



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:23 pm GMT

PDB ID : 7BEO
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 Spike glycoprotein in a ternary complex with COVOX-253H55L and COVOX-75 Fabs
Authors : Zhou, D.; Zhao, Y.; Ren, J.; Stuart, D.
Deposited on : 2020-12-24
Resolution : 3.19 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

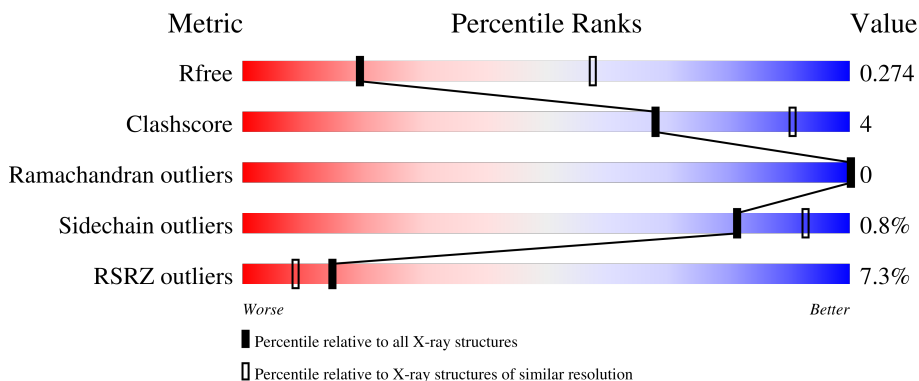
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	R	205	
1	X	205	
2	C	228	
2	H	228	
3	D	215	

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Mol	Chain	Length	Quality of chain
3	L	215	<p>4% 89% 10%</p>
4	A	245	<p>3% 83% 8% 9%</p>
4	E	245	<p>3% 84% 7% 9%</p>
5	B	227	<p>4% 83% 11% 6%</p>
5	F	227	<p>4% 82% 12% 6%</p>
6	G	3	<p>67% 33%</p>
6	I	3	<p>67% 33%</p>
6	J	3	<p>67% 33%</p>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 16313 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	R	183	1462	937	243	275	7	0	0	0
1	X	182	1454	933	241	273	7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	324	GLU	-	expression tag	UNP P0DTC2
R	325	THR	-	expression tag	UNP P0DTC2
R	326	GLY	-	expression tag	UNP P0DTC2
R	327	HIS	-	expression tag	UNP P0DTC2
R	328	HIS	-	expression tag	UNP P0DTC2
R	329	HIS	-	expression tag	UNP P0DTC2
R	330	HIS	-	expression tag	UNP P0DTC2
R	331	HIS	-	expression tag	UNP P0DTC2
R	332	HIS	-	expression tag	UNP P0DTC2
R	527	LYS	PRO	engineered mutation	UNP P0DTC2
X	324	GLU	-	expression tag	UNP P0DTC2
X	325	THR	-	expression tag	UNP P0DTC2
X	326	GLY	-	expression tag	UNP P0DTC2
X	327	HIS	-	expression tag	UNP P0DTC2
X	328	HIS	-	expression tag	UNP P0DTC2
X	329	HIS	-	expression tag	UNP P0DTC2
X	330	HIS	-	expression tag	UNP P0DTC2
X	331	HIS	-	expression tag	UNP P0DTC2
X	332	HIS	-	expression tag	UNP P0DTC2
X	527	LYS	PRO	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called COVOX-253H55L heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1639	1031	276	323	9			
2	C	219	Total	C	N	O	S	0	0	0
			1639	1031	276	323	9			

- Molecule 3 is a protein called COVOX-253H55L light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	2	0
			1646	1029	279	332	6			
3	D	214	Total	C	N	O	S	0	2	0
			1646	1029	279	332	6			

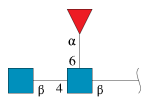
- Molecule 4 is a protein called COVOX-75 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	224	Total	C	N	O	S	0	1	0
			1694	1068	293	327	6			
4	E	224	Total	C	N	O	S	0	1	0
			1694	1068	293	327	6			

- Molecule 5 is a protein called COVOX-75 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	213	Total	C	N	O	S	0	1	0
			1633	1029	272	328	4			
5	F	213	Total	C	N	O	S	0	0	0
			1629	1025	272	328	4			

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



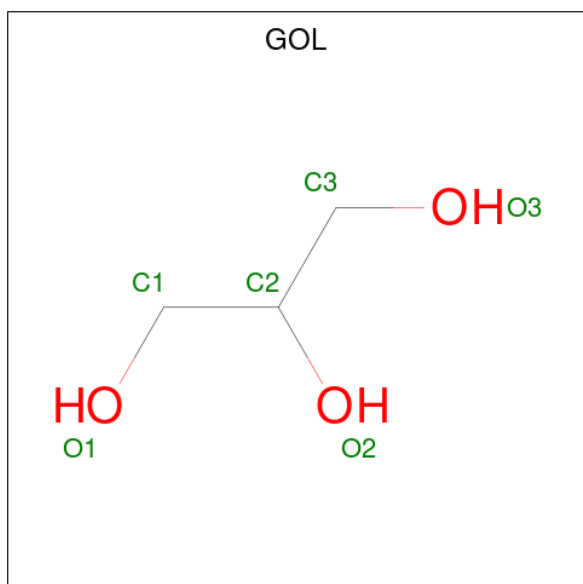
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



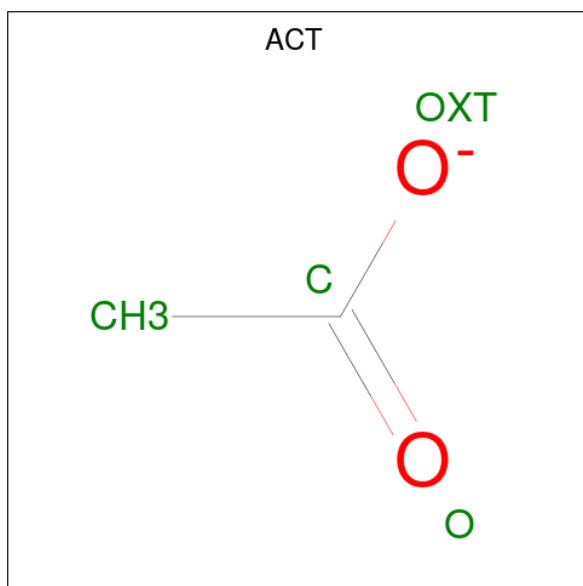
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	H	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	X	1	6	3	3	0	0

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	L	1	4	2	2	0	0
9	A	1	4	2	2	0	0
9	A	1	4	2	2	0	0
9	A	1	4	2	2	0	0
9	C	1	4	2	2	0	0
9	D	1	4	2	2	0	0
9	D	1	4	2	2	0	0
9	E	1	4	2	2	0	0
9	E	1	4	2	2	0	0

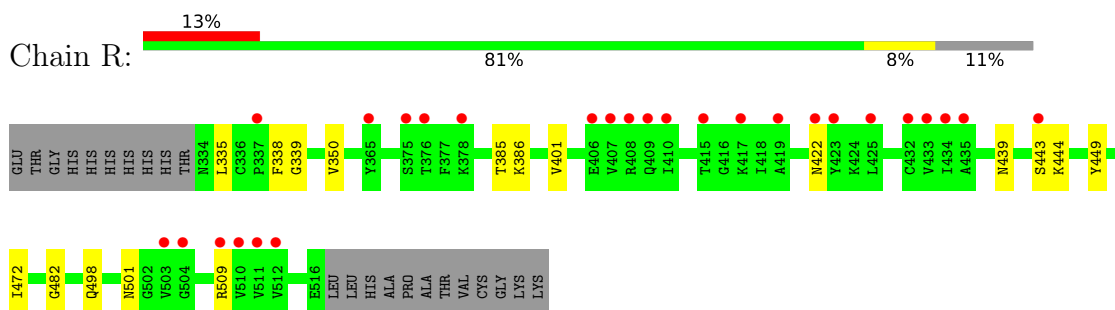
- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

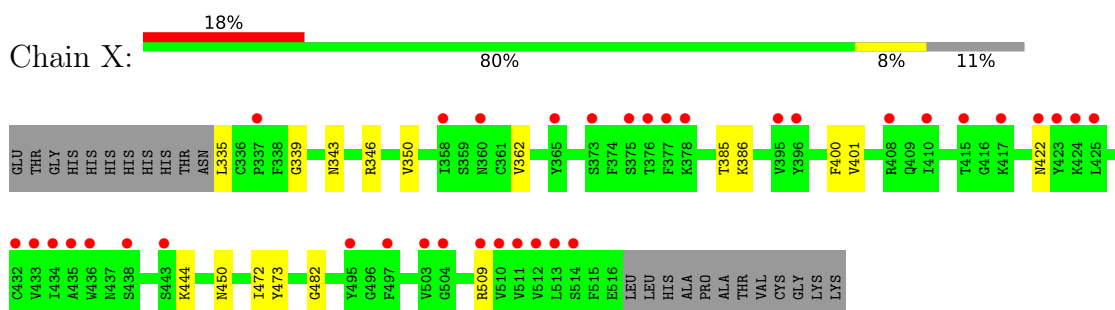
3 Residue-property plots [i](#)

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.

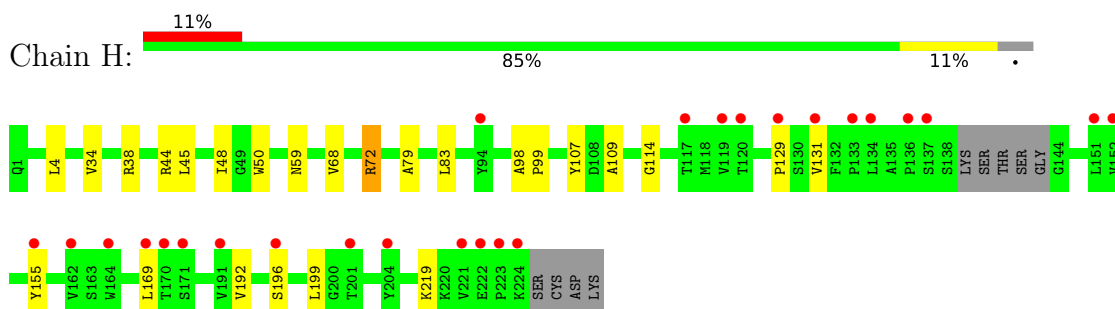
- Molecule 1: Spike glycoprotein



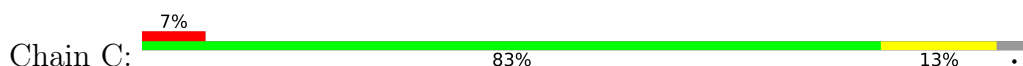
- Molecule 1: Spike glycoprotein

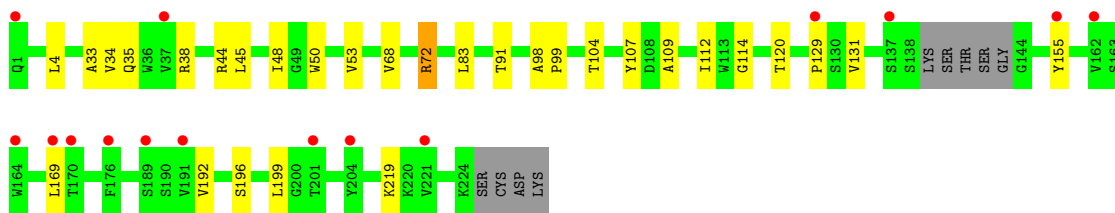


- Molecule 2: COVOX-253H55L heavy chain

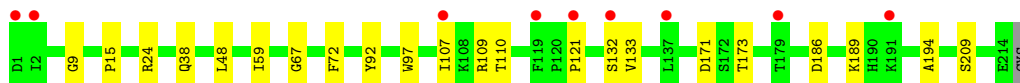
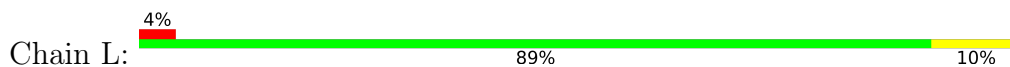


- Molecule 2: COVOX-253H55L heavy chain

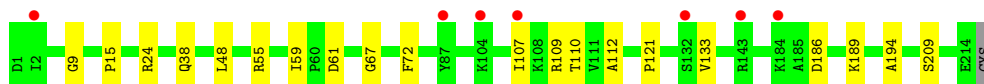
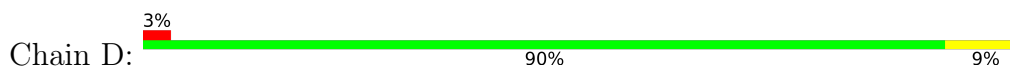




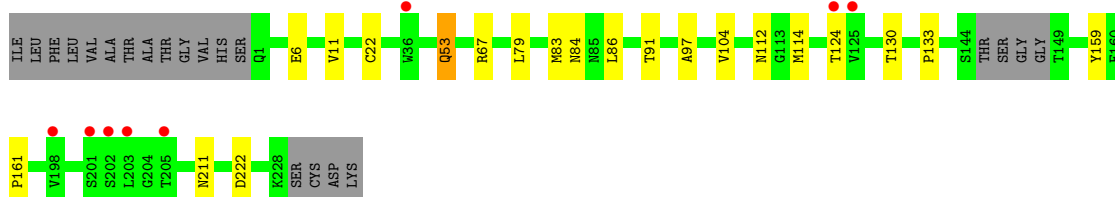
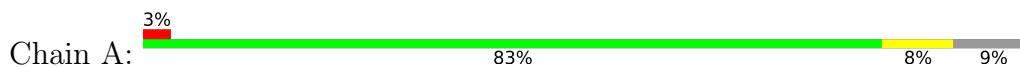
- Molecule 3: COVOX-253H55L light chain



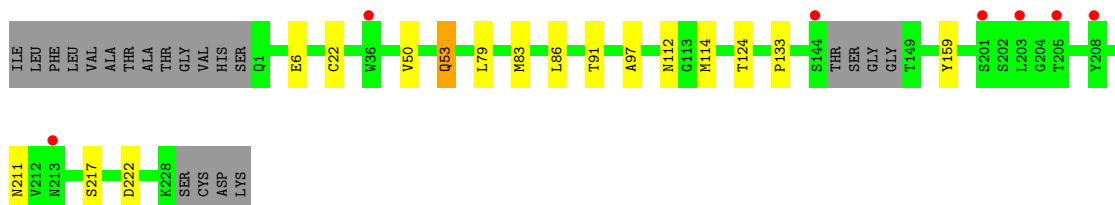
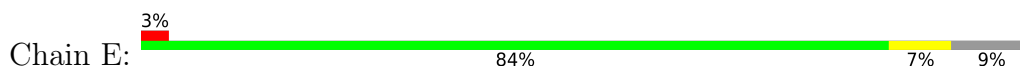
- Molecule 3: COVOX-253H55L light chain



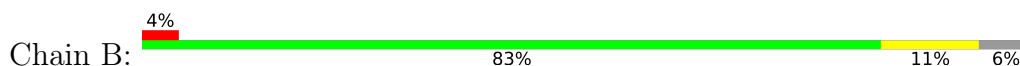
- Molecule 4: COVOX-75 heavy chain



- Molecule 4: COVOX-75 heavy chain

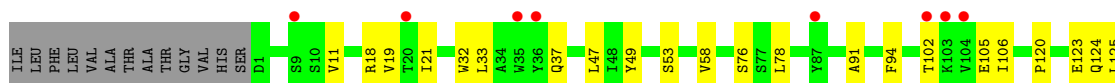
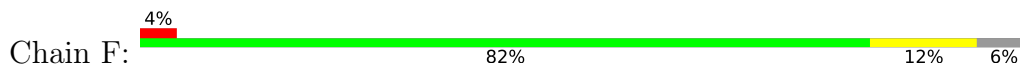


- Molecule 5: COVOX-75 light chain





- Molecule 5: COVOX-75 light chain



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.42Å 150.07Å 116.08Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	58.01 – 3.19 66.37 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.01-3.19) 99.8 (66.37-3.19)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.234 , 0.274 0.234 , 0.274	Depositor DCC
R_{free} test set	2659 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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: ACT, FUC, CL, GOL, NAG

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	R	0.26	0/1503	0.44	0/2043
1	X	0.25	0/1495	0.42	0/2032
2	C	0.25	0/1677	0.46	0/2289
2	H	0.25	0/1677	0.46	0/2289
3	D	0.25	0/1689	0.45	0/2293
3	L	0.24	0/1689	0.45	0/2293
4	A	0.25	0/1737	0.46	0/2370
4	E	0.25	0/1737	0.46	0/2370
5	B	0.25	0/1673	0.44	0/2273
5	F	0.25	0/1666	0.44	0/2263
All	All	0.25	0/16543	0.45	0/22515

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	R	1462	0	1377	12	0
1	X	1454	0	1371	13	0
2	C	1639	0	1595	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1639	0	1595	14	0
3	D	1646	0	1594	14	0
3	L	1646	0	1594	14	0
4	A	1694	0	1662	12	0
4	E	1694	0	1662	10	0
5	B	1633	0	1601	12	0
5	F	1629	0	1592	14	0
6	G	38	0	34	1	0
6	I	38	0	34	0	0
6	J	38	0	34	1	0
7	R	14	0	13	2	0
8	H	6	0	8	0	0
8	X	6	0	8	1	0
9	A	12	0	9	1	0
9	C	4	0	3	0	0
9	D	8	0	6	0	0
9	E	8	0	6	1	0
9	L	4	0	3	0	0
10	C	1	0	0	0	0
All	All	16313	0	15801	121	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 4.

All (121) 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:X:346:ARG:HH22	1:X:450:ASN:HB3	1.54	0.71
2:C:38:ARG:HB3	2:C:48:ILE:HD11	1.77	0.66
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.78	0.65
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.77	0.65
4:A:53:GLN:NE2	9:A:402:ACT:O	2.30	0.65
1:X:335:LEU:N	1:X:362:VAL:O	2.29	0.65
3:D:121:PRO:HD3	3:D:133:VAL:HG22	1.81	0.62
3:D:109:ARG:NH2	3:D:110:THR:O	2.34	0.61
1:X:473:TYR:OH	2:C:104:THR:O	2.17	0.61
4:A:133:PRO:HB3	4:A:159:TYR:HB3	1.83	0.61
4:A:211:ASN:ND2	4:A:222:ASP:OD2	2.34	0.59
1:X:444:LYS:NZ	5:F:91:ALA:O	2.35	0.59
3:D:38:GLN:HB2	3:D:48:LEU:HD11	1.83	0.59
5:F:21:ILE:HD12	5:F:102:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.83	0.59
2:C:129:PRO:HB3	2:C:155:TYR:HB3	1.84	0.59
1:R:472:ILE:HD13	1:R:482:GLY:HA2	1.84	0.58
4:A:22:CYS:HB3	4:A:79:LEU:HB3	1.86	0.57
4:E:211:ASN:ND2	4:E:222:ASP:OD2	2.37	0.57
1:R:385:THR:OG1	1:R:386:LYS:N	2.37	0.57
4:E:133:PRO:HB3	4:E:159:TYR:HB3	1.86	0.57
1:R:444:LYS:NZ	5:B:91:ALA:O	2.38	0.57
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.86	0.57
4:E:91:THR:HG23	4:E:124:THR:HA	1.87	0.57
4:E:83:MET:HB3	4:E:86:LEU:HD21	1.85	0.56
1:X:343:ASN:OD1	8:X:701:GOL:O1	2.23	0.55
5:B:21:ILE:HD12	5:B:102:THR:HG21	1.89	0.55
2:C:131:VAL:O	2:C:219:LYS:NZ	2.41	0.55
1:R:339:GLY:HA2	7:R:601:NAG:O7	2.08	0.54
3:L:15:PRO:HD3	3:L:107:ILE:HG23	1.90	0.54
4:A:83:MET:HB3	4:A:86:LEU:HD21	1.88	0.54
2:H:44:ARG:NH2	2:H:45:LEU:O	2.41	0.54
3:D:186:ASP:HA	3:D:189:LYS:HD3	1.92	0.52
2:C:107:TYR:HD1	6:J:3:FUC:H63	1.75	0.51
1:R:338:PHE:O	7:R:601:NAG:H81	2.11	0.51
4:E:22:CYS:HB3	4:E:79:LEU:HB3	1.92	0.51
1:X:350:VAL:HG22	1:X:422:ASN:HB3	1.94	0.51
5:F:18:ARG:HG2	5:F:76:SER:O	2.12	0.50
4:A:91:THR:HG23	4:A:124:THR:HA	1.94	0.50
3:D:109:ARG:HG2	3:D:110:THR:H	1.76	0.50
3:D:67:GLY:HA3	3:D:72:PHE:HA	1.94	0.50
1:R:350:VAL:HG22	1:R:422:ASN:HB3	1.93	0.49
2:H:107:TYR:HD1	6:G:3:FUC:H63	1.77	0.49
5:F:120:PRO:HD3	5:F:132:VAL:HG22	1.95	0.49
5:F:37:GLN:HB2	5:F:47:LEU:HD11	1.95	0.49
3:D:15:PRO:HD3	3:D:107:ILE:HG23	1.94	0.48
2:C:44:ARG:NH2	2:C:45:LEU:O	2.46	0.48
1:X:444:LYS:HD2	5:F:32:TRP:CD1	2.49	0.47
1:X:472:ILE:HD13	1:X:482:GLY:HA2	1.95	0.47
2:H:131:VAL:O	2:H:219:LYS:NZ	2.45	0.47
2:C:169:LEU:HD21	2:C:192:VAL:HG21	1.96	0.47
3:L:186:ASP:HA	3:L:189:LYS:HD3	1.96	0.47
5:B:37:GLN:HB2	5:B:47:LEU:HD11	1.97	0.47
2:C:34:VAL:HG22	2:C:98:ALA:HB2	1.96	0.47
4:E:53:GLN:NE2	9:E:302:ACT:OXT	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:121:PRO:HB3	3:L:132:SER:H	1.80	0.46
5:F:19:VAL:HG21	5:F:78:LEU:HD12	1.97	0.46
5:B:120:PRO:HD3	5:B:132:VAL:HG22	1.96	0.46
1:X:339:GLY:O	1:X:343:ASN:HB2	2.15	0.46
1:R:439:ASN:O	1:R:443:SER:OG	2.21	0.46
2:H:34:VAL:HG22	2:H:98:ALA:HB2	1.97	0.46
3:L:48:LEU:HD23	3:L:59:ILE:HD12	1.98	0.46
4:A:130:THR:HB	4:E:217:SER:HA	1.96	0.46
3:D:194:ALA:HB2	3:D:209:SER:HB3	1.98	0.46
2:C:53:VAL:O	2:C:72:ARG:HD3	2.16	0.45
3:D:48:LEU:HD23	3:D:59:ILE:HD12	1.99	0.45
3:L:24:ARG:CZ	3:D:9:GLY:HA2	2.46	0.45
2:C:91:THR:HG23	2:C:120:THR:HA	1.98	0.45
2:H:169:LEU:HD21	2:H:192:VAL:HG21	1.98	0.45
3:L:109:ARG:HG2	3:L:110:THR:H	1.82	0.45
1:R:444:LYS:HD2	5:B:32:TRP:CD1	2.52	0.44
2:H:68:VAL:HG22	2:H:83:LEU:HD13	2.00	0.44
2:H:72:ARG:HA	2:H:79:ALA:HA	1.99	0.44
2:C:35:GLN:HA	2:C:50:TRP:HA	2.00	0.44
2:C:196:SER:HA	2:C:199:LEU:HD23	1.99	0.44
3:D:55:ARG:NH1	3:D:61:ASP:O	2.50	0.44
2:H:196:SER:HA	2:H:199:LEU:HD23	2.00	0.43
5:B:19:VAL:HG21	5:B:78:LEU:HD12	1.99	0.43
2:C:4:LEU:O	2:C:114:GLY:HA2	2.18	0.43
1:R:401:VAL:HG22	1:R:509:ARG:HG2	2.01	0.43
3:L:194:ALA:HB2	3:L:209:SER:HB3	2.00	0.43
5:B:105:GLU:HG2	5:B:106:ILE:N	2.34	0.43
5:F:105:GLU:HG2	5:F:106:ILE:N	2.34	0.43
2:C:99:PRO:HB3	2:C:109:ALA:O	2.18	0.43
3:L:67:GLY:HA3	3:L:72:PHE:HA	2.01	0.43
3:L:9:GLY:HA2	3:D:24:ARG:CZ	2.49	0.43
2:C:68:VAL:HG22	2:C:83:LEU:HD13	2.01	0.43
1:R:444:LYS:HE2	4:A:112:ASN:OD1	2.19	0.42
1:R:498:GLN:HB2	1:R:501:ASN:OD1	2.19	0.42
2:H:199:LEU:HD13	2:H:199:LEU:HA	1.80	0.42
5:B:120:PRO:HB3	5:B:131:SER:H	1.84	0.42
3:D:109:ARG:HG2	3:D:110:THR:N	2.34	0.42
2:H:99:PRO:HB3	2:H:109:ALA:O	2.19	0.42
1:X:401:VAL:HG22	1:X:509:ARG:HG2	2.01	0.42
4:E:97:ALA:HB1	4:E:114:MET:HB3	2.00	0.42
1:X:444:LYS:HE2	4:E:112:ASN:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:115:VAL:O	5:B:207:LYS:HE2	2.19	0.42
2:H:50:TRP:CD1	2:H:59:ASN:HB2	2.54	0.42
1:X:350:VAL:HA	1:X:400:PHE:HB2	2.02	0.42
4:A:97:ALA:HB1	4:A:114:MET:HB3	2.02	0.42
5:B:47:LEU:HA	5:B:58:VAL:HG21	2.02	0.42
3:L:171:ASP:OD2	3:L:173:THR:OG1	2.26	0.41
3:D:109:ARG:NH2	3:D:112:ALA:HB2	2.35	0.41
1:R:449:TYR:HB2	4:A:104:VAL:HG21	2.02	0.41
2:C:4:LEU:HB2	2:C:112:ILE:HG22	2.01	0.41
5:F:49:TYR:O	5:F:53:SER:HB2	2.20	0.41
5:F:145:LYS:HB3	5:F:197:THR:OG1	2.21	0.41
1:X:385:THR:OG1	1:X:386:LYS:N	2.53	0.41
3:L:92:TYR:HA	3:L:97:TRP:CG	2.55	0.41
5:F:47:LEU:HA	5:F:58:VAL:HG21	2.02	0.41
3:L:48:LEU:HA	3:L:59:ILE:HG13	2.02	0.41
4:A:67:ARG:HB3	4:A:84:ASN:O	2.21	0.41
5:F:125:LEU:O	5:F:183:LYS:HD2	2.21	0.41
2:C:199:LEU:HA	2:C:199:LEU:HD13	1.82	0.41
5:F:124:GLN:HG2	5:F:129:THR:O	2.21	0.41
2:H:4:LEU:O	2:H:114:GLY:HA2	2.21	0.40
4:A:11:VAL:HG21	4:A:161:PRO:HG3	2.03	0.40
5:B:125:LEU:O	5:B:183:LYS:HD2	2.22	0.40
2:C:33:ALA:O	2:C:99:PRO:HD2	2.21	0.40
5:B:49:TYR:O	5:B:53:SER:HB2	2.20	0.40
4:E:50:VAL:HG11	5:F:94:PHE:CZ	2.57	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	R	181/205 (88%)	168 (93%)	13 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	180/205 (88%)	169 (94%)	11 (6%)	0	100	100
2	C	215/228 (94%)	204 (95%)	11 (5%)	0	100	100
2	H	215/228 (94%)	204 (95%)	11 (5%)	0	100	100
3	D	214/215 (100%)	206 (96%)	8 (4%)	0	100	100
3	L	214/215 (100%)	206 (96%)	8 (4%)	0	100	100
4	A	221/245 (90%)	217 (98%)	4 (2%)	0	100	100
4	E	221/245 (90%)	217 (98%)	4 (2%)	0	100	100
5	B	212/227 (93%)	202 (95%)	10 (5%)	0	100	100
5	F	211/227 (93%)	200 (95%)	11 (5%)	0	100	100
All	All	2084/2240 (93%)	1993 (96%)	91 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	159/177 (90%)	158 (99%)	1 (1%)	86	94
1	X	158/177 (89%)	158 (100%)	0	100	100
2	C	186/196 (95%)	185 (100%)	1 (0%)	88	95
2	H	186/196 (95%)	185 (100%)	1 (0%)	88	95
3	D	186/186 (100%)	186 (100%)	0	100	100
3	L	186/186 (100%)	186 (100%)	0	100	100
4	A	190/206 (92%)	188 (99%)	2 (1%)	73	88
4	E	190/206 (92%)	188 (99%)	2 (1%)	73	88
5	B	187/197 (95%)	183 (98%)	4 (2%)	53	79
5	F	186/197 (94%)	183 (98%)	3 (2%)	62	84
All	All	1814/1924 (94%)	1800 (99%)	14 (1%)	81	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	335	LEU
2	H	72	ARG
4	A	6	GLU
4	A	53	GLN
5	B	1	ASP
5	B	11	VAL
5	B	33	LEU
5	B	123	GLU
2	C	72	ARG
4	E	6	GLU
4	E	53	GLN
5	F	11	VAL
5	F	33	LEU
5	F	123	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	388	ASN
3	D	3	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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
6	NAG	G	1	6,2	14,14,15	0.25	0	17,19,21	0.36	0
6	NAG	G	2	6	14,14,15	0.35	0	17,19,21	0.54	0
6	FUC	G	3	6	10,10,11	0.78	0	14,14,16	0.73	0
6	NAG	I	1	1,6	14,14,15	0.48	0	17,19,21	0.56	0
6	NAG	I	2	6	14,14,15	0.20	0	17,19,21	0.45	0
6	FUC	I	3	6	10,10,11	1.17	1 (10%)	14,14,16	1.13	1 (7%)
6	NAG	J	1	6,2	14,14,15	0.27	0	17,19,21	0.35	0
6	NAG	J	2	6	14,14,15	0.39	0	17,19,21	0.56	0
6	FUC	J	3	6	10,10,11	0.78	0	14,14,16	0.73	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	G	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	2/6/23/26	0/1/1/1
6	FUC	G	3	6	-	-	0/1/1/1
6	NAG	I	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	FUC	I	3	6	-	-	0/1/1/1
6	NAG	J	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	FUC	J	3	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	3	FUC	O5-C1	-2.78	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	3	FUC	O2-C2-C1	2.55	114.36	109.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

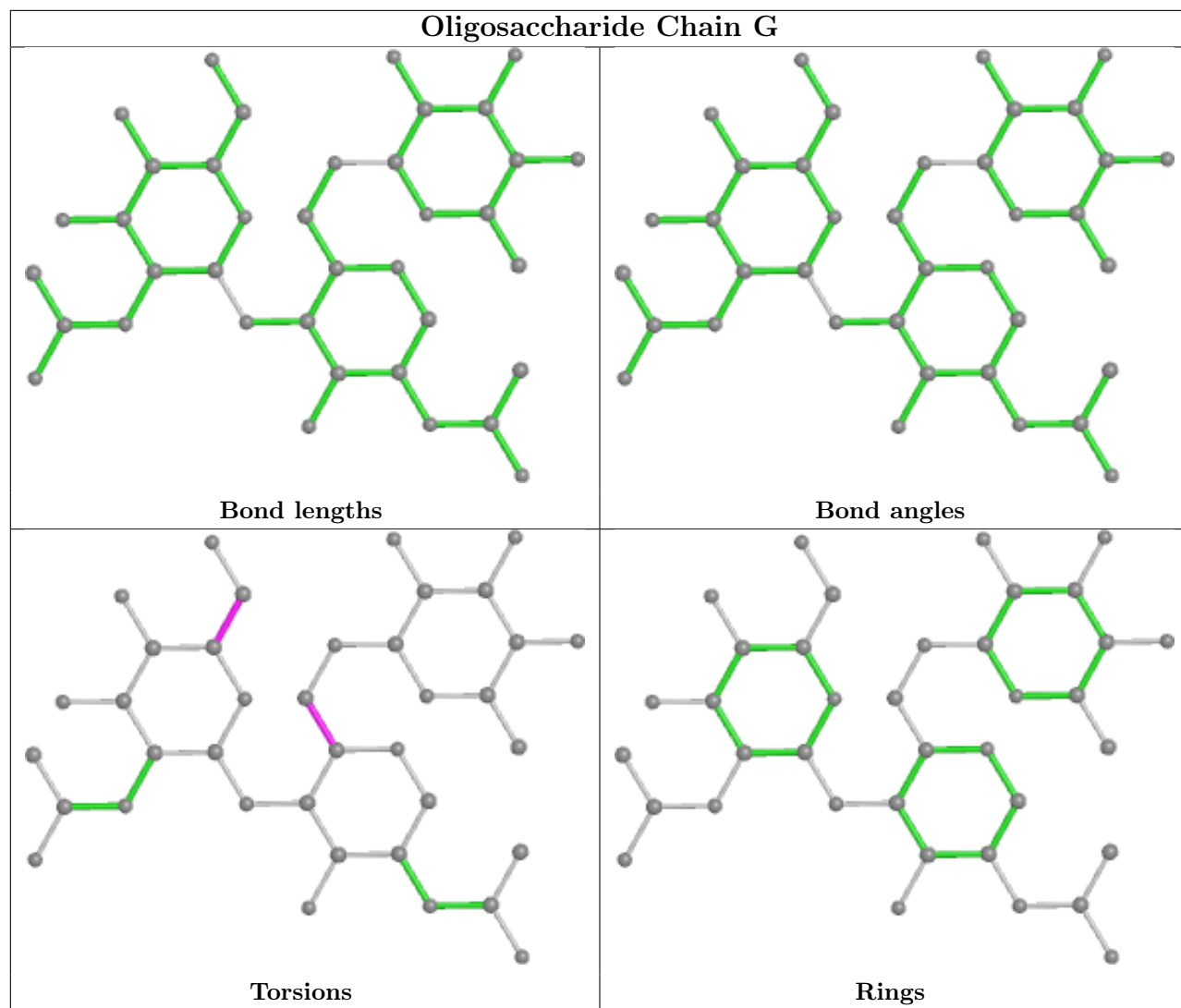
Mol	Chain	Res	Type	Atoms
6	J	2	NAG	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6

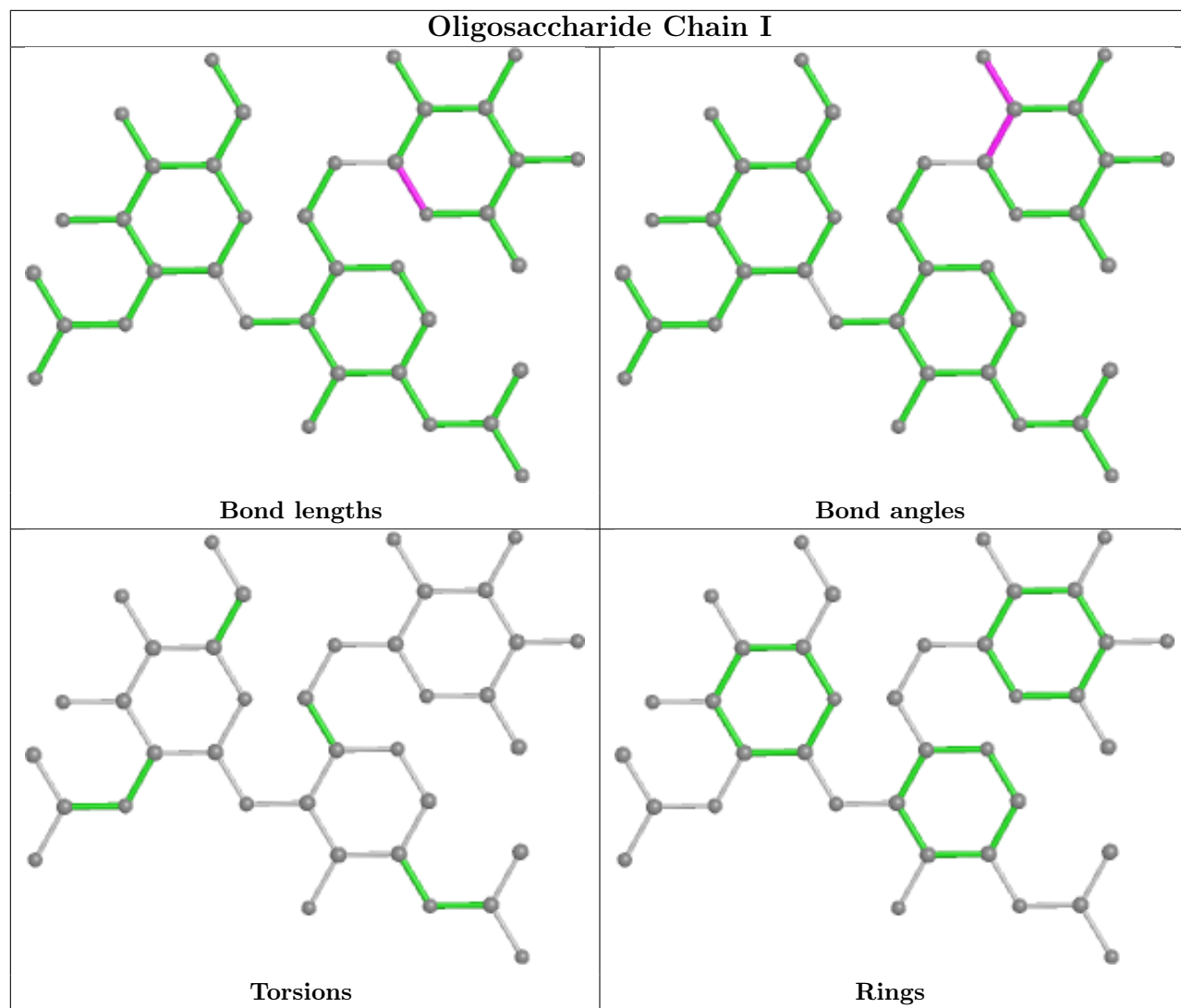
There are no ring outliers.

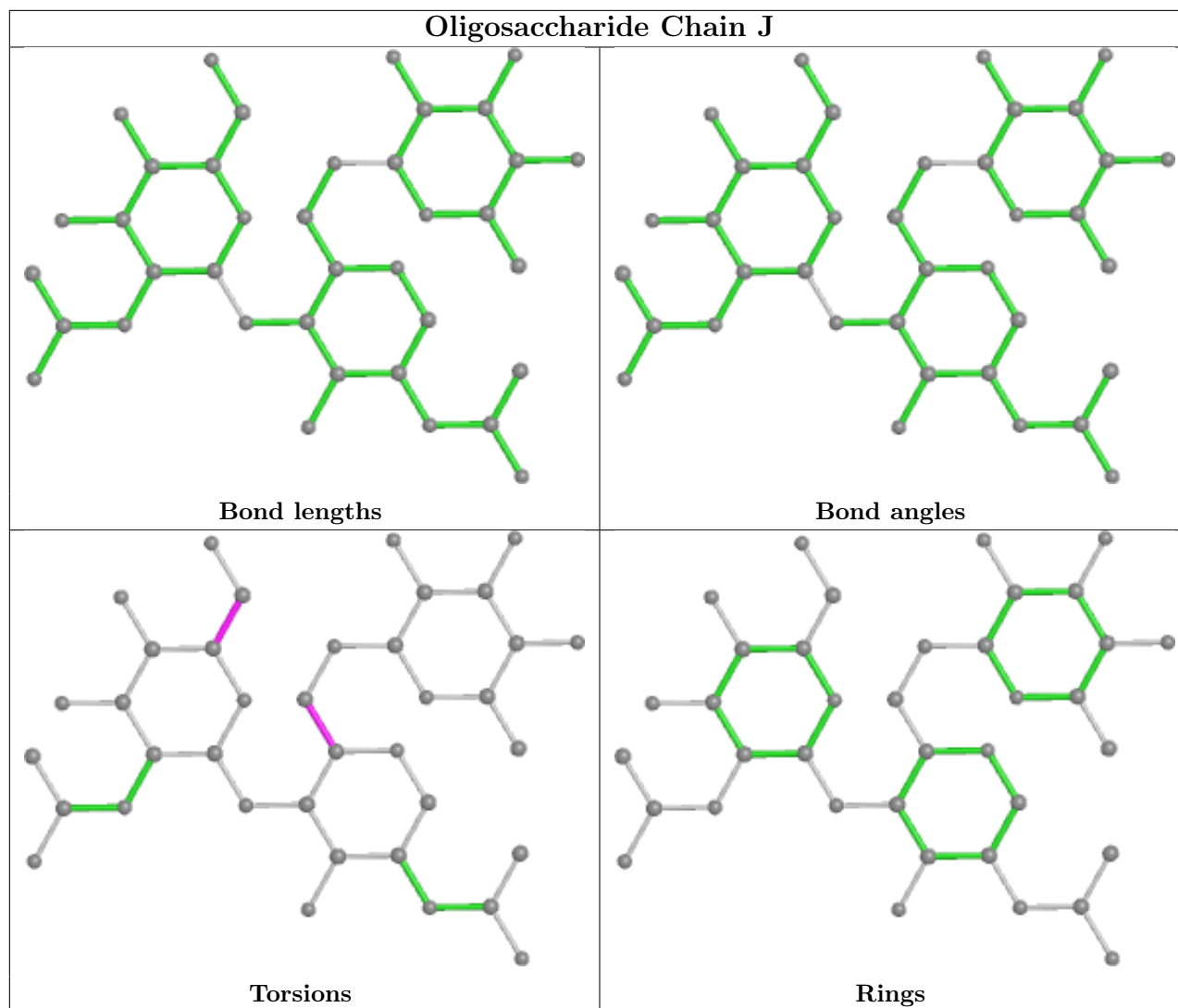
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	3	FUC	1	0
6	G	3	FUC	1	0

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







5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	ACT	C	501	-	3,3,3	1.35	0	3,3,3	1.38	0
7	NAG	R	601	1	14,14,15	0.49	0	17,19,21	0.65	1 (5%)
9	ACT	D	302	-	3,3,3	1.38	1 (33%)	3,3,3	1.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ACT	A	401	-	3,3,3	1.29	0	3,3,3	1.38	0
9	ACT	A	403	-	3,3,3	1.33	0	3,3,3	1.51	0
9	ACT	D	301	-	3,3,3	1.38	1 (33%)	3,3,3	1.50	0
8	GOL	X	701	-	5,5,5	0.72	0	5,5,5	1.08	0
8	GOL	H	501	-	5,5,5	0.70	0	5,5,5	1.08	0
9	ACT	E	302	-	3,3,3	1.40	1 (33%)	3,3,3	1.36	0
9	ACT	L	301	-	3,3,3	1.32	0	3,3,3	1.36	0
9	ACT	E	301	-	3,3,3	1.41	1 (33%)	3,3,3	1.52	0
9	ACT	A	402	-	3,3,3	1.27	0	3,3,3	1.53	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	GOL	H	501	-	-	0/4/4/4	-
7	NAG	R	601	1	-	0/6/23/26	0/1/1/1
8	GOL	X	701	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	301	ACT	CH3-C	2.11	1.57	1.49
9	E	302	ACT	CH3-C	2.09	1.57	1.49
9	E	301	ACT	CH3-C	2.08	1.57	1.49
9	D	302	ACT	CH3-C	2.04	1.57	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	601	NAG	C1-O5-C5	2.24	115.23	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

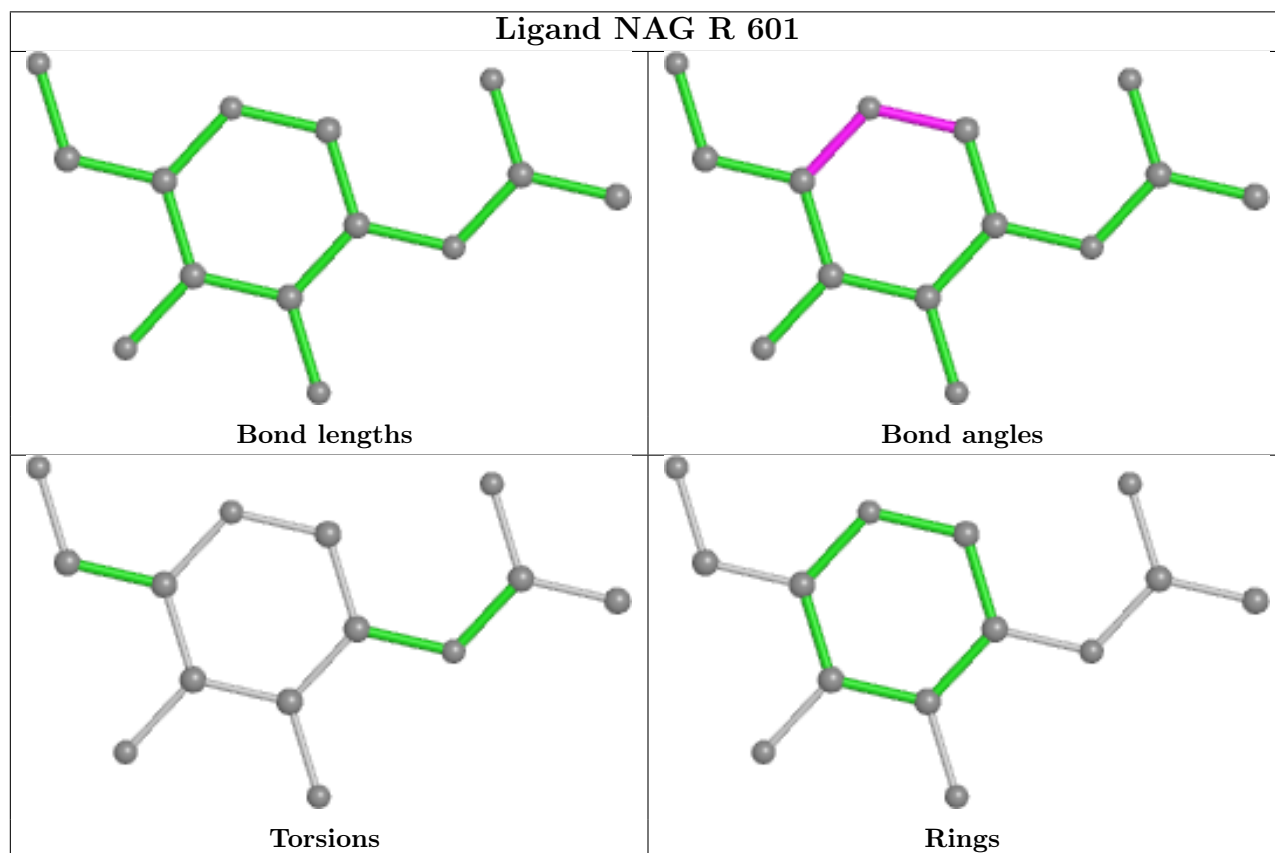
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	601	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	701	GOL	1	0
9	E	302	ACT	1	0
9	A	402	ACT	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 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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	183/205 (89%)	0.92	27 (14%) 2 1	61, 86, 138, 164	0
1	X	182/205 (88%)	1.13	36 (19%) 1 1	57, 83, 137, 158	0
2	C	219/228 (96%)	0.42	15 (6%) 17 10	60, 100, 143, 170	0
2	H	219/228 (96%)	0.66	26 (11%) 4 2	62, 106, 155, 215	0
3	D	214/215 (99%)	0.41	7 (3%) 46 30	61, 94, 128, 158	0
3	L	214/215 (99%)	0.40	9 (4%) 36 23	52, 98, 136, 173	0
4	A	224/245 (91%)	0.47	8 (3%) 42 27	45, 71, 115, 146	0
4	E	224/245 (91%)	0.42	7 (3%) 49 32	50, 69, 115, 154	0
5	B	213/227 (93%)	0.40	10 (4%) 31 19	56, 82, 118, 168	0
5	F	213/227 (93%)	0.37	8 (3%) 40 26	56, 83, 111, 156	0
All	All	2105/2240 (93%)	0.55	153 (7%) 15 9	45, 86, 138, 215	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	410	ILE	5.9
1	R	503	VAL	5.2
3	L	119	PHE	5.0
2	H	222	GLU	5.0
1	R	511	VAL	4.8
1	X	514	SER	4.8
1	X	425	LEU	4.8
1	R	415	THR	4.7
1	R	433	VAL	4.7
1	R	407	VAL	4.7
2	C	129	PRO	4.7
1	X	410	ILE	4.7
2	H	221	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	R	432	CYS	4.6
2	H	164	TRP	4.5
5	F	102	THR	4.4
1	X	438	SER	4.3
1	X	511	VAL	4.2
2	H	201	THR	4.0
1	X	435	ALA	4.0
1	X	415	THR	3.8
1	X	337	PRO	3.8
1	R	510	VAL	3.7
5	B	130	ALA	3.7
1	X	443	SER	3.7
1	X	423	TYR	3.6
1	X	503	VAL	3.6
1	R	434	ILE	3.5
2	H	223	PRO	3.5
2	C	221	VAL	3.5
2	C	137	SER	3.5
1	X	434	ILE	3.4
1	X	512	VAL	3.4
1	X	432	CYS	3.4
1	R	435	ALA	3.3
2	H	137	SER	3.3
1	R	423	TYR	3.2
1	X	433	VAL	3.2
1	X	513	LEU	3.2
5	B	103	LYS	3.2
1	R	422	ASN	3.1
2	C	189	SER	3.1
1	R	376	THR	3.0
4	E	205	THR	3.0
1	X	510	VAL	3.0
4	E	144	SER	3.0
1	R	443	SER	3.0
4	A	205	THR	3.0
5	F	20	THR	2.9
2	H	151	LEU	2.9
4	A	203	LEU	2.9
2	H	136	PRO	2.9
4	E	201	SER	2.9
1	X	509	ARG	2.9
1	R	337	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	107	ILE	2.8
2	C	164	TRP	2.8
5	B	141	PRO	2.8
1	X	365	TYR	2.8
1	X	422	ASN	2.8
5	B	69	THR	2.8
1	X	396	TYR	2.8
2	H	131	VAL	2.7
5	F	9	SER	2.7
3	L	107	ILE	2.7
2	H	134	LEU	2.7
2	C	201	THR	2.7
2	H	129	PRO	2.7
4	A	125	VAL	2.7
5	B	20	THR	2.7
5	F	103	LYS	2.7
3	L	132	SER	2.7
5	B	102	THR	2.6
1	X	360	ASN	2.6
3	D	2	ILE	2.6
4	E	213	ASN	2.6
4	E	203	LEU	2.6
1	X	378	LYS	2.6
2	C	169	LEU	2.6
2	H	204	TYR	2.6
2	H	169	LEU	2.6
2	C	170	THR	2.6
2	H	196	SER	2.6
2	H	120	THR	2.5
4	A	124	THR	2.5
1	X	497	PHE	2.5
1	R	512	VAL	2.5
5	B	11	VAL	2.5
1	R	406	GLU	2.5
4	A	201	SER	2.5
2	H	94	TYR	2.5
1	R	509	ARG	2.5
3	D	132	SER	2.5
2	C	1	GLN	2.5
1	X	373	SER	2.5
2	H	191	VAL	2.5
5	B	35	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
5	F	35	TRP	2.4
1	X	495	TYR	2.4
3	L	137	LEU	2.4
5	B	36	TYR	2.4
3	L	179	THR	2.3
3	L	2	ILE	2.3
5	B	87	TYR	2.3
5	F	36	TYR	2.3
3	L	191	LYS	2.3
1	X	377	PHE	2.3
1	R	378	LYS	2.3
1	X	376	THR	2.3
2	H	152	VAL	2.3
4	A	36	TRP	2.3
4	E	208	TYR	2.3
1	R	417	LYS	2.3
2	H	170	THR	2.2
2	C	191	VAL	2.2
1	R	419	ALA	2.2
3	D	87	TYR	2.2
1	X	436	TRP	2.2
2	C	37	VAL	2.2
5	F	104	VAL	2.2
2	H	155	TYR	2.2
1	R	375	SER	2.2
1	X	395	VAL	2.2
1	X	358	ILE	2.2
2	C	162	VAL	2.2
1	X	504	GLY	2.2
2	H	171	SER	2.2
2	H	162	VAL	2.2
2	H	133	PRO	2.2
2	C	176	PHE	2.2
1	R	365	TYR	2.1
3	D	104	LYS	2.1
4	A	198	VAL	2.1
1	R	504	GLY	2.1
1	X	375	SER	2.1
3	D	184	LYS	2.1
2	C	204	TYR	2.1
2	H	119	VAL	2.1
2	H	224	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	1	ASP	2.1
1	R	409	GLN	2.1
1	X	424	LYS	2.1
1	R	408	ARG	2.1
1	R	425	LEU	2.1
2	C	155	TYR	2.0
3	L	121	PRO	2.0
1	X	408	ARG	2.0
3	D	143	ARG	2.0
2	H	117	THR	2.0
1	X	417	LYS	2.0
5	F	87	TYR	2.0
4	A	202	SER	2.0
4	E	36	TRP	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](#)

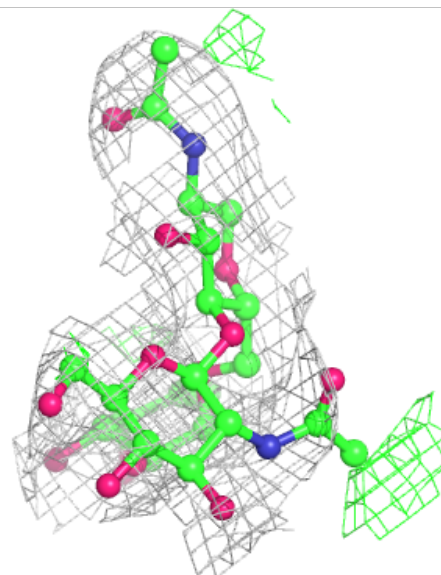
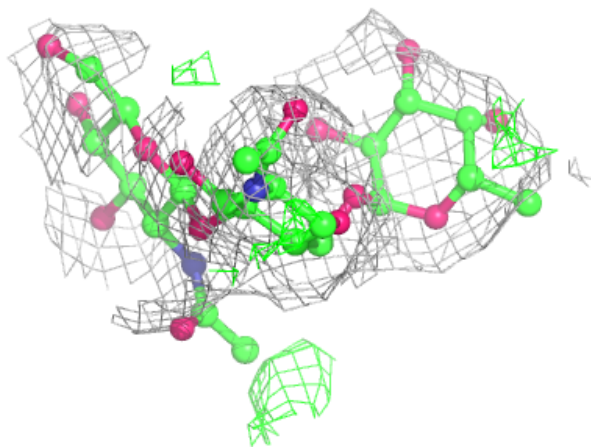
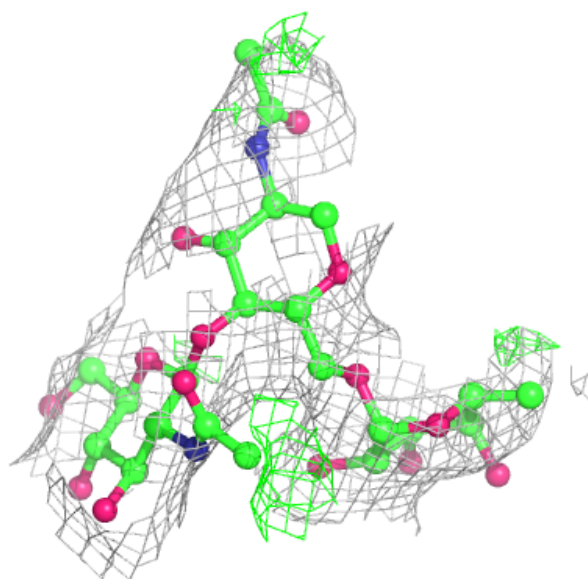
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	G	2	14/15	0.76	0.22	113,125,139,140	0
6	NAG	I	2	14/15	0.76	0.32	122,136,148,152	0
6	FUC	G	3	10/11	0.77	0.26	100,113,116,118	0
6	NAG	J	2	14/15	0.78	0.23	115,124,130,139	0
6	FUC	J	3	10/11	0.83	0.26	99,117,120,122	0
6	FUC	I	3	10/11	0.89	0.35	137,143,152,156	0
6	NAG	I	1	14/15	0.91	0.18	94,121,143,150	0
6	NAG	G	1	14/15	0.92	0.15	90,101,112,116	0
6	NAG	J	1	14/15	0.92	0.15	94,104,113,118	0

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

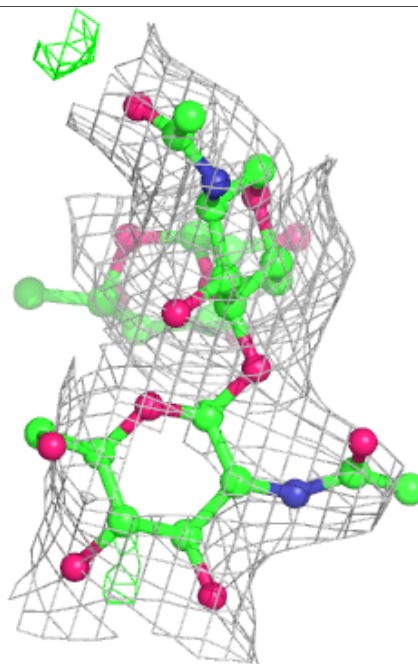
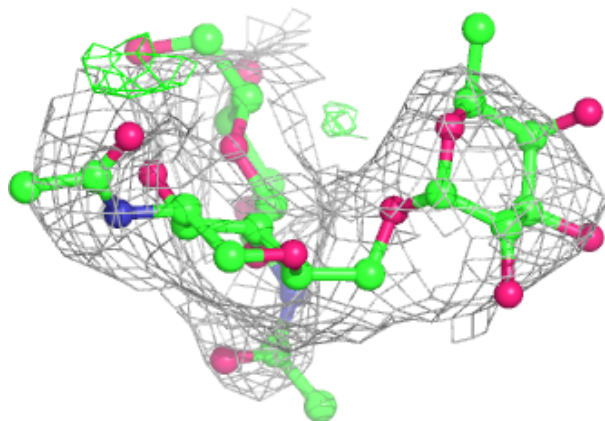
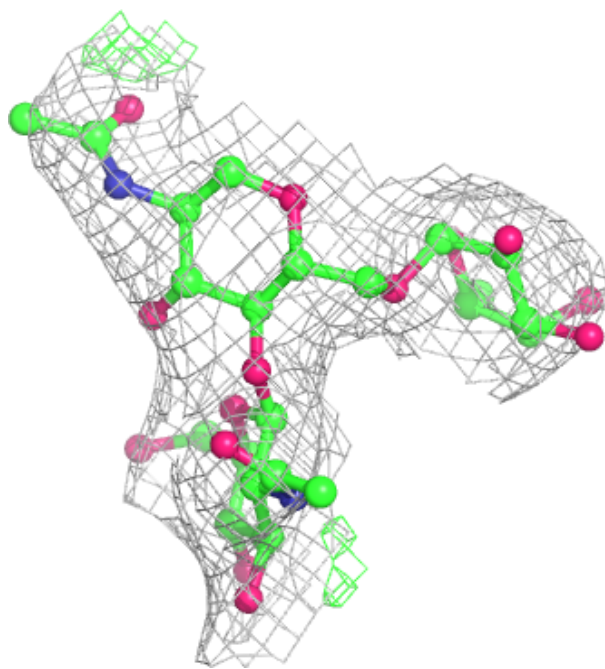
Electron density around Chain G:

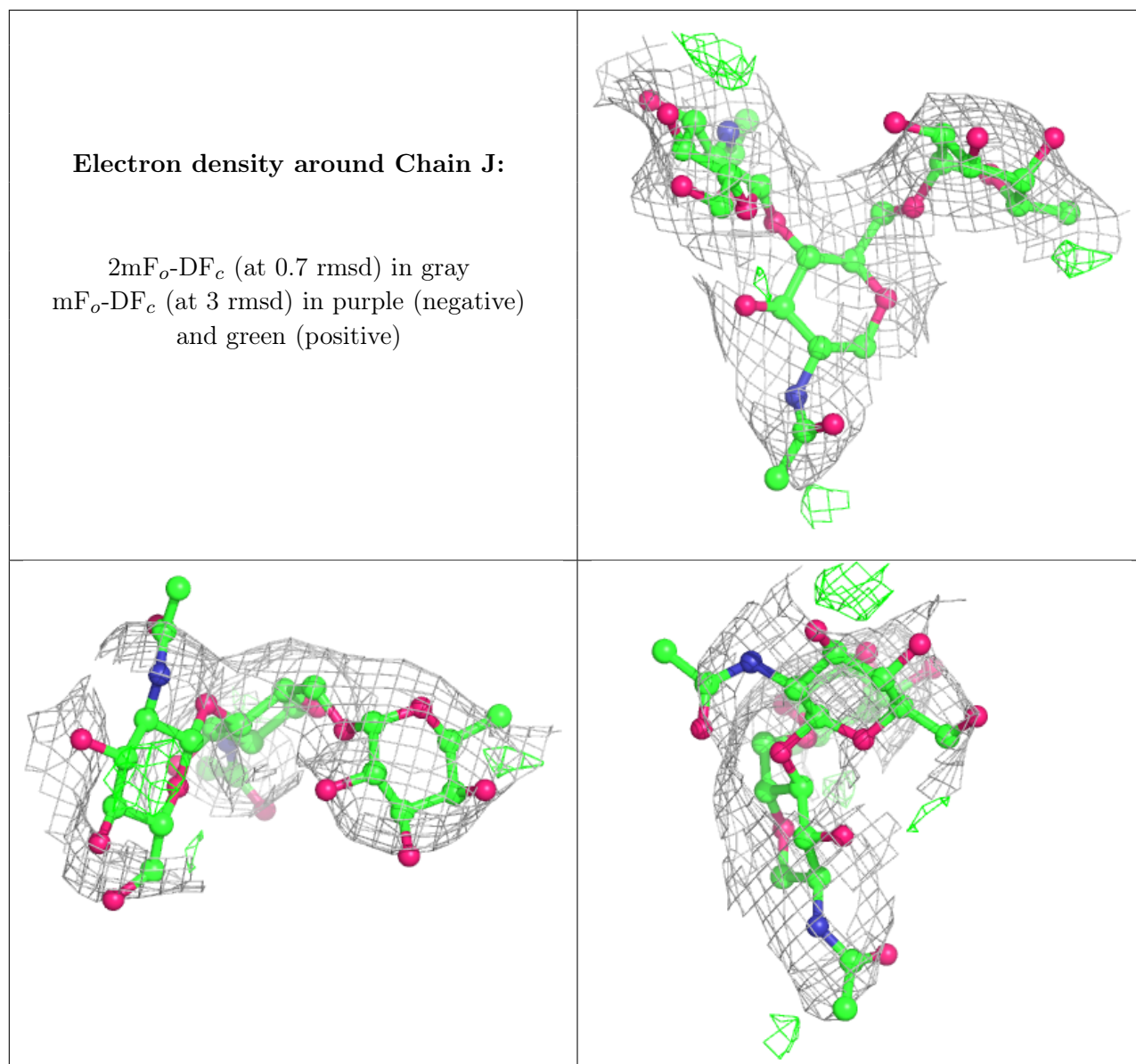
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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.

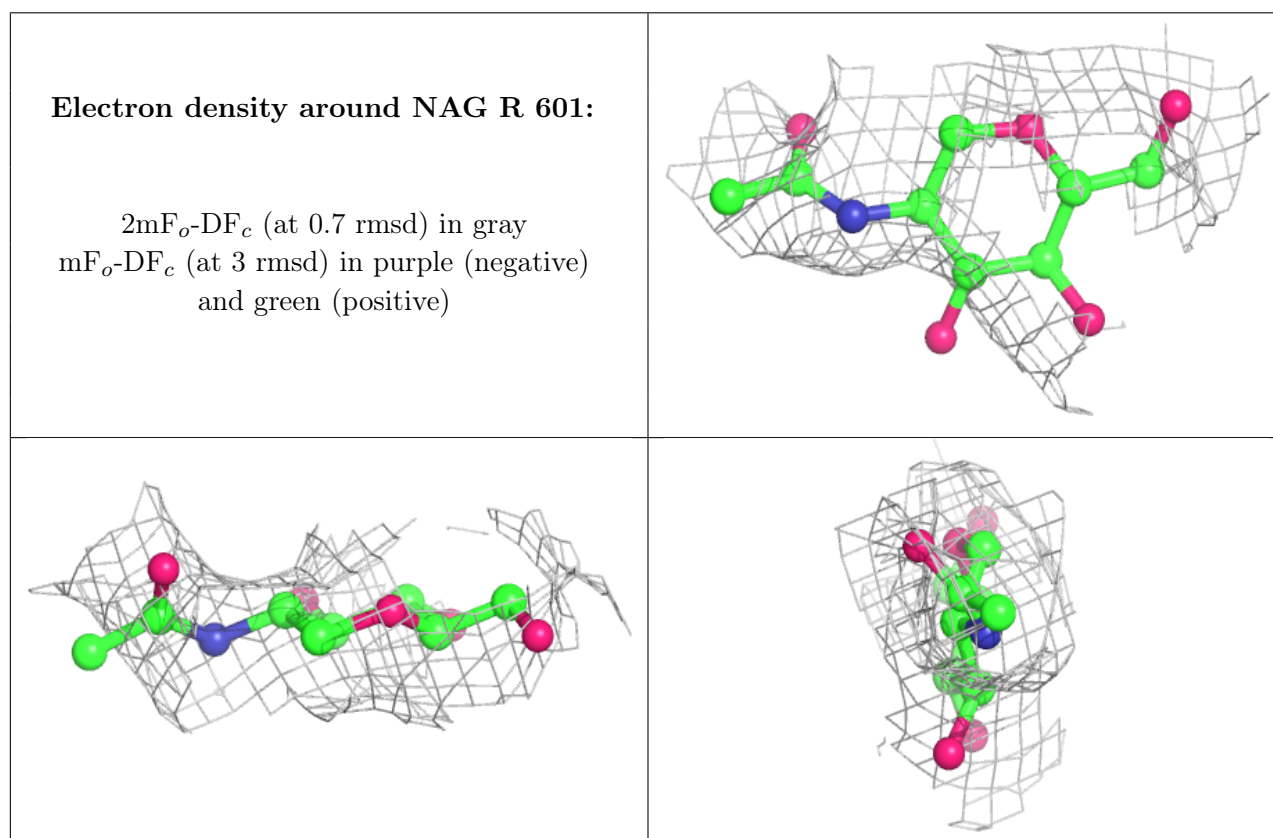
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	R	601	14/15	0.66	0.31	116,127,142,143	0
9	ACT	E	301	4/4	0.79	0.27	60,80,108,123	0
9	ACT	D	302	4/4	0.82	0.61	106,107,117,124	0
9	ACT	E	302	4/4	0.83	0.29	70,114,114,115	0
9	ACT	D	301	4/4	0.84	0.29	85,107,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	ACT	A	402	4/4	0.84	0.20	74,95,95,95	0
9	ACT	A	401	4/4	0.88	0.21	61,62,78,79	0
9	ACT	L	301	4/4	0.89	0.29	50,67,83,93	0
10	CL	C	502	1/1	0.89	0.19	63,63,63,63	0
9	ACT	A	403	4/4	0.90	0.24	56,73,74,77	0
8	GOL	X	701	6/6	0.91	0.25	68,95,101,136	0
8	GOL	H	501	6/6	0.93	0.23	81,84,101,127	0
9	ACT	C	501	4/4	0.95	0.25	50,73,86,101	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.