



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:25 AM EDT

PDB ID : 7L0N / pdb_0000710n
Title : Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity
Authors : Snell, G.; Czudnochowski, N.; Dillen, J.; Nix, J.C.; Croll, T.I.; Corti, D.
Deposited on : 2020-12-11
Resolution : 2.78 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:

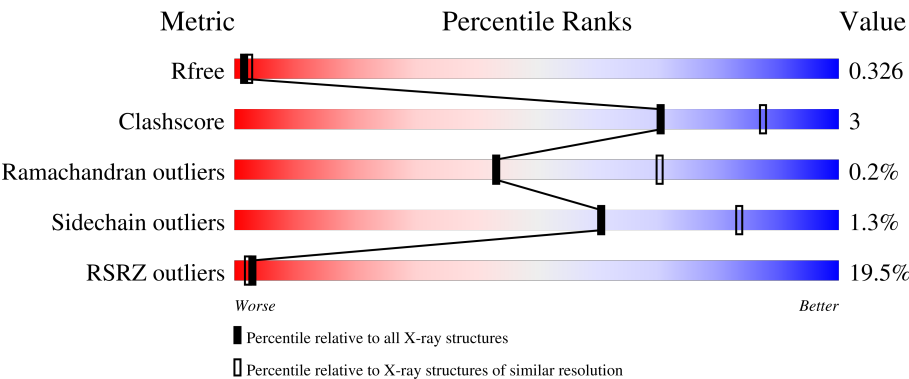
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	214	
1	D	214	
2	A	230	
2	C	230	
3	L	215	

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Mol	Chain	Length	Quality of chain
3	N	215	
4	H	223	
4	M	223	
5	E	597	
5	F	597	
6	R	204	
6	S	204	
7	G	6	
8	I	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	G	5	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 26468 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 Monoclonal antibody S309 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			
1	D	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			

- Molecule 2 is a protein called Monoclonal antibody S309 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	222	Total	C	N	O	S	0	0	0
			1674	1058	282	327	7			
2	C	224	Total	C	N	O	S	0	0	0
			1692	1069	286	330	7			

- Molecule 3 is a protein called Monoclonal antibody S304 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1627	1021	271	330	5			
3	N	213	Total	C	N	O	S	0	0	0
			1627	1021	271	330	5			

- Molecule 4 is a protein called Monoclonal antibody S304 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	212	Total	C	N	O	S	0	0	0
			1600	1016	263	315	6			
4	M	215	Total	C	N	O	S	0	0	0
			1619	1026	266	321	6			

- Molecule 5 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	579	Total	C	N	O	S	0	0	0
			4733	3031	784	891	27			
5	F	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			

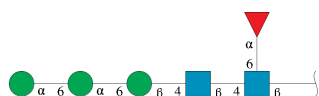
- Molecule 6 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	203	Total	C	N	O	S	0	0	0
			1609	1034	268	299	8			
6	S	201	Total	C	N	O	S	0	0	0
			1598	1027	268	295	8			

There are 2 discrepancies between the modelled and reference sequences:

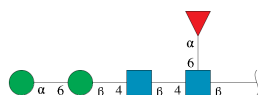
Chain	Residue	Modelled	Actual	Comment	Reference
R	439	LYS	ASN	variant	UNP P0DTC2
S	439	LYS	ASN	variant	UNP P0DTC2

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-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
7	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.

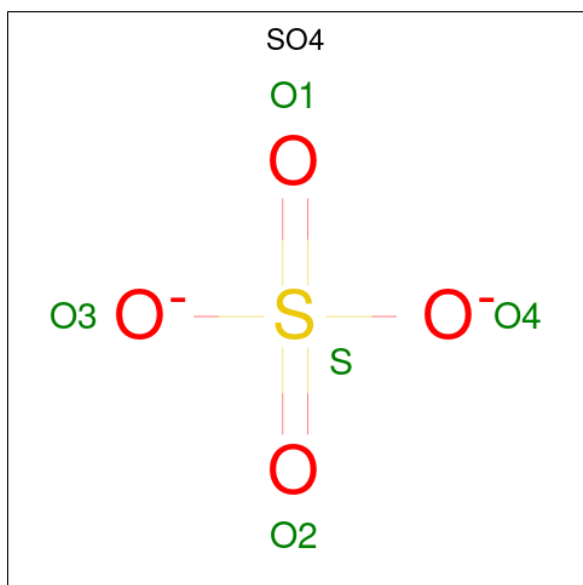


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cl 1 1	0	0
9	A	1	Total Cl 1 1	0	0
9	D	1	Total Cl 1 1	0	0
9	C	2	Total Cl 2 2	0	0
9	H	3	Total Cl 3 3	0	0
9	N	2	Total Cl 2 2	0	0
9	M	5	Total Cl 5 5	0	0
9	E	1	Total Cl 1 1	0	0
9	F	6	Total Cl 6 6	0	0
9	R	2	Total Cl 2 2	0	0
9	S	3	Total Cl 3 3	0	0

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

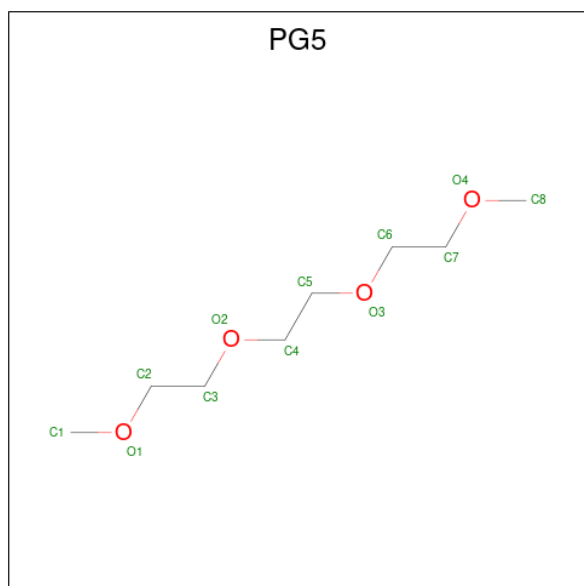


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	O	S	0	0
			5	4	1		
10	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

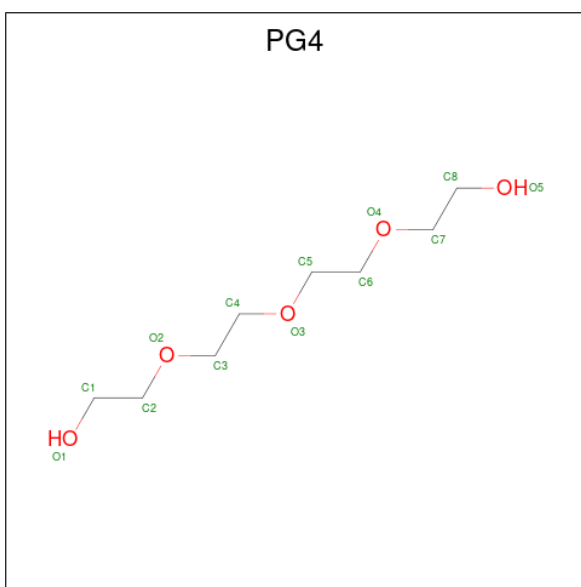
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	3	Total	Na	0	0
			3	3		
11	F	2	Total	Na	0	0
			2	2		
11	R	1	Total	Na	0	0
			1	1		

- Molecule 12 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	H	1	Total	C	O	0	0
			12	8	4		

- Molecule 13 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).

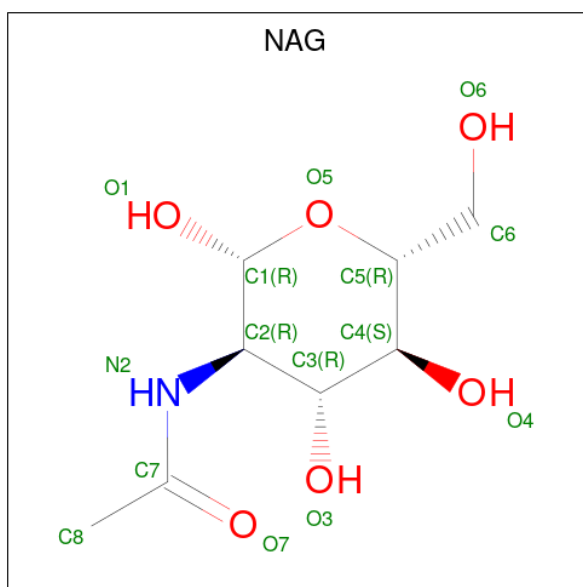


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	N	1	Total	C	O	0	0
			13	8	5		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

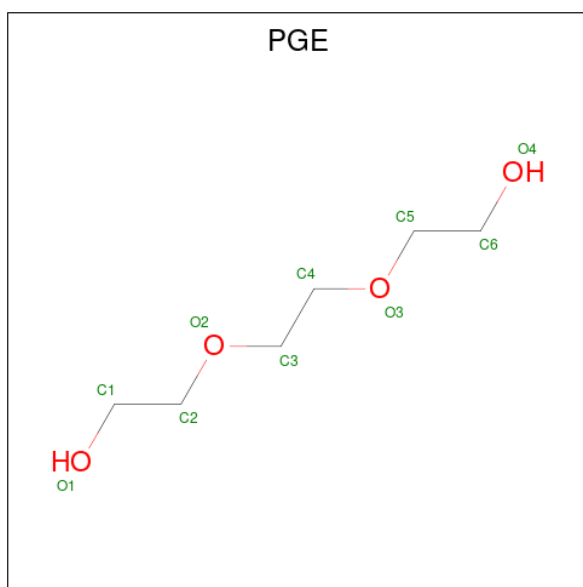
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	E	1	Total	Zn	0	0
			1	1		
14	F	1	Total	Zn	0	0
			1	1		

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	E	1	Total	C	N	O	0	0
			14	8	1	5		
15	E	1	Total	C	N	O	0	0
			14	8	1	5		
15	E	1	Total	C	N	O	0	0
			14	8	1	5		
15	E	1	Total	C	N	O	0	0
			14	8	1	5		
15	F	1	Total	C	N	O	0	0
			14	8	1	5		
15	F	1	Total	C	N	O	0	0
			14	8	1	5		
15	F	1	Total	C	N	O	0	0
			14	8	1	5		
15	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 16 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	C	O	0	0
			10	6	4		
16	S	1	Total	C	O	0	0
			10	6	4		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	32	Total	O	0	0
			32	32		
17	A	8	Total	O	0	0
			8	8		
17	D	19	Total	O	0	0
			19	19		
17	C	8	Total	O	0	0
			8	8		
17	L	22	Total	O	0	0
			22	22		
17	H	12	Total	O	0	0
			12	12		
17	N	11	Total	O	0	0
			11	11		
17	M	15	Total	O	0	0
			15	15		
17	E	15	Total	O	0	0
			15	15		
17	F	37	Total	O	0	0
			37	37		

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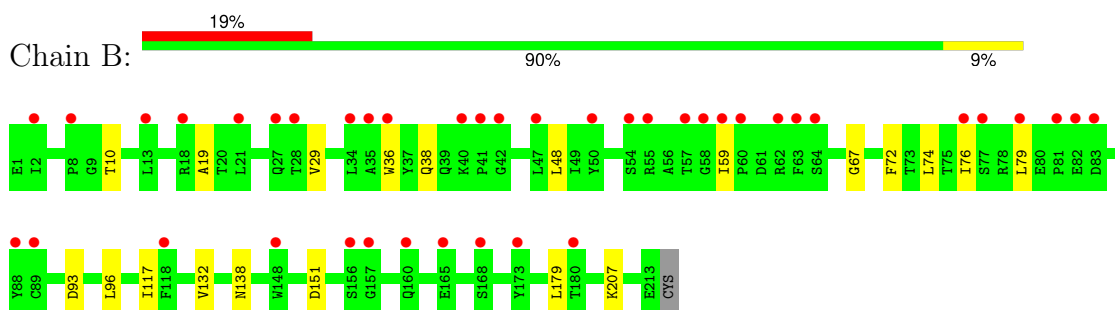
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	R	24	Total 24	O 24	0	0
17	S	29	Total 29	O 29	0	0

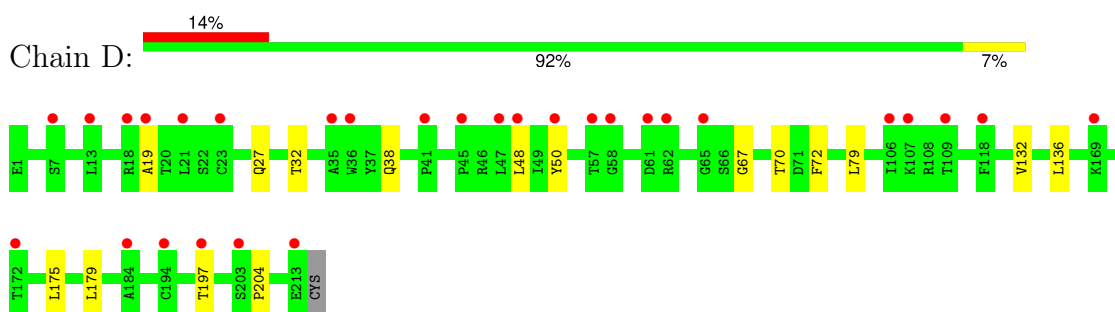
3 Residue-property plots [i](#)

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

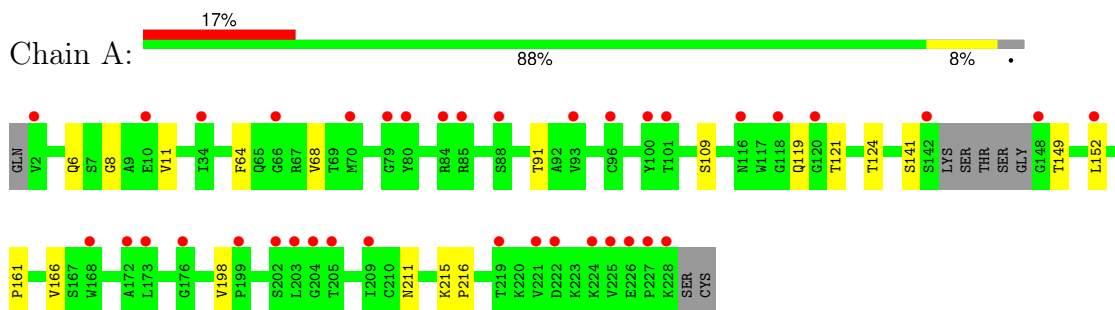
- Molecule 1: Monoclonal antibody S309 Fab light chain



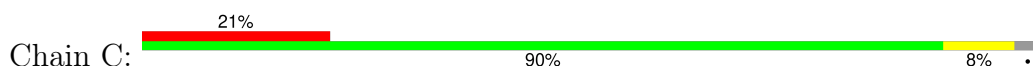
- Molecule 1: Monoclonal antibody S309 Fab light chain

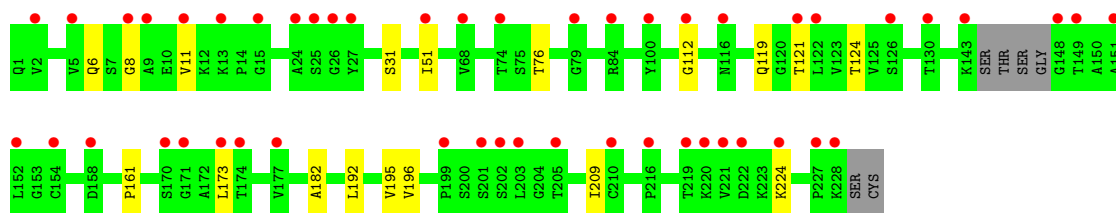


- Molecule 2: Monoclonal antibody S309 Fab heavy chain

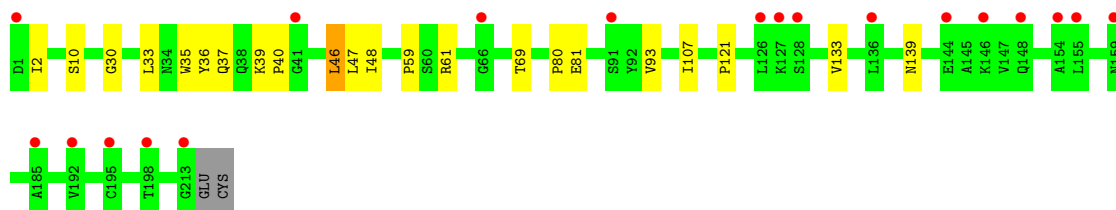
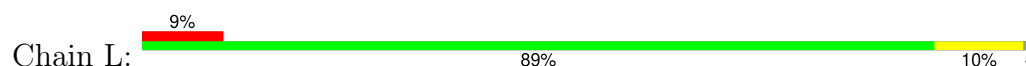


- Molecule 2: Monoclonal antibody S309 Fab heavy chain

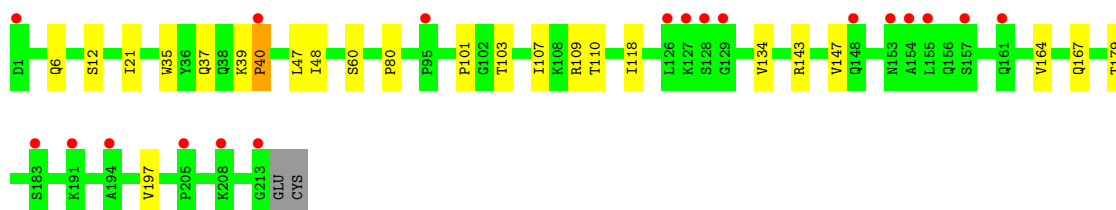
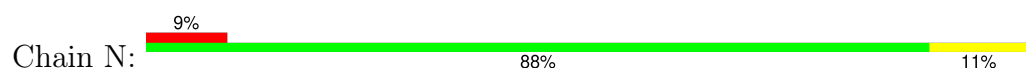




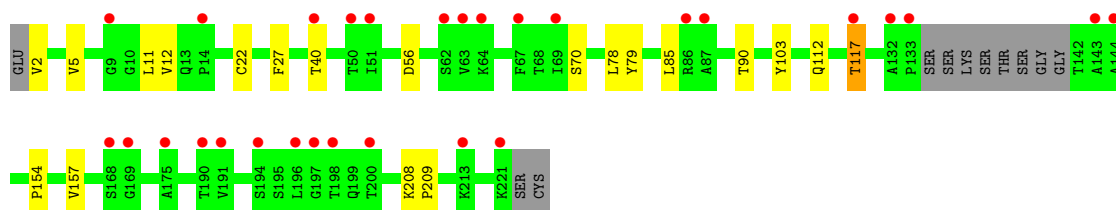
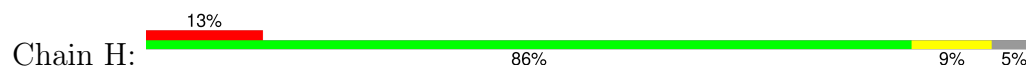
• Molecule 3: Monoclonal antibody S304 Fab light chain



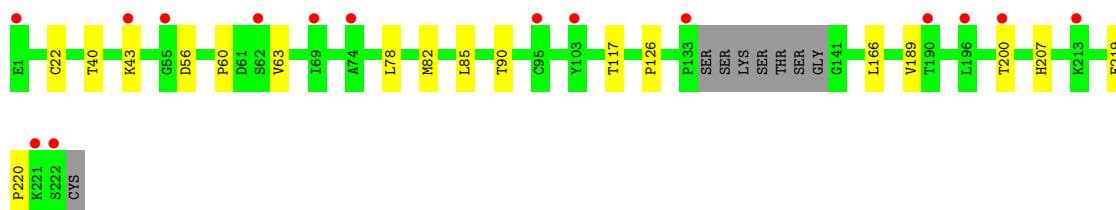
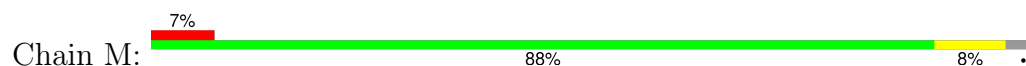
• Molecule 3: Monoclonal antibody S304 Fab light chain



• Molecule 4: Monoclonal antibody S304 Fab heavy chain

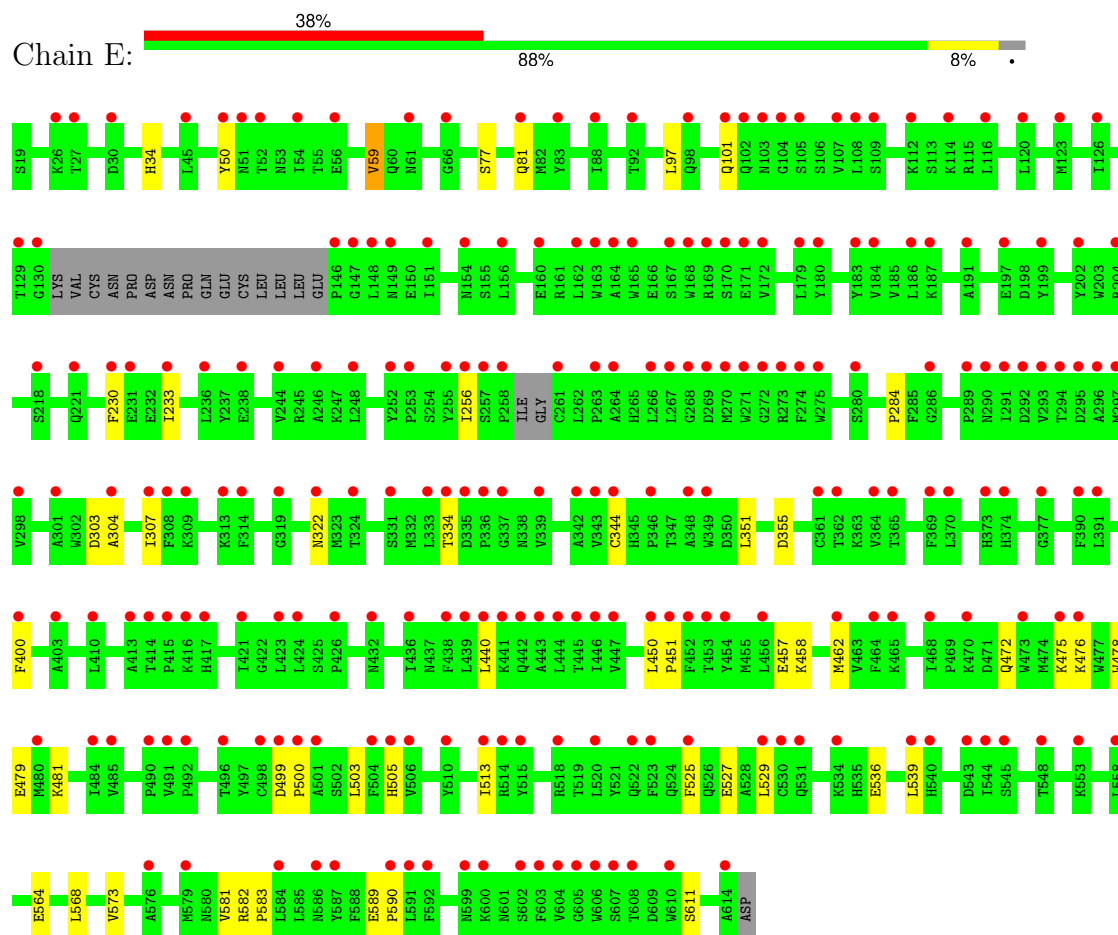


• Molecule 4: Monoclonal antibody S304 Fab heavy chain



• Molecule 5: Angiotensin-converting enzyme 2

Chain E:

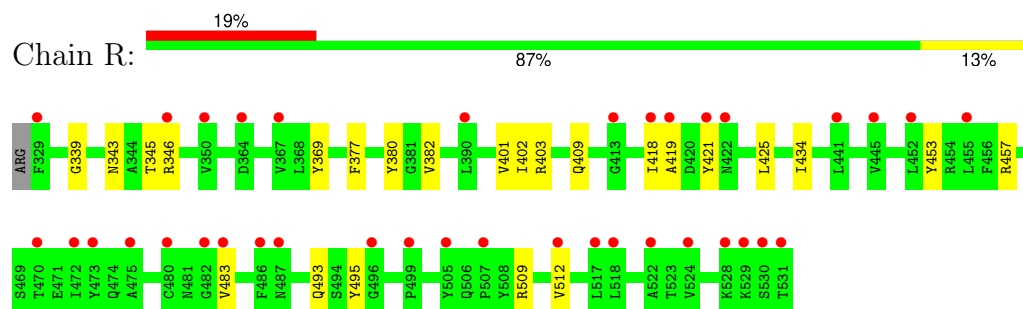


• Molecule 5: Angiotensin-converting enzyme 2

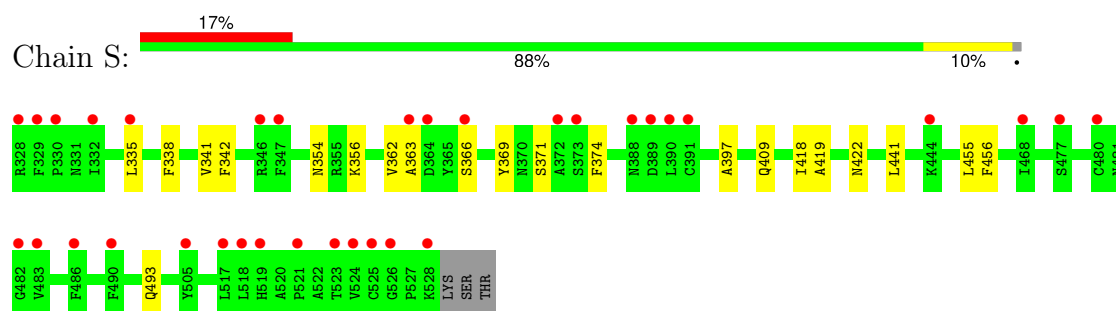
Chain F:



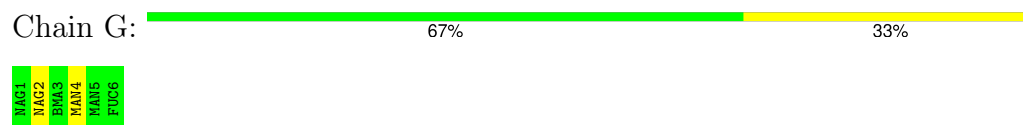
- Molecule 6: Spike protein S1



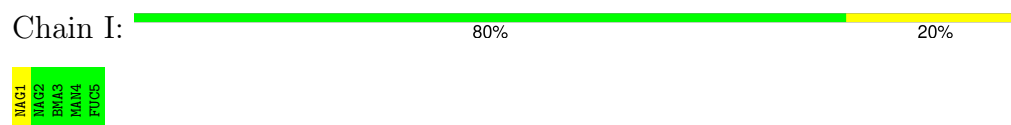
- Molecule 6: Spike protein S1



- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-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



- Molecule 8: alpha-D-mannopyranose-(1-6)-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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.98Å 186.58Å 194.52Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	48.90 – 2.78 48.90 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.9 (48.90-2.78) 92.9 (48.90-2.78)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.290 , 0.325 0.291 , 0.326	Depositor DCC
R_{free} test set	6375 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	26468	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7733e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG5, SO4, NAG, CL, ZN, PG4, FUC, PGE, BMA, NA, MAN

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	B	0.45	0/1657	0.77	0/2250
1	D	0.45	0/1657	0.78	0/2250
2	A	0.44	0/1716	0.78	0/2338
2	C	0.45	0/1734	0.78	0/2361
3	L	0.45	0/1663	0.77	0/2260
3	N	0.46	0/1663	0.79	0/2260
4	H	0.45	0/1641	0.77	0/2236
4	M	0.45	0/1660	0.74	0/2261
5	E	0.40	0/4866	0.94	0/6606
5	F	0.41	0/4999	0.95	0/6792
6	R	0.42	0/1655	0.82	0/2251
6	S	0.42	0/1644	0.80	0/2236
All	All	0.43	0/26555	0.84	0/36101

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1624	0	1582	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1624	0	1582	9	0
2	A	1674	0	1628	12	0
2	C	1692	0	1652	12	0
3	L	1627	0	1587	10	0
3	N	1627	0	1587	15	0
4	H	1600	0	1545	10	0
4	M	1619	0	1562	9	0
5	E	4733	0	4507	23	0
5	F	4862	0	4634	44	0
6	R	1609	0	1537	19	0
6	S	1598	0	1525	12	0
7	G	71	0	61	1	0
8	I	60	0	52	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	6	0	0	0	0
9	H	3	0	0	0	0
9	M	5	0	0	0	0
9	N	2	0	0	0	0
9	R	2	0	0	0	0
9	S	3	0	0	0	0
10	L	5	0	0	0	0
10	N	5	0	0	0	0
11	F	2	0	0	0	0
11	H	3	0	0	0	0
11	R	1	0	0	0	0
12	H	12	0	18	0	0
13	N	13	0	18	1	0
14	E	1	0	0	0	0
14	F	1	0	0	0	0
15	E	56	0	52	0	0
15	F	70	0	65	0	0
16	E	10	0	14	0	0
16	S	10	0	14	0	0
17	A	8	0	0	0	0
17	B	32	0	0	0	0
17	C	8	0	0	0	0
17	D	19	0	0	0	0
17	E	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	F	37	0	0	0	0
17	H	12	0	0	0	0
17	L	22	0	0	0	0
17	M	15	0	0	0	0
17	N	11	0	0	0	0
17	R	24	0	0	0	0
17	S	29	0	0	0	0
All	All	26468	0	25222	174	0

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

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:323:MET:HE1	5:F:379:ILE:HG21	1.58	0.84
4:M:219:GLU:HG2	4:M:220:PRO:HD2	1.67	0.75
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.66	0.74
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.71	0.72
6:R:409:GLN:HB3	6:R:419:ALA:HB2	1.75	0.68
2:A:6:GLN:HB3	2:A:121:THR:HG23	1.77	0.65
6:S:354:ASN:HD21	6:S:356:LYS:HE2	1.62	0.65
4:H:70:SER:HB2	4:H:79:TYR:HB2	1.79	0.64
1:B:67:GLY:HA3	1:B:72:PHE:HA	1.80	0.62
5:F:284:PRO:HG3	5:F:440:LEU:HD13	1.80	0.62
2:C:31:SER:HB3	6:S:335:LEU:HD21	1.81	0.61
4:M:166:LEU:HD21	4:M:189:VAL:HG21	1.83	0.60
3:N:21:ILE:HD12	3:N:103:THR:HG21	1.83	0.60
2:C:11:VAL:HG11	2:C:161:PRO:HG3	1.84	0.60
5:F:499:ASP:N	5:F:500:PRO:HD2	2.16	0.59
3:N:107:ILE:HB	3:N:167:GLN:HE22	1.68	0.58
5:F:458:LYS:HG3	5:F:462:MET:HE2	1.85	0.58
6:R:402:ILE:HD12	6:R:418:ILE:HD13	1.86	0.58
5:F:50:TYR:CE1	5:F:59:VAL:HG13	2.38	0.58
2:A:6:GLN:H	2:A:119:GLN:HE22	1.52	0.57
3:N:39:LYS:HB3	3:N:40:PRO:HD2	1.87	0.57
1:B:38:GLN:HB2	1:B:48:LEU:HD11	1.87	0.56
5:E:284:PRO:HG3	5:E:440:LEU:HD13	1.86	0.56
4:M:90:THR:HG23	4:M:117:THR:HA	1.86	0.56
6:S:418:ILE:HA	6:S:422:ASN:HD22	1.70	0.56
2:C:6:GLN:H	2:C:119:GLN:HE22	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:VAL:HG12	2:C:124:THR:HB	1.88	0.55
6:R:402:ILE:HG22	6:R:403:ARG:N	2.22	0.55
5:F:389:PRO:HG2	5:F:392:LEU:HD12	1.89	0.54
4:M:40:THR:HB	4:M:43:LYS:HB2	1.89	0.54
6:R:339:GLY:O	6:R:343:ASN:HB2	2.07	0.54
5:F:490:PRO:HA	5:F:612:PRO:HG2	1.89	0.54
5:F:476:LYS:HG3	5:F:480:MET:HE2	1.90	0.54
5:F:524:GLN:HG2	5:F:583:PRO:HG2	1.90	0.54
3:N:134:VAL:HG22	3:N:179:THR:HG22	1.88	0.54
2:A:11:VAL:HG21	2:A:161:PRO:HG3	1.90	0.54
1:D:50:TYR:HB2	2:C:112:GLY:HA2	1.89	0.53
4:M:56:ASP:HB3	6:S:369:TYR:CG	2.43	0.53
5:E:527:GLU:HA	5:E:539:LEU:HD11	1.90	0.53
5:F:529:LEU:HD11	5:F:554:LEU:HD13	1.90	0.53
4:H:90:THR:HG23	4:H:117:THR:HA	1.88	0.53
6:R:345:THR:HG23	6:R:346:ARG:HG2	1.89	0.53
3:N:35:TRP:HB2	3:N:48:ILE:HB	1.90	0.52
5:E:450:LEU:HB2	5:E:451:PRO:HD3	1.92	0.52
5:E:564:GLU:HB3	5:E:568:LEU:HD23	1.92	0.52
6:R:461:LEU:HD22	6:R:465:GLU:HB3	1.91	0.52
2:C:173:LEU:HD21	2:C:196:VAL:HG21	1.92	0.52
3:L:80:PRO:HA	3:L:107:ILE:HD13	1.90	0.52
4:H:103:TYR:HD1	6:R:382:VAL:HG12	1.75	0.51
3:N:80:PRO:HA	3:N:107:ILE:HD13	1.92	0.51
5:E:525:PHE:HD1	5:E:573:VAL:HG11	1.75	0.51
5:E:499:ASP:N	5:E:500:PRO:CD	2.73	0.51
3:L:39:LYS:HB3	3:L:40:PRO:HD2	1.92	0.51
5:F:455:MET:HG2	5:F:485:VAL:CG2	2.41	0.51
5:F:248:LEU:HD21	5:F:278:LEU:HD11	1.92	0.51
5:F:407:ILE:HA	5:F:410:LEU:HD12	1.92	0.51
7:G:2:NAG:H83	7:G:4:MAN:H61	1.92	0.51
3:N:107:ILE:HB	3:N:167:GLN:NE2	2.26	0.51
5:F:212:VAL:HG11	5:F:565:PRO:HG3	1.93	0.50
5:E:230:PHE:HA	5:E:233:ILE:HD12	1.94	0.50
3:L:10:SER:HB3	3:N:12:SER:HB3	1.94	0.50
6:R:401:VAL:HG22	6:R:509:ARG:HG2	1.93	0.50
2:C:8:GLY:H	2:C:121:THR:HG22	1.77	0.50
5:F:457:GLU:HG2	5:F:513:ILE:HB	1.94	0.50
3:N:147:VAL:HG12	3:N:197:VAL:HG22	1.94	0.50
6:R:421:TYR:CD1	6:R:457:ARG:HB2	2.47	0.49
5:F:564:GLU:HG3	5:F:565:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:THR:HG22	1:D:204:PRO:HG3	1.95	0.49
5:E:503:LEU:HD23	5:E:505:HIS:H	1.78	0.49
5:F:133:CYS:HA	5:F:141:CYS:HA	1.95	0.49
2:A:109:SER:HB2	6:R:345:THR:CG2	2.43	0.49
4:M:22:CYS:HB3	4:M:78:LEU:HB3	1.94	0.49
5:E:472:GLN:HG2	5:E:475:LYS:HE3	1.95	0.49
5:F:455:MET:HG2	5:F:485:VAL:HG21	1.95	0.48
2:A:8:GLY:H	2:A:121:THR:HG22	1.77	0.48
5:F:323:MET:HE1	5:F:379:ILE:CG2	2.37	0.48
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.95	0.48
4:H:2:VAL:HG13	4:H:27:PHE:CD1	2.49	0.48
5:E:77:SER:O	5:E:81:GLN:HG2	2.14	0.48
5:E:97:LEU:O	5:E:101:GLN:HG2	2.14	0.47
5:E:525:PHE:O	5:E:529:LEU:HG	2.14	0.47
5:F:122:THR:O	5:F:126:ILE:HG12	2.15	0.47
2:A:91:THR:HG23	2:A:124:THR:HA	1.95	0.47
3:L:2:ILE:HD12	3:L:93:VAL:HG23	1.96	0.47
6:R:453:TYR:HB3	6:R:495:TYR:CE2	2.49	0.47
6:S:366:SER:HA	6:S:369:TYR:CD2	2.49	0.47
4:M:82:MET:HB3	4:M:85:LEU:HD21	1.96	0.47
5:E:457:GLU:HG2	5:E:513:ILE:HB	1.96	0.47
1:D:132:VAL:HG13	1:D:179:LEU:HB3	1.97	0.46
3:N:6:GLN:HG2	3:N:101:PRO:HD2	1.97	0.46
1:D:67:GLY:HA3	1:D:72:PHE:HA	1.97	0.46
5:E:304:ALA:HA	5:E:307:ILE:HD12	1.97	0.46
4:H:12:VAL:HG11	4:H:85:LEU:HD12	1.97	0.46
5:F:459:TRP:HD1	5:F:480:MET:HE1	1.81	0.46
2:A:166:VAL:HA	2:A:211:ASN:O	2.16	0.46
4:H:22:CYS:HB3	4:H:78:LEU:HB3	1.97	0.46
5:F:200:GLY:O	5:F:204:ARG:HG3	2.15	0.46
4:M:60:PRO:HG2	4:M:63:VAL:HG22	1.97	0.46
2:C:209:ILE:HG12	2:C:224:LYS:HG3	1.98	0.46
5:E:476:LYS:HA	5:E:479:GLU:HB2	1.98	0.46
3:L:93:VAL:HG22	6:R:380:TYR:CE1	2.51	0.45
5:F:233:ILE:HD13	5:F:450:LEU:HD13	1.98	0.45
5:F:459:TRP:HD1	5:F:480:MET:CE	2.29	0.45
1:D:32:THR:HG22	6:S:441:LEU:HD22	1.97	0.45
5:F:582:ARG:N	5:F:583:PRO:CD	2.80	0.45
3:N:109:ARG:HG2	3:N:110:THR:N	2.31	0.45
2:C:8:GLY:H	2:C:121:THR:CG2	2.29	0.45
5:F:108:LEU:O	5:F:109:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:455:LEU:HD22	6:S:493:GLN:HG3	1.99	0.45
1:B:132:VAL:HG13	1:B:179:LEU:HB3	1.99	0.45
2:A:109:SER:HB2	6:R:345:THR:HG21	1.99	0.45
2:A:6:GLN:HB3	2:A:121:THR:CG2	2.44	0.44
2:A:64:PHE:O	2:A:68:VAL:HG12	2.17	0.44
5:E:589:GLU:N	5:E:590:PRO:HD2	2.32	0.44
1:D:38:GLN:HB2	1:D:48:LEU:HD11	1.98	0.44
5:E:458:LYS:HG3	5:E:462:MET:HE2	1.98	0.44
2:C:192:LEU:C	2:C:192:LEU:HD12	2.42	0.44
1:D:19:ALA:HB2	1:D:79:LEU:HD11	2.00	0.44
3:N:143:ARG:HH11	3:N:164:VAL:HG11	1.82	0.44
4:M:126:PRO:HD3	4:M:207:HIS:ND1	2.33	0.44
1:B:36:TRP:CE2	1:B:74:LEU:HB2	2.52	0.44
2:A:215:LYS:N	2:A:216:PRO:CD	2.80	0.44
1:D:136:LEU:HB2	1:D:175:LEU:HB3	2.00	0.43
5:F:554:LEU:HG	5:F:558:LEU:HD11	2.00	0.43
5:E:101:GLN:O	5:E:101:GLN:HG3	2.18	0.43
5:F:589:GLU:N	5:F:590:PRO:HD2	2.34	0.43
1:B:19:ALA:HB2	1:B:79:LEU:HD11	2.00	0.43
2:C:6:GLN:H	2:C:119:GLN:NE2	2.16	0.43
5:E:582:ARG:N	5:E:583:PRO:CD	2.82	0.43
6:S:409:GLN:HB3	6:S:419:ALA:HB2	2.00	0.43
4:H:56:ASP:HB3	6:R:369:TYR:CG	2.54	0.43
3:N:39:LYS:HB3	3:N:40:PRO:CD	2.48	0.43
5:E:351:LEU:HB2	5:E:355:ASP:HB3	1.99	0.43
5:F:261:CYS:HB2	5:F:488:VAL:HB	2.00	0.43
3:L:59:PRO:C	3:L:61:ARG:N	2.77	0.42
4:H:11:LEU:HB2	4:H:154:PRO:HG3	2.02	0.42
6:R:402:ILE:HG22	6:R:403:ARG:O	2.20	0.42
5:F:419:LYS:HG3	5:F:424:LEU:HD23	2.00	0.42
2:C:182:ALA:HA	2:C:192:LEU:HB3	2.01	0.42
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.00	0.42
5:F:501:ALA:O	5:F:507:SER:OG	2.36	0.42
1:B:19:ALA:HB3	1:B:76:ILE:HB	2.01	0.42
3:N:60:SER:HB2	13:N:703:PG4:H72	2.01	0.42
5:F:304:ALA:HA	5:F:307:ILE:HD12	2.02	0.42
5:F:349:TRP:HB3	5:F:351:LEU:HD12	2.02	0.42
5:F:573:VAL:HG13	5:F:574:VAL:HG23	2.02	0.42
1:B:48:LEU:HD23	1:B:59:ILE:HD12	2.01	0.41
5:F:288:LYS:HD2	5:F:433:GLU:HB2	2.01	0.41
5:F:315:PHE:CD1	5:F:380:GLN:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:36:TYR:CE2	3:L:46:LEU:HD23	2.56	0.41
5:F:215:TYR:CZ	5:F:568:LEU:HD13	2.55	0.41
5:F:336:PRO:HB2	5:F:340:GLN:CG	2.50	0.41
1:B:29:VAL:HG13	1:B:93:ASP:HB2	2.02	0.41
4:H:208:LYS:N	4:H:209:PRO:CD	2.84	0.41
5:F:104:GLY:C	5:F:106:SER:H	2.29	0.41
5:F:252:TYR:CZ	5:F:266:LEU:HD22	2.55	0.41
5:F:459:TRP:CD1	5:F:480:MET:HE1	2.56	0.41
6:S:341:VAL:HG11	6:S:397:ALA:HB1	2.03	0.41
2:A:6:GLN:H	2:A:119:GLN:NE2	2.18	0.41
6:S:338:PHE:HE2	6:S:363:ALA:HB1	1.86	0.41
6:S:342:PHE:HB2	8:I:1:NAG:H82	2.03	0.41
5:F:324:THR:HG23	5:F:327:PHE:H	1.86	0.41
6:R:377:PHE:CD1	6:R:434:ILE:HG12	2.56	0.41
6:S:371:SER:HB2	6:S:374:PHE:CD2	2.56	0.41
5:F:312:GLU:O	5:F:316:VAL:HG23	2.21	0.41
6:R:425:LEU:HD21	6:R:512:VAL:HG11	2.02	0.41
4:H:5:VAL:HG13	4:H:112:GLN:HE22	1.86	0.40
5:E:34:HIS:CE1	6:R:493:GLN:HB3	2.56	0.40
5:E:50:TYR:CE1	5:E:59:VAL:HG13	2.56	0.40
1:D:27:GLN:O	1:D:70:THR:HG22	2.21	0.40
1:B:117:ILE:HB	1:B:207:LYS:HB3	2.02	0.40
5:E:478:TRP:HA	5:E:481:LYS:HB2	2.02	0.40
5:F:554:LEU:O	5:F:558:LEU:HG	2.22	0.40
6:R:402:ILE:CG2	6:R:403:ARG:N	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	211/214 (99%)	192 (91%)	17 (8%)	2 (1%)	14 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
2	A	218/230 (95%)	206 (94%)	11 (5%)	1 (0%)	24	52
2	C	220/230 (96%)	210 (96%)	10 (4%)	0	100	100
3	L	211/215 (98%)	197 (93%)	12 (6%)	2 (1%)	14	37
3	N	211/215 (98%)	198 (94%)	12 (6%)	1 (0%)	24	52
4	H	208/223 (93%)	196 (94%)	12 (6%)	0	100	100
4	M	211/223 (95%)	198 (94%)	13 (6%)	0	100	100
5	E	573/597 (96%)	547 (96%)	26 (4%)	0	100	100
5	F	594/597 (100%)	571 (96%)	23 (4%)	0	100	100
6	R	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
6	S	199/204 (98%)	187 (94%)	12 (6%)	0	100	100
All	All	3268/3366 (97%)	3095 (95%)	167 (5%)	6 (0%)	43	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ASP
3	L	30	GLY
1	B	138	ASN
2	A	141	SER
3	L	139	ASN
3	N	40	PRO

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	B	184/185 (100%)	182 (99%)	2 (1%)	65	85
1	D	184/185 (100%)	184 (100%)	0	100	100
2	A	185/192 (96%)	182 (98%)	3 (2%)	55	81
2	C	187/192 (97%)	184 (98%)	3 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	186/188 (99%)	182 (98%)	4 (2%)	45	75
3	N	186/188 (99%)	185 (100%)	1 (0%)	81	92
4	H	177/186 (95%)	174 (98%)	3 (2%)	53	80
4	M	179/186 (96%)	178 (99%)	1 (1%)	78	91
5	E	510/527 (97%)	500 (98%)	10 (2%)	48	77
5	F	526/527 (100%)	518 (98%)	8 (2%)	57	81
6	R	176/177 (99%)	175 (99%)	1 (1%)	78	91
6	S	174/177 (98%)	172 (99%)	2 (1%)	65	85
All	All	2854/2910 (98%)	2816 (99%)	38 (1%)	61	83

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	THR
1	B	96	LEU
2	A	149	THR
2	A	152	LEU
2	A	198	VAL
2	C	51	ILE
2	C	76	THR
2	C	195	VAL
3	L	33	LEU
3	L	46	LEU
3	L	69	THR
3	L	81	GLU
4	H	40	THR
4	H	117	THR
4	H	157	VAL
3	N	118	ILE
4	M	200	THR
5	E	59	VAL
5	E	256	ILE
5	E	303	ASP
5	E	322	ASN
5	E	334	THR
5	E	344	CYS
5	E	400	PHE
5	E	536	GLU
5	E	581	VAL

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Mol	Chain	Res	Type
5	E	611	SER
5	F	22	GLU
5	F	59	VAL
5	F	335	ASP
5	F	385	TYR
5	F	400	PHE
5	F	401	HIS
5	F	573	VAL
5	F	601	ASN
6	R	483	VAL
6	S	362	VAL
6	S	456	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	B	43	GLN
1	B	138	ASN
2	A	39	GLN
2	A	116	ASN
2	A	178	HIS
1	D	39	GLN
1	D	137	ASN
2	C	39	GLN
2	C	116	ASN
2	C	178	HIS
3	L	138	ASN
3	L	148	GLN
3	L	161	GLN
4	H	112	GLN
4	H	171	HIS
3	N	27	GLN
3	N	138	ASN
3	N	167	GLN
3	N	190	HIS
3	N	211	ASN
4	M	171	HIS
4	M	178	GLN
4	M	206	ASN
5	E	24	GLN
5	E	159	ASN

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Mol	Chain	Res	Type
5	E	175	GLN
5	E	210	ASN
5	E	305	GLN
5	E	340	GLN
5	E	508	ASN
5	E	522	GLN
5	E	531	GLN
5	F	42	GLN
5	F	51	ASN
5	F	76	GLN
5	F	159	ASN
5	F	239	HIS
5	F	417	HIS
5	F	522	GLN
5	F	531	GLN
5	F	535	HIS
5	F	572	ASN
5	F	599	ASN
6	R	450	ASN
6	R	460	ASN
6	S	334	ASN
6	S	354	ASN
6	S	360	ASN
6	S	450	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 ⓘ

11 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	$\# Z > 2$
7	NAG	G	1	7,6	14,14,15	0.40	0	17,19,21	0.61	0
7	NAG	G	2	7	14,14,15	0.35	0	17,19,21	0.60	0
7	BMA	G	3	7	11,11,12	0.41	0	15,15,17	0.83	0
7	MAN	G	4	7	11,11,12	0.39	0	15,15,17	0.60	0
7	MAN	G	5	7	11,11,12	0.39	0	15,15,17	0.72	0
7	FUC	G	6	7	10,10,11	0.45	0	14,14,16	0.64	0
8	NAG	I	1	8,6	14,14,15	0.36	0	17,19,21	0.49	0
8	NAG	I	2	8	14,14,15	0.39	0	17,19,21	0.72	0
8	BMA	I	3	8	11,11,12	0.41	0	15,15,17	0.64	0
8	MAN	I	4	8	11,11,12	0.44	0	15,15,17	0.81	0
8	FUC	I	5	8	10,10,11	0.39	0	14,14,16	0.47	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
7	NAG	G	1	7,6	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	MAN	G	5	7	1/1/4/5	0/2/19/22	0/1/1/1
7	FUC	G	6	7	-	-	0/1/1/1
8	NAG	I	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	4/6/23/26	0/1/1/1
8	BMA	I	3	8	-	2/2/19/22	0/1/1/1
8	MAN	I	4	8	-	2/2/19/22	0/1/1/1
8	FUC	I	5	8	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	5	MAN	C1

All (12) torsion outliers are listed below:

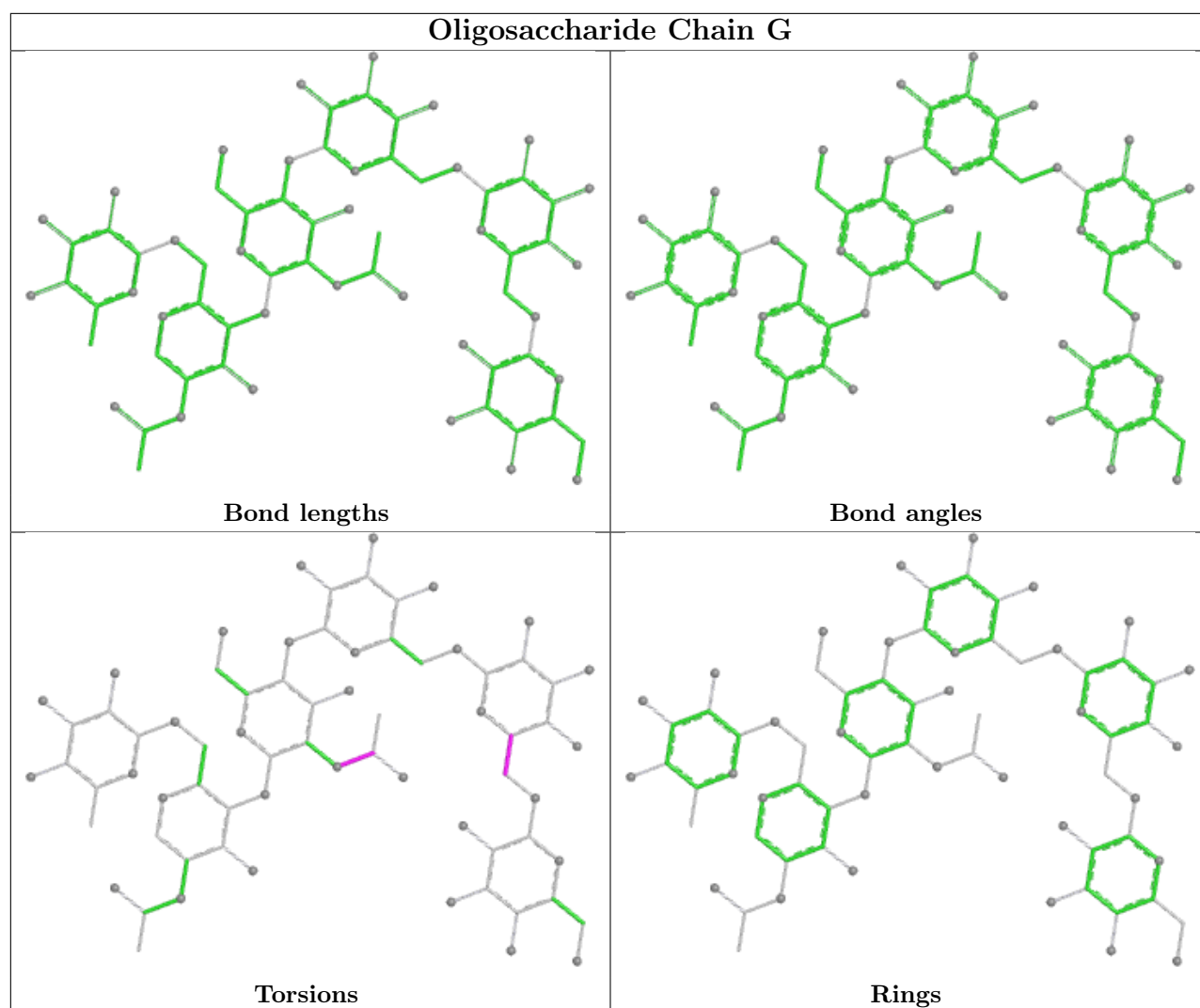
Mol	Chain	Res	Type	Atoms
8	I	2	NAG	O7-C7-N2-C2
8	I	2	NAG	C8-C7-N2-C2
7	G	4	MAN	O5-C5-C6-O6
8	I	2	NAG	O5-C5-C6-O6
7	G	4	MAN	C4-C5-C6-O6
8	I	2	NAG	C4-C5-C6-O6
8	I	4	MAN	O5-C5-C6-O6
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
8	I	4	MAN	C4-C5-C6-O6
8	I	3	BMA	C4-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6

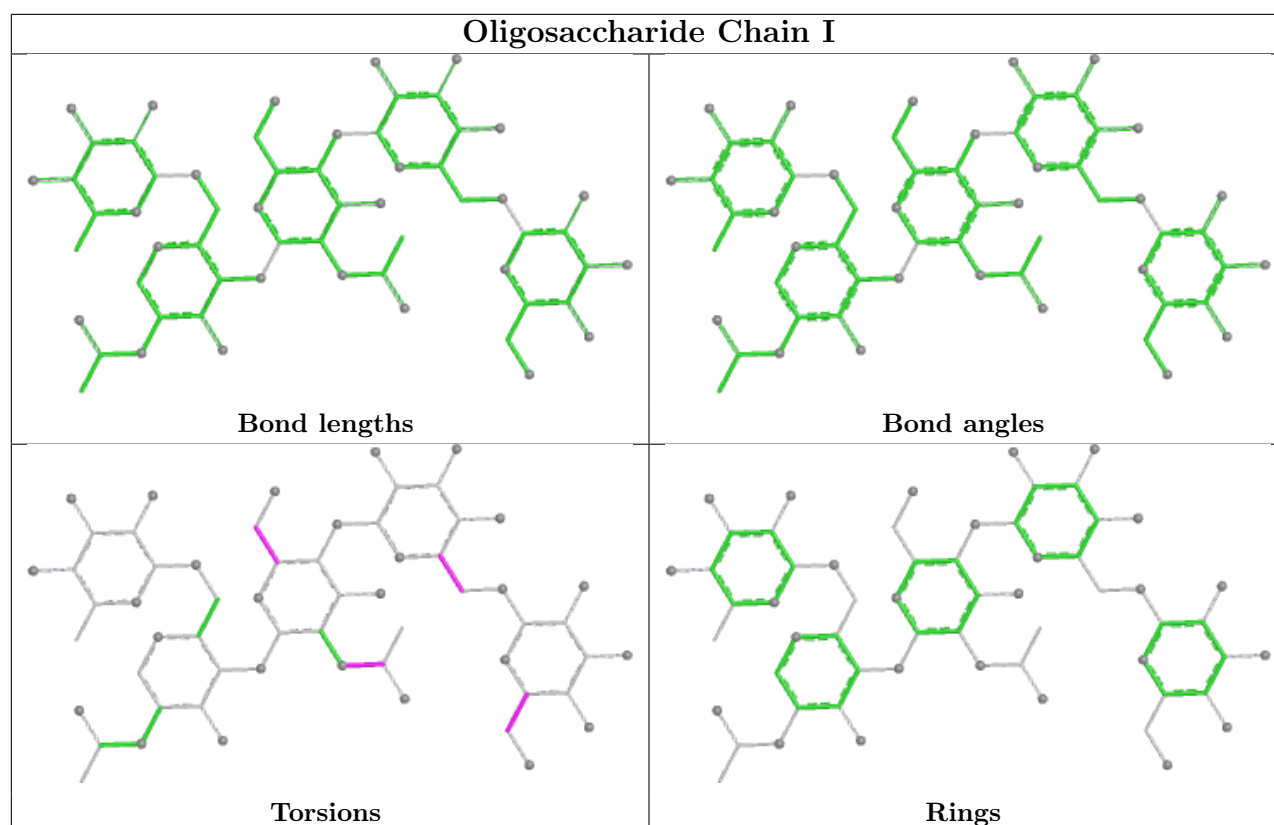
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	NAG	1	0
7	G	4	MAN	1	0
7	G	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](#)

Of 50 ligands modelled in this entry, 35 are monoatomic - leaving 15 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
15	NAG	F	705	5	14,14,15	0.35	0	17,19,21	0.85	1 (5%)
10	SO4	N	700	-	4,4,4	0.34	0	6,6,6	0.07	0
12	PG5	H	702	-	11,11,11	0.19	0	10,10,10	0.09	0
10	SO4	L	700	-	4,4,4	0.34	0	6,6,6	0.07	0
15	NAG	F	703	5	14,14,15	0.37	0	17,19,21	0.69	0
13	PG4	N	703	-	12,12,12	0.18	0	11,11,11	0.07	0
16	PGE	S	602	-	9,9,9	0.17	0	8,8,8	0.10	0
16	PGE	E	706	-	9,9,9	0.14	0	8,8,8	0.09	0
15	NAG	E	704	5	14,14,15	0.49	0	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	E	703	5	14,14,15	0.37	0	17,19,21	0.86	1 (5%)
15	NAG	E	702	5	14,14,15	0.45	0	17,19,21	0.91	1 (5%)
15	NAG	F	702	5	14,14,15	0.38	0	17,19,21	0.71	0
15	NAG	F	704	5	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
15	NAG	E	705	5	14,14,15	0.43	0	17,19,21	1.31	1 (5%)
15	NAG	F	706	5	14,14,15	0.34	0	17,19,21	0.83	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
15	NAG	F	705	5	-	2/6/23/26	0/1/1/1
12	PG5	H	702	-	-	6/9/9/9	-
16	PGE	S	602	-	-	5/7/7/7	-
15	NAG	F	703	5	-	2/6/23/26	0/1/1/1
13	PG4	N	703	-	-	5/10/10/10	-
16	PGE	E	706	-	-	2/7/7/7	-
15	NAG	E	704	5	-	4/6/23/26	0/1/1/1
15	NAG	E	703	5	-	2/6/23/26	0/1/1/1
15	NAG	E	702	5	-	2/6/23/26	0/1/1/1
15	NAG	F	702	5	-	2/6/23/26	0/1/1/1
15	NAG	F	704	5	-	0/6/23/26	0/1/1/1
15	NAG	E	705	5	-	2/6/23/26	0/1/1/1
15	NAG	F	706	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	705	NAG	C1-O5-C5	4.64	118.40	112.19
15	F	705	NAG	C1-O5-C5	2.77	115.90	112.19
15	E	704	NAG	C4-C3-C2	2.71	115.00	111.02
15	E	702	NAG	C4-C3-C2	2.59	114.81	111.02
15	E	703	NAG	C4-C3-C2	2.40	114.54	111.02
15	F	704	NAG	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	702	NAG	C8-C7-N2-C2
15	E	702	NAG	O7-C7-N2-C2
15	E	703	NAG	C8-C7-N2-C2
15	E	703	NAG	O7-C7-N2-C2
15	E	704	NAG	C8-C7-N2-C2
15	E	704	NAG	O7-C7-N2-C2
15	F	705	NAG	C8-C7-N2-C2
15	F	705	NAG	O7-C7-N2-C2
15	F	706	NAG	C4-C5-C6-O6
12	H	702	PG5	O2-C4-C5-O3
13	N	703	PG4	O3-C5-C6-O4
15	F	706	NAG	O5-C5-C6-O6
16	S	602	PGE	O2-C3-C4-O3
12	H	702	PG5	O1-C2-C3-O2
15	F	702	NAG	O5-C5-C6-O6
15	E	705	NAG	O5-C5-C6-O6
16	S	602	PGE	O3-C5-C6-O4
15	F	702	NAG	C4-C5-C6-O6
13	N	703	PG4	O4-C7-C8-O5
15	F	703	NAG	C8-C7-N2-C2
15	E	705	NAG	C4-C5-C6-O6
15	F	706	NAG	C8-C7-N2-C2
15	E	704	NAG	C1-C2-N2-C7
16	S	602	PGE	C3-C4-O3-C5
13	N	703	PG4	C1-C2-O2-C3
16	E	706	PGE	C6-C5-O3-C4
15	F	703	NAG	O7-C7-N2-C2
15	F	706	NAG	O7-C7-N2-C2
12	H	702	PG5	C4-C5-O3-C6
12	H	702	PG5	C6-C7-O4-C8
15	E	704	NAG	C3-C2-N2-C7
12	H	702	PG5	O3-C6-C7-O4
16	E	706	PGE	C3-C4-O3-C5
12	H	702	PG5	C3-C2-O1-C1
13	N	703	PG4	C8-C7-O4-C6
13	N	703	PG4	C5-C6-O4-C7
16	S	602	PGE	O1-C1-C2-O2
16	S	602	PGE	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N	703	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	B	213/214 (99%)	1.26	41 (19%) 3 2	58, 74, 97, 109	0
1	D	213/214 (99%)	1.20	29 (13%) 7 5	55, 73, 92, 106	0
2	A	222/230 (96%)	1.30	38 (17%) 4 3	61, 78, 96, 114	0
2	C	224/230 (97%)	1.45	49 (21%) 2 2	61, 85, 101, 106	0
3	L	213/215 (99%)	0.95	19 (8%) 15 12	49, 68, 122, 133	0
3	N	213/215 (99%)	0.88	19 (8%) 15 12	45, 66, 108, 126	0
4	H	212/223 (95%)	1.15	29 (13%) 6 5	47, 83, 105, 126	0
4	M	215/223 (96%)	1.00	15 (6%) 22 18	45, 72, 94, 128	0
5	E	579/597 (96%)	1.87	228 (39%) 1 0	64, 116, 162, 189	0
5	F	596/597 (99%)	1.31	105 (17%) 4 3	55, 84, 111, 149	0
6	R	203/204 (99%)	1.35	38 (18%) 3 2	50, 73, 101, 125	0
6	S	201/204 (98%)	1.23	34 (16%) 4 3	47, 71, 99, 114	0
All	All	3304/3366 (98%)	1.32	644 (19%) 3 2	45, 80, 138, 189	0

All (644) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	146	PRO	5.5
1	B	63	PHE	5.4
5	E	506	VAL	5.2
2	C	26	GLY	5.1
5	E	298	VAL	5.1
3	L	213	GLY	5.0
6	S	528	LYS	5.0
5	E	258	PRO	4.9
5	E	267	LEU	4.9
5	F	614	ALA	4.9
5	F	430	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
2	C	203	LEU	4.7
3	N	213	GLY	4.6
5	E	180	TYR	4.6
5	E	168	TRP	4.6
5	E	271	TRP	4.5
6	S	505	TYR	4.5
6	R	530	SER	4.3
2	C	143	LYS	4.3
5	E	256	ILE	4.3
5	F	135	PRO	4.3
5	E	272	GLY	4.3
2	A	228	LYS	4.3
5	E	257	SER	4.3
5	E	603	PHE	4.2
5	E	297	MET	4.2
6	R	529	LYS	4.2
2	C	130	THR	4.2
5	F	339	VAL	4.2
5	E	614	ALA	4.1
2	C	202	SER	4.1
5	F	103	ASN	4.1
5	E	446	ILE	4.1
6	R	475	ALA	4.1
1	B	35	ALA	4.0
2	C	148	GLY	4.0
5	E	592	PHE	4.0
5	F	428	PHE	4.0
5	E	130	GLY	3.9
6	S	346	ARG	3.9
5	F	344	CYS	3.9
4	M	222	SER	3.9
6	S	490	PHE	3.9
6	R	505	TYR	3.9
5	E	289	PRO	3.9
5	E	496	THR	3.9
5	E	266	LEU	3.9
2	C	228	LYS	3.8
3	N	126	LEU	3.8
5	E	116	LEU	3.8
5	E	183	TYR	3.8
5	F	92	THR	3.7
5	E	590	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	148	GLN	3.7
5	E	454	TYR	3.7
6	R	413	GLY	3.7
5	E	126	ILE	3.7
5	E	123	MET	3.6
2	A	225	VAL	3.6
5	E	30	ASP	3.6
5	E	104	GLY	3.6
5	E	441	LYS	3.6
5	E	105	SER	3.6
5	E	290	ASN	3.5
4	M	221	LYS	3.5
5	E	484	ILE	3.5
5	E	447	VAL	3.5
5	E	365	THR	3.5
2	C	121	THR	3.5
5	E	432	ASN	3.5
5	E	600	LYS	3.5
5	F	416	LYS	3.5
5	E	548	THR	3.4
6	S	518	LEU	3.4
6	R	329	PHE	3.4
6	R	468	ILE	3.4
4	M	196	LEU	3.4
2	C	224	LYS	3.4
4	H	200	THR	3.4
5	E	56	GLU	3.4
5	E	485	VAL	3.4
5	F	498	CYS	3.3
5	E	274	PHE	3.3
5	E	451	PRO	3.3
5	E	342	ALA	3.3
6	S	526	GLY	3.3
5	E	187	LYS	3.3
5	E	523	PHE	3.3
5	F	364	VAL	3.3
5	E	606	TRP	3.3
5	F	336	PRO	3.3
6	R	517	LEU	3.3
2	A	204	GLY	3.3
5	E	301	ALA	3.3
5	E	275	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
6	R	482	GLY	3.3
1	D	65	GLY	3.2
5	F	343	VAL	3.2
5	E	440	LEU	3.2
5	F	102	GLN	3.2
2	C	2	VAL	3.2
5	E	544	ILE	3.2
2	C	74	THR	3.2
5	E	473	TRP	3.2
5	E	314	PHE	3.2
5	E	339	VAL	3.2
5	E	470	LYS	3.2
5	E	605	GLY	3.2
5	E	103	ASN	3.1
6	S	523	THR	3.1
5	E	291	ILE	3.1
5	E	308	PHE	3.1
3	N	127	LYS	3.1
5	E	169	ARG	3.1
5	E	238	GLU	3.1
6	R	528	LYS	3.1
1	B	21	LEU	3.1
5	E	162	LEU	3.1
2	A	227	PRO	3.1
4	H	198	THR	3.1
5	E	304	ALA	3.1
5	E	108	LEU	3.1
5	E	322	ASN	3.1
5	E	263	PRO	3.1
5	E	337	GLY	3.1
5	F	603	PHE	3.1
5	E	450	LEU	3.0
5	E	453	THR	3.0
5	E	504	PHE	3.0
5	E	186	LEU	3.0
5	F	180	TYR	3.0
5	F	194	ASN	3.0
5	E	421	ILE	3.0
5	F	270	MET	3.0
5	F	132	VAL	3.0
5	E	346	PRO	3.0
2	C	9	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	413	ALA	3.0
2	C	221	VAL	3.0
3	L	195	CYS	3.0
5	E	149	ASN	3.0
5	E	50	TYR	3.0
1	D	61	ASP	3.0
1	D	18	ARG	3.0
5	E	438	PHE	3.0
5	E	410	LEU	2.9
6	S	517	LEU	2.9
2	C	227	PRO	2.9
5	E	112	LYS	2.9
4	H	132	ALA	2.9
6	R	483	VAL	2.9
5	E	520	LEU	2.9
1	B	82	GLU	2.9
1	D	107	LYS	2.9
2	A	168	TRP	2.9
1	B	89	CYS	2.9
2	A	85	ARG	2.9
6	S	328	ARG	2.9
5	E	513	ILE	2.9
5	E	445	THR	2.9
5	F	52	THR	2.9
5	E	264	ALA	2.9
1	B	64	SER	2.9
1	B	58	GLY	2.9
5	E	336	PRO	2.9
2	A	202	SER	2.9
5	E	252	TYR	2.9
5	E	248	LEU	2.9
5	F	424	LEU	2.9
2	A	199	PRO	2.8
1	D	36	TRP	2.8
5	F	50	TYR	2.8
5	E	370	LEU	2.8
5	E	452	PHE	2.8
1	B	41	PRO	2.8
2	C	199	PRO	2.8
5	E	518	ARG	2.8
3	N	157	SER	2.8
5	F	307	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	586	ASN	2.8
2	C	174	THR	2.8
5	E	362	THR	2.8
5	E	501	ALA	2.8
5	F	304	ALA	2.8
6	R	473	TYR	2.8
2	C	51	ILE	2.8
2	A	142	SER	2.8
2	C	171	GLY	2.8
2	A	96	CYS	2.8
4	M	95	CYS	2.8
5	E	492	PRO	2.8
5	E	442	GLN	2.8
6	S	468	ILE	2.8
2	C	170	SER	2.8
5	F	269	ASP	2.8
3	L	192	VAL	2.8
5	E	52	THR	2.8
5	E	369	PHE	2.8
2	C	216	PRO	2.7
5	F	131	LYS	2.7
2	C	201	SER	2.7
5	E	286	GLY	2.7
5	E	364	VAL	2.7
6	S	486	PHE	2.7
5	E	83	TYR	2.7
4	H	64	LYS	2.7
2	A	173	LEU	2.7
4	H	196	LEU	2.7
5	F	345	HIS	2.7
5	E	293	VAL	2.7
5	E	343	VAL	2.7
5	F	390	PHE	2.7
3	N	205	PRO	2.7
6	S	480	CYS	2.7
5	F	152	MET	2.7
5	E	268	GLY	2.7
6	S	519	HIS	2.7
5	F	163	TRP	2.7
4	H	143	ALA	2.7
6	R	522	ALA	2.7
5	F	471	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
6	S	364	ASP	2.7
6	S	389	ASP	2.7
5	E	426	PRO	2.7
6	R	421	TYR	2.7
5	E	261	CYS	2.7
2	A	66	GLY	2.7
4	M	1	GLU	2.7
2	A	205	THR	2.7
3	N	1	ASP	2.7
5	E	490	PRO	2.7
1	D	50	TYR	2.6
5	E	202	TYR	2.6
5	F	183	TYR	2.6
5	E	391	LEU	2.6
5	E	498	CYS	2.6
2	A	79	GLY	2.6
2	A	226	GLU	2.6
4	H	221	LYS	2.6
2	C	24	ALA	2.6
2	C	151	ALA	2.6
5	F	109	SER	2.6
5	F	302	TRP	2.6
6	R	367	VAL	2.6
5	F	346	PRO	2.6
2	C	158	ASP	2.6
5	E	199	TYR	2.6
5	E	179	LEU	2.6
5	E	333	LEU	2.6
5	F	456	LEU	2.6
5	E	530	CYS	2.6
6	R	480	CYS	2.6
5	E	147	GLY	2.6
5	E	231	GLU	2.6
5	E	553	LYS	2.6
5	F	489	GLU	2.6
2	C	68	VAL	2.6
4	H	87	ALA	2.6
5	F	434	THR	2.6
3	N	161	GLN	2.6
5	F	30	ASP	2.6
5	E	88	ILE	2.6
1	D	48	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	444	LEU	2.6
5	F	108	LEU	2.6
1	B	55	ARG	2.6
2	A	224	LYS	2.6
5	E	475	LYS	2.6
1	B	157	GLY	2.6
2	A	176	GLY	2.6
4	H	197	GLY	2.6
1	B	36	TRP	2.6
2	C	219	THR	2.6
5	E	269	ASP	2.6
5	E	579	MET	2.6
5	F	259	ILE	2.6
5	E	273	ARG	2.6
2	A	2	VAL	2.6
5	E	107	VAL	2.6
5	E	491	VAL	2.6
6	R	486	PHE	2.6
1	D	57	THR	2.5
5	E	109	SER	2.5
5	E	349	TRP	2.5
1	B	59	ILE	2.5
1	B	47	LEU	2.5
2	A	152	LEU	2.5
5	E	255	TYR	2.5
5	E	184	VAL	2.5
6	R	445	VAL	2.5
5	E	464	PHE	2.5
1	D	197	THR	2.5
5	F	334	THR	2.5
6	R	470	THR	2.5
5	F	136	ASP	2.5
2	A	34	ILE	2.5
5	E	468	ILE	2.5
2	C	220	LYS	2.5
6	R	518	LEU	2.5
2	C	100	TYR	2.5
4	H	9	GLY	2.5
5	F	399	GLY	2.5
5	E	296	ALA	2.5
1	D	172	THR	2.5
4	H	40	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	128	SER	2.5
2	A	84	ARG	2.5
5	E	514	ARG	2.5
5	E	584	LEU	2.5
5	E	515	TYR	2.5
1	D	58	GLY	2.5
1	D	41	PRO	2.5
1	B	160	GLN	2.5
3	N	154	ALA	2.5
5	F	305	GLN	2.5
6	S	329	PHE	2.5
2	A	116	ASN	2.5
5	E	476	LYS	2.5
5	E	151	ILE	2.5
6	R	418	ILE	2.5
5	E	335	ASP	2.5
5	E	610	TRP	2.5
6	R	364	ASP	2.5
3	L	144	GLU	2.5
5	E	500	PRO	2.5
5	E	510	TYR	2.5
5	E	462	MET	2.5
2	C	5	VAL	2.5
5	E	26	LYS	2.4
4	M	190	THR	2.4
5	E	529	LEU	2.4
6	S	332	ILE	2.4
5	F	168	TRP	2.4
2	C	8	GLY	2.4
5	E	587	TYR	2.4
1	B	40	LYS	2.4
2	C	11	VAL	2.4
5	E	416	LYS	2.4
5	F	98	GLN	2.4
5	F	112	LYS	2.4
4	H	175	ALA	2.4
5	E	246	ALA	2.4
5	E	443	ALA	2.4
6	R	419	ALA	2.4
5	E	324	THR	2.4
5	E	51	ASN	2.4
5	E	280	SER	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	505	HIS	2.4
5	E	160	GLU	2.4
5	F	435	GLU	2.4
4	M	133	PRO	2.4
3	L	127	LYS	2.4
6	R	524	VAL	2.4
6	R	452	LEU	2.4
6	R	472	ILE	2.4
5	E	374	HIS	2.4
1	B	77	SER	2.4
2	C	126	SER	2.4
5	F	138	PRO	2.4
4	H	67	PHE	2.4
5	F	403	ALA	2.4
5	F	413	ALA	2.4
5	F	533	ALA	2.4
6	R	346	ARG	2.4
1	B	76	ILE	2.4
1	D	47	LEU	2.4
5	F	423	LEU	2.4
6	R	390	LEU	2.4
1	B	168	SER	2.4
5	F	19	SER	2.4
5	F	105	SER	2.4
3	L	146	LYS	2.4
4	M	43	LYS	2.4
1	B	81	PRO	2.4
5	F	258	PRO	2.4
2	A	93	VAL	2.4
5	E	204	ARG	2.4
2	A	172	ALA	2.4
5	E	348	ALA	2.4
5	E	403	ALA	2.4
5	E	525	PHE	2.4
1	B	50	TYR	2.3
5	E	45	LEU	2.3
5	F	143	LEU	2.3
4	H	117	THR	2.3
5	E	294	THR	2.3
6	R	531	THR	2.3
5	E	197	GLU	2.3
4	H	213	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	309	LYS	2.3
5	F	111	ASP	2.3
1	D	194	CYS	2.3
4	H	133	PRO	2.3
5	E	415	PRO	2.3
6	R	499	PRO	2.3
5	E	221	GLN	2.3
5	F	164	ALA	2.3
6	S	363	ALA	2.3
2	A	101	THR	2.3
4	H	50	THR	2.3
1	D	213	GLU	2.3
1	D	7	SER	2.3
2	A	148	GLY	2.3
3	N	148	GLN	2.3
4	H	86	ARG	2.3
5	E	377	GLY	2.3
5	E	361	CYS	2.3
1	D	21	LEU	2.3
5	E	539	LEU	2.3
5	F	550	ALA	2.3
6	R	441	LEU	2.3
5	E	233	ILE	2.3
4	M	103	TYR	2.3
5	E	27	THR	2.3
5	F	548	THR	2.3
2	A	10	GLU	2.3
5	F	238	GLU	2.3
5	F	341	LYS	2.3
6	S	444	LYS	2.3
2	C	116	ASN	2.3
5	E	292	ASP	2.3
6	S	330	PRO	2.3
1	D	23	CYS	2.3
5	E	172	VAL	2.3
6	R	350	VAL	2.3
5	E	120	LEU	2.3
6	R	455	LEU	2.3
6	S	390	LEU	2.3
5	F	25	ALA	2.3
5	F	301	ALA	2.3
5	F	348	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	569	ALA	2.3
3	L	198	THR	2.3
3	N	191	LYS	2.3
4	M	213	LYS	2.3
5	E	270	MET	2.3
5	E	313	LYS	2.3
1	B	83	ASP	2.3
2	A	88	SER	2.3
3	N	40	PRO	2.3
5	E	98	GLN	2.3
1	B	148	TRP	2.3
2	C	15	GLY	2.3
3	L	41	GLY	2.3
4	H	169	GLY	2.3
1	B	34	LEU	2.3
5	E	236	LEU	2.3
6	R	512	VAL	2.3
5	E	230	PHE	2.3
5	E	390	PHE	2.3
1	D	35	ALA	2.2
3	L	154	ALA	2.2
3	L	185	ALA	2.2
1	B	28	THR	2.2
4	M	200	THR	2.2
1	B	173	TYR	2.2
1	B	18	ARG	2.2
2	C	84	ARG	2.2
1	B	8	PRO	2.2
1	B	156	SER	2.2
3	L	91	SER	2.2
5	E	170	SER	2.2
5	F	340	GLN	2.2
6	S	366	SER	2.2
5	F	268	GLY	2.2
2	C	173	LEU	2.2
5	E	424	LEU	2.2
4	H	69	ILE	2.2
5	F	553	LYS	2.2
6	S	347	PHE	2.2
4	H	144	ALA	2.2
5	E	191	ALA	2.2
5	E	540	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	576	ALA	2.2
6	S	525	CYS	2.2
1	D	109	THR	2.2
2	C	149	THR	2.2
5	E	253	PRO	2.2
1	B	42	GLY	2.2
2	C	25	SER	2.2
3	N	129	GLY	2.2
4	H	168	SER	2.2
4	M	62	SER	2.2
2	A	203	LEU	2.2
5	E	604	VAL	2.2
5	F	298	VAL	2.2
6	S	483	VAL	2.2
1	B	2	ILE	2.2
2	A	209	ILE	2.2
1	D	184	ALA	2.2
1	B	165	GLU	2.2
5	E	129	THR	2.2
5	E	414	THR	2.2
5	F	141	CYS	2.2
5	F	146	PRO	2.2
2	C	79	GLY	2.2
2	C	122	LEU	2.2
5	E	114	LYS	2.2
5	F	286	GLY	2.2
5	F	335	ASP	2.2
6	R	496	GLY	2.2
5	E	545	SER	2.2
5	F	511	SER	2.2
6	S	335	LEU	2.2
2	A	221	VAL	2.2
2	C	177	VAL	2.2
5	E	171	GLU	2.2
5	E	334	THR	2.2
5	E	344	CYS	2.2
3	L	159	ASN	2.2
5	F	134	ASN	2.2
6	S	521	PRO	2.2
5	E	102	GLN	2.2
5	E	522	GLN	2.2
5	E	534	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	N	155	LEU	2.2
5	E	156	LEU	2.2
5	E	439	LEU	2.2
5	E	591	LEU	2.2
6	S	482	GLY	2.2
5	E	499	ASP	2.2
4	H	194	SER	2.2
6	S	477	SER	2.2
5	E	417	HIS	2.2
5	F	34	HIS	2.2
3	N	194	ALA	2.1
5	F	311	ALA	2.1
5	E	92	THR	2.1
2	C	154	CYS	2.1
1	B	60	PRO	2.1
5	E	61	ASN	2.1
5	E	531	GLN	2.1
5	F	601	ASN	2.1
2	C	27	TYR	2.1
5	F	237	TYR	2.1
2	A	70	MET	2.1
5	E	456	LEU	2.1
5	F	142	LEU	2.1
5	F	520	LEU	2.1
5	E	319	GLY	2.1
4	M	69	ILE	2.1
5	E	373	HIS	2.1
5	E	436	ILE	2.1
5	E	543	ASP	2.1
6	S	373	SER	2.1
5	F	512	PHE	2.1
1	D	19	ALA	2.1
1	B	180	THR	2.1
2	C	205	THR	2.1
1	D	45	PRO	2.1
2	C	13	LYS	2.1
4	H	14	PRO	2.1
5	E	465	LYS	2.1
6	R	507	PRO	2.1
1	B	13	LEU	2.1
1	B	79	LEU	2.1
3	L	126	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	153	ASN	2.1
6	R	422	ASN	2.1
6	S	388	ASN	2.1
2	A	118	GLY	2.1
2	C	112	GLY	2.1
5	E	295	ASP	2.1
5	E	307	ILE	2.1
5	F	421	ILE	2.1
1	B	118	PHE	2.1
1	D	118	PHE	2.1
3	N	128	SER	2.1
4	H	62	SER	2.1
5	E	607	SER	2.1
5	F	525	PHE	2.1
5	E	163	TRP	2.1
2	A	219	THR	2.1
3	N	208	LYS	2.1
5	E	558	LEU	2.1
5	F	267	LEU	2.1
2	C	210	CYS	2.1
5	F	210	ASN	2.1
3	L	66	GLY	2.1
4	H	51	ILE	2.1
5	E	244	VAL	2.1
2	C	222	ASP	2.1
1	B	54	SER	2.1
1	D	203	SER	2.1
4	M	74	ALA	2.1
5	E	164	ALA	2.1
5	F	547	SER	2.1
6	S	372	ALA	2.1
1	D	169	LYS	2.1
1	B	57	THR	2.1
4	H	190	THR	2.1
5	F	78	THR	2.1
3	N	95	PRO	2.1
5	E	480	MET	2.1
5	F	579	MET	2.1
1	D	13	LEU	2.1
2	C	152	LEU	2.1
5	E	148	LEU	2.1
5	F	144	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	66	GLY	2.1
1	D	106	ILE	2.1
5	E	54	ILE	2.1
5	F	88	ILE	2.1
5	F	544	ILE	2.1
4	H	191	VAL	2.1
2	A	222	ASP	2.0
3	L	1	ASP	2.0
5	E	167	SER	2.0
5	E	218	SER	2.0
5	E	165	TRP	2.0
5	F	389	PRO	2.0
3	L	155	LEU	2.0
5	E	81	GLN	2.0
5	E	101	GLN	2.0
5	E	423	LEU	2.0
5	F	333	LEU	2.0
5	E	154	ASN	2.0
5	E	599	ASN	2.0
2	A	120	GLY	2.0
4	M	55	GLY	2.0
5	F	104	GLY	2.0
1	B	88	TYR	2.0
2	A	80	TYR	2.0
2	A	100	TYR	2.0
5	F	485	VAL	2.0
5	F	497	TYR	2.0
5	F	515	TYR	2.0
5	F	587	TYR	2.0
6	S	391	CYS	2.0
6	S	524	VAL	2.0
1	B	62	ARG	2.0
5	E	400	PHE	2.0
5	F	464	PHE	2.0
3	N	183	SER	2.0
5	E	331	SER	2.0
5	E	602	SER	2.0
5	F	425	SER	2.0
5	E	608	THR	2.0
5	F	294	THR	2.0
1	B	27	GLN	2.0
3	L	136	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
6	R	487	ASN	2.0
1	D	62	ARG	2.0
4	H	63	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](#)

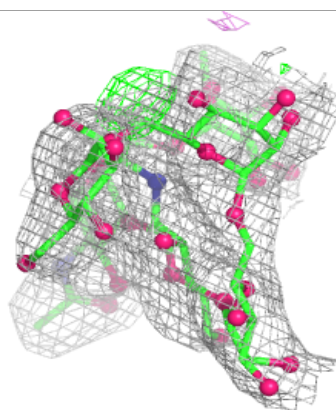
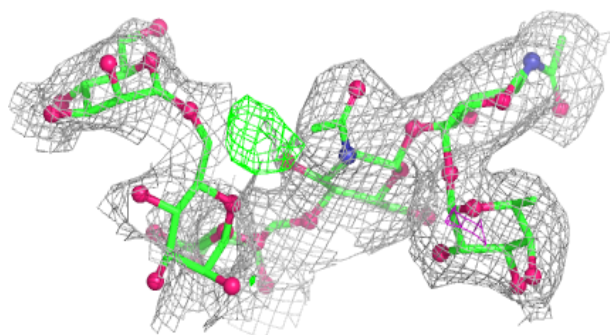
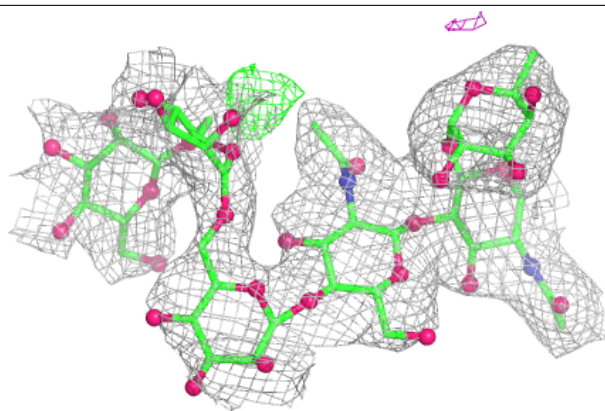
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	G	1	14/15	-	-	72,75,79,82	0
7	NAG	G	2	14/15	-	-	89,92,95,102	0
7	BMA	G	3	11/12	-	-	117,123,128,135	0
7	MAN	G	4	11/12	-	-	148,150,152,152	0
7	MAN	G	5	11/12	-	-	144,149,150,150	0
7	FUC	G	6	10/11	-	-	79,80,80,81	0
8	NAG	I	1	14/15	-	-	78,80,82,87	0
8	NAG	I	2	14/15	-	-	91,98,102,108	0
8	BMA	I	3	11/12	-	-	122,127,131,132	0
8	MAN	I	4	11/12	-	-	140,144,146,147	0
8	FUC	I	5	10/11	-	-	74,75,76,76	0

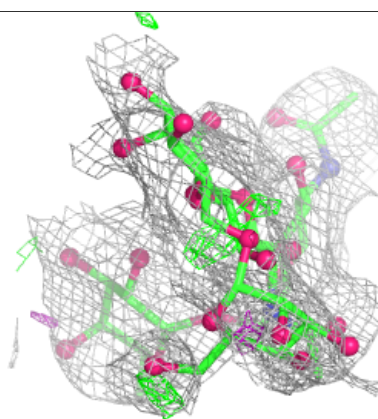
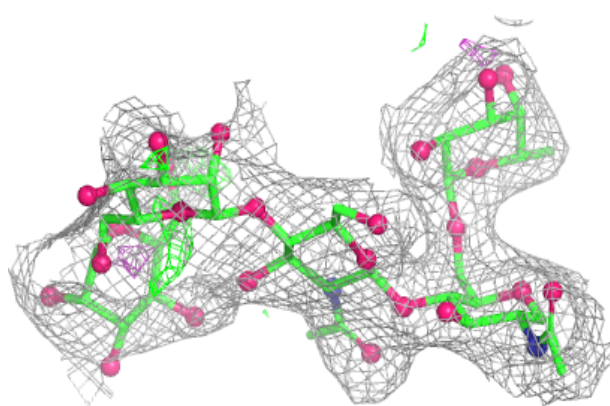
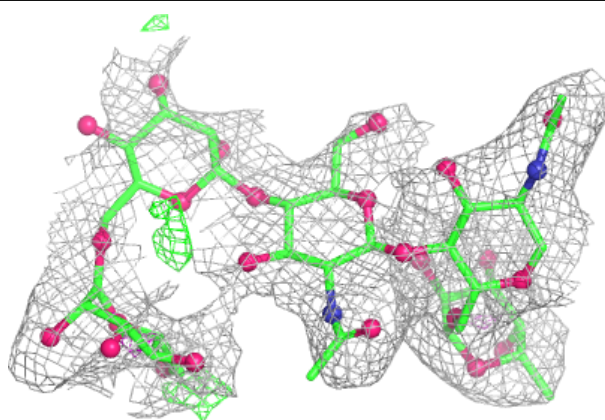
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 ⓘ

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
15	NAG	E	704	14/15	0.54	0.23	121,127,130,131	0
15	NAG	F	705	14/15	0.68	0.16	99,101,102,103	0
15	NAG	E	702	14/15	0.70	0.18	133,140,143,145	0
15	NAG	F	706	14/15	0.74	0.15	135,137,137,138	0
15	NAG	E	703	14/15	0.76	0.19	97,98,99,100	0
15	NAG	F	703	14/15	0.77	0.18	85,86,88,89	0
15	NAG	E	705	14/15	0.78	0.15	99,102,105,105	0
9	CL	M	303	1/1	0.80	0.14	113,113,113,113	0
15	NAG	F	702	14/15	0.81	0.16	100,102,106,107	0
12	PG5	H	702	12/12	0.81	0.34	116,120,122,122	0
16	PGE	S	602	10/10	0.81	0.23	97,103,109,110	0
9	CL	N	702	1/1	0.82	0.29	114,114,114,114	0
10	SO4	L	700	5/5	0.83	0.20	158,158,159,159	0
16	PGE	E	706	10/10	0.83	0.18	91,96,98,98	0
11	NA	F	711	1/1	0.83	0.14	84,84,84,84	0
9	CL	F	713	1/1	0.84	0.17	117,117,117,117	0
13	PG4	N	703	13/13	0.84	0.19	84,94,96,96	0
10	SO4	N	700	5/5	0.85	0.15	139,139,139,139	0
9	CL	C	701	1/1	0.86	0.16	105,105,105,105	0
15	NAG	F	704	14/15	0.86	0.13	94,97,99,100	0
9	CL	M	305	1/1	0.88	0.19	97,97,97,97	0
11	NA	R	603	1/1	0.89	0.08	50,50,50,50	0
11	NA	F	708	1/1	0.90	0.25	90,90,90,90	0
9	CL	H	707	1/1	0.91	0.16	113,113,113,113	0
9	CL	R	602	1/1	0.91	0.18	105,105,105,105	0
9	CL	M	302	1/1	0.91	0.11	88,88,88,88	0
9	CL	F	709	1/1	0.91	0.19	101,101,101,101	0
9	CL	A	301	1/1	0.92	0.16	98,98,98,98	0
9	CL	M	301	1/1	0.93	0.08	67,67,67,67	0
9	CL	F	710	1/1	0.94	0.09	66,66,66,66	0
9	CL	R	601	1/1	0.94	0.12	95,95,95,95	0
9	CL	F	712	1/1	0.94	0.12	91,91,91,91	0
9	CL	S	604	1/1	0.95	0.14	103,103,103,103	0
11	NA	H	704	1/1	0.95	0.07	56,56,56,56	0
9	CL	M	304	1/1	0.95	0.16	95,95,95,95	0
9	CL	H	706	1/1	0.96	0.07	82,82,82,82	0
9	CL	E	707	1/1	0.96	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	D	700	1/1	0.96	0.07	92,92,92,92	0
9	CL	S	601	1/1	0.96	0.15	94,94,94,94	0
9	CL	N	701	1/1	0.96	0.09	75,75,75,75	0
9	CL	B	700	1/1	0.96	0.06	83,83,83,83	0
9	CL	C	700	1/1	0.97	0.13	76,76,76,76	0
11	NA	H	701	1/1	0.97	0.07	38,38,38,38	0
9	CL	S	603	1/1	0.97	0.09	88,88,88,88	0
11	NA	H	705	1/1	0.97	0.11	52,52,52,52	0
9	CL	F	707	1/1	0.98	0.08	64,64,64,64	0
9	CL	F	714	1/1	0.98	0.12	76,76,76,76	0
14	ZN	E	701	1/1	0.98	0.05	95,95,95,95	0
14	ZN	F	701	1/1	0.98	0.05	77,77,77,77	0
9	CL	H	703	1/1	0.98	0.07	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.