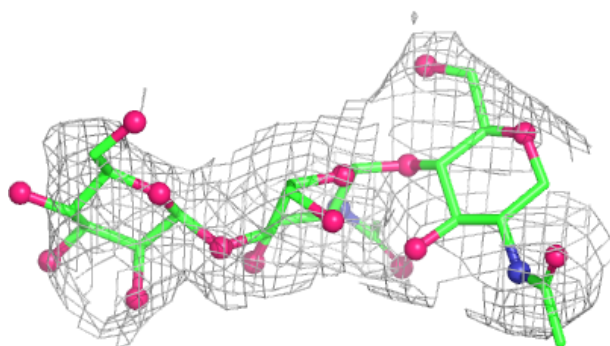
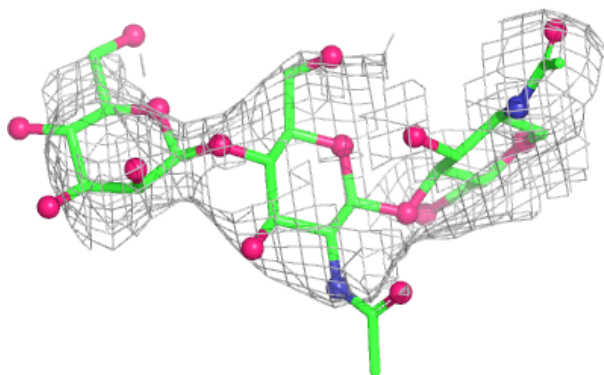
**Electron density around Chain K:**

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

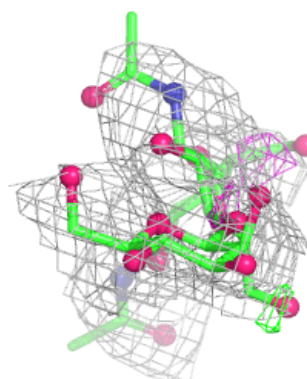
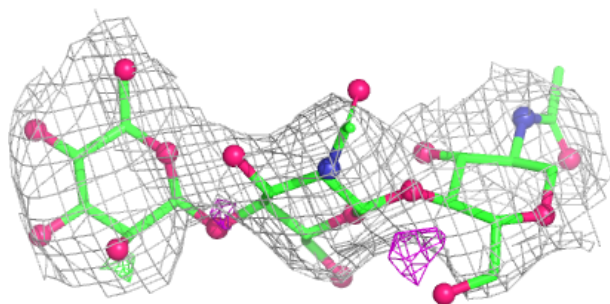
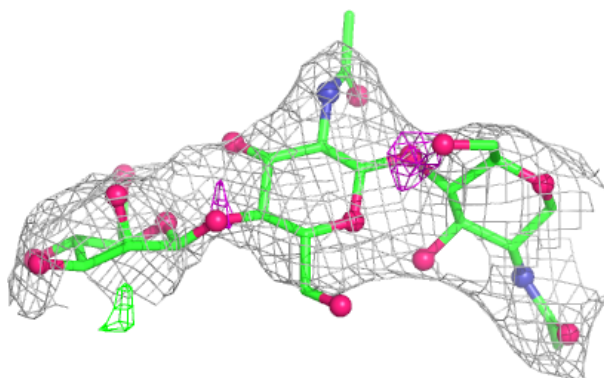


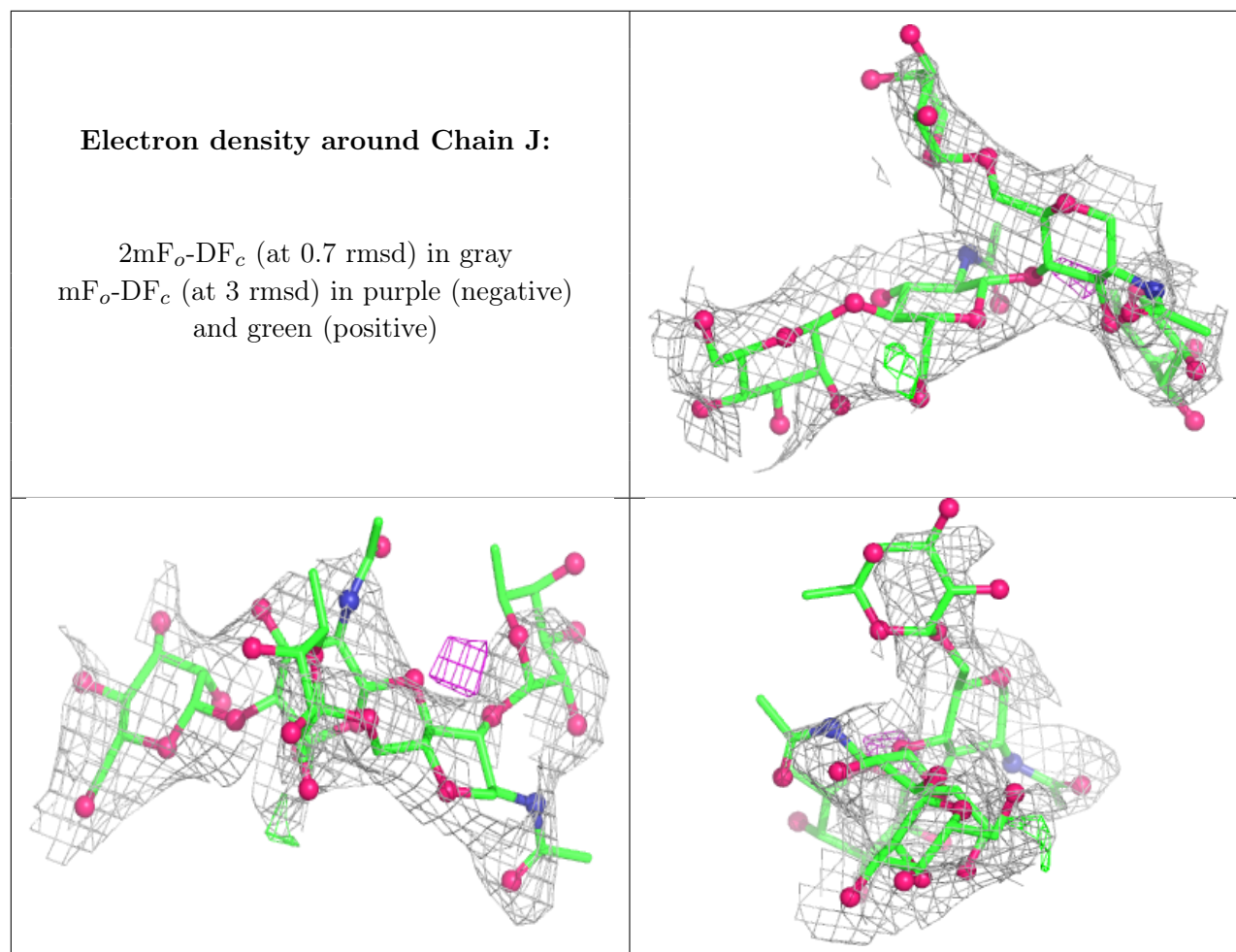
Electron density around Chain I:

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

**Electron density around Chain L:**

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





6.4 Ligands [i](#)

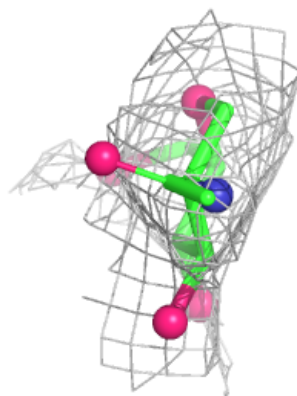
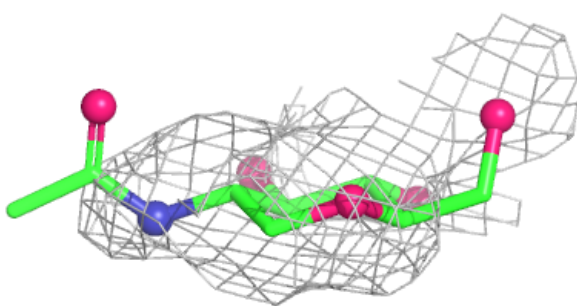
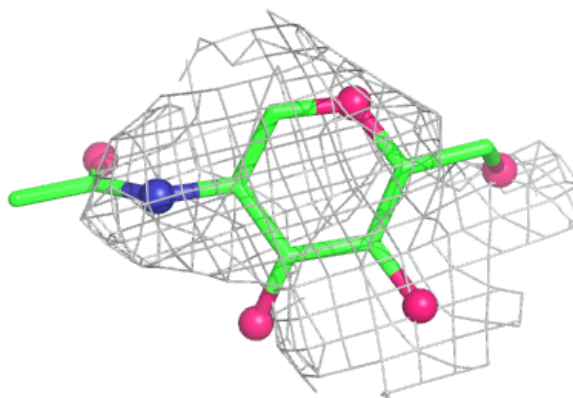
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
8	NAG	A	701	14/15	0.67	0.14	134,150,155,156	0
8	NAG	B	701	14/15	0.67	0.15	150,166,172,174	0

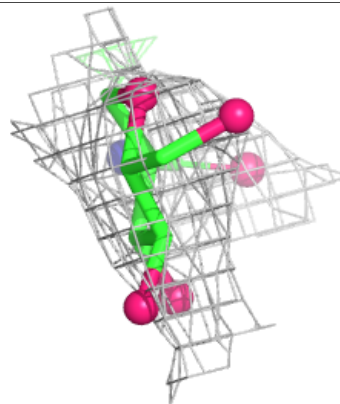
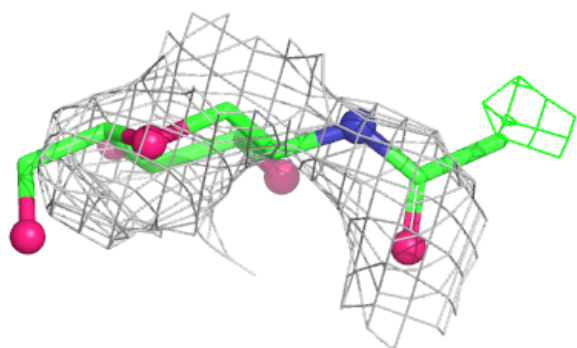
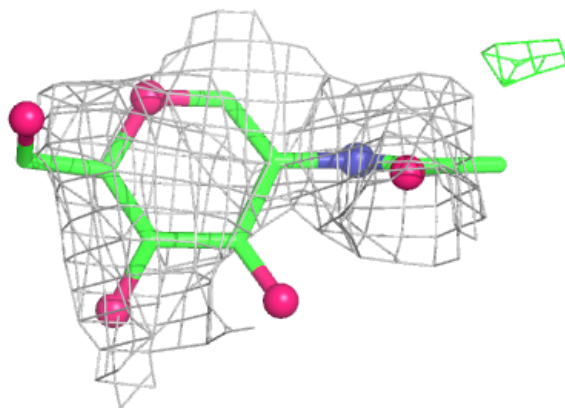
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 701:

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

**Electron density around NAG B 701:**

$2mF_o-DF_c$ (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.