



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2021 – 10:21 AM EDT

PDB ID : 7LDJ
Title : SARS-CoV-2 receptor binding domain in complex with WNb-2
Authors : Pymm, P.; Dietrich, M.H.; Tan, L.L.; Adair, A.; Tham, W.H.
Deposited on : 2021-01-13
Resolution : 2.36 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

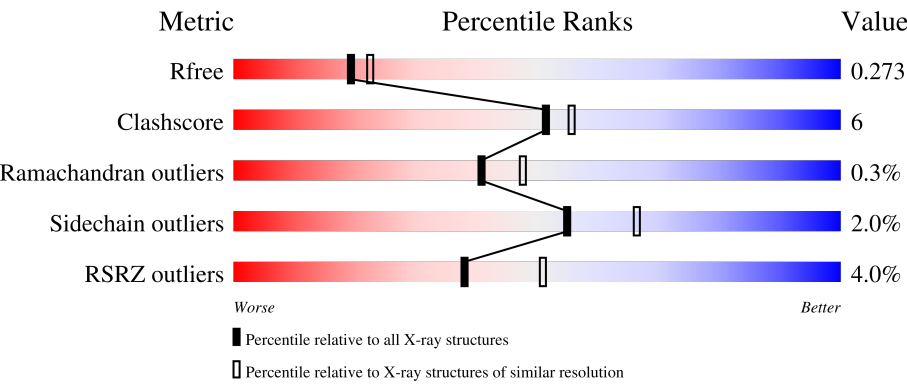
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

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 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	199	<div><div>2%</div><div>85%</div><div>10%</div><div>• •</div></div>
1	B	199	<div><div>3%</div><div>83%</div><div>16%</div><div>• •</div></div>
1	C	199	<div><div>5%</div><div>84%</div><div>12%</div><div>•</div></div>
1	D	199	<div><div>10%</div><div>80%</div><div>12%</div><div>• 8%</div></div>
2	E	131	<div><div>2%</div><div>91%</div><div>8%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
2	F	131	
2	G	131	
2	H	131	
3	I	4	
3	K	4	
4	J	6	

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
3	BMA	I	3	-	-	-	X
4	FUL	J	6	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10429 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
1	B	198	Total	C	N	O	S	0	1	0
			1567	1004	260	295	8			
1	A	193	Total	C	N	O	S	0	0	0
			1520	972	253	287	8			
1	C	191	Total	C	N	O	S	0	0	0
			1510	967	252	284	7			
1	D	184	Total	C	N	O	S	0	1	0
			1478	948	247	276	7			

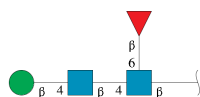
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	528	GLY	-	expression tag	UNP P0DTC2
B	529	SER	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	SER	-	expression tag	UNP P0DTC2
C	528	GLY	-	expression tag	UNP P0DTC2
C	529	SER	-	expression tag	UNP P0DTC2
D	528	GLY	-	expression tag	UNP P0DTC2
D	529	SER	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody 2.

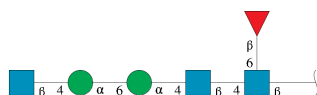
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	130	Total	C	N	O	S	0	1	0
			1002	628	171	197	6			
2	F	130	Total	C	N	O	S	0	0	0
			987	620	166	195	6			
2	G	131	Total	C	N	O	S	0	1	0
			1006	631	171	198	6			
2	H	130	Total	C	N	O	S	0	0	0
			990	622	167	195	6			

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



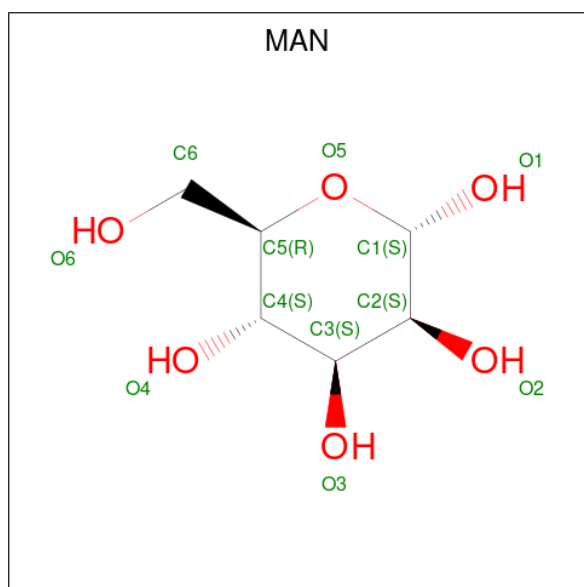
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	K	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



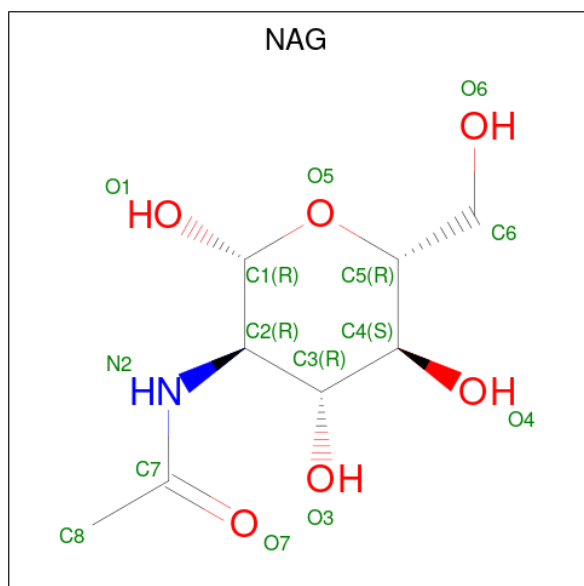
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	6	Total	C	N	O	0	0	0
			74	42	3	29			

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



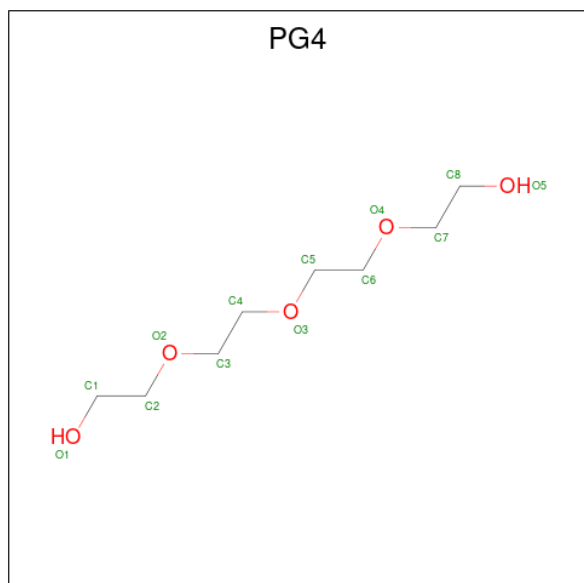
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			8	5	3		


- Molecule 8 is water.

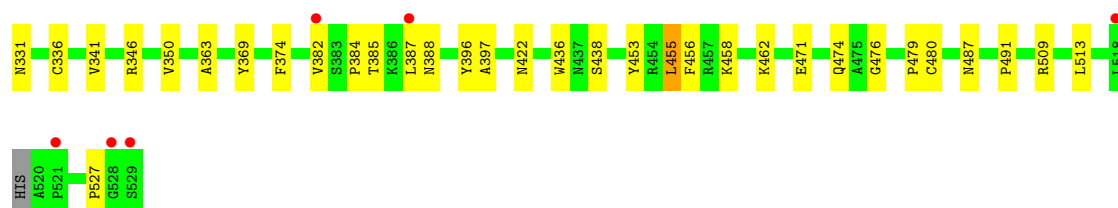
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	19	Total	O	0	0
			19	19		
8	A	19	Total	O	0	0
			19	19		
8	C	31	Total	O	0	0
			31	31		
8	D	17	Total	O	0	0
			17	17		
8	E	19	Total	O	0	0
			19	19		
8	F	18	Total	O	0	0
			18	18		
8	G	28	Total	O	0	0
			28	28		
8	H	13	Total	O	0	0
			13	13		

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

Chain B: 




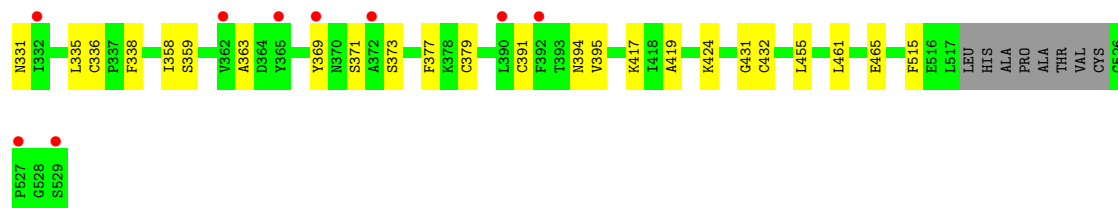
- Molecule 1: Spike glycoprotein

Chain A: 



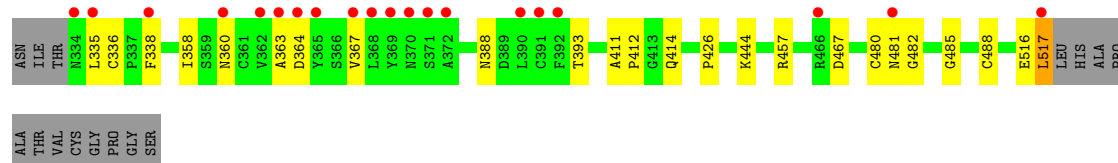
- Molecule 1: Spike glycoprotein

Chain C: 

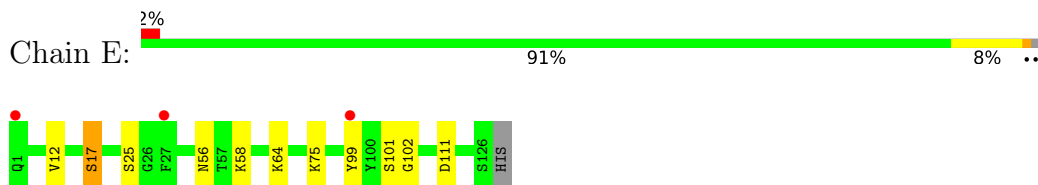


- Molecule 1: Spike glycoprotein

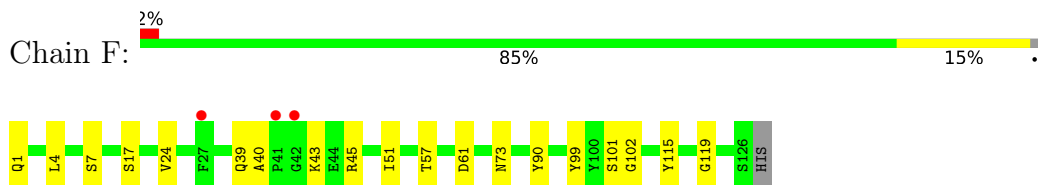
Chain D: 



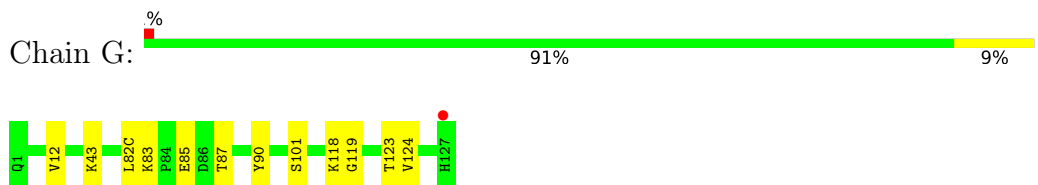
- Molecule 2: Nanobody 2



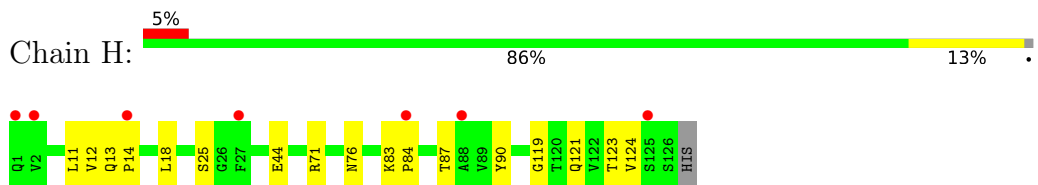
- Molecule 2: Nanobody 2



- Molecule 2: Nanobody 2



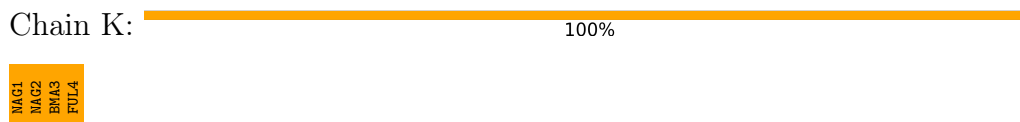
- Molecule 2: Nanobody 2



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



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



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



MAG1
MAG2
MAG3
MAG4
MAG5
FUL6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.12Å 88.51Å 107.49Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	45.94 – 2.36 45.94 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.94-2.36) 99.9 (45.94-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.210 , 0.268 0.216 , 0.273	Depositor DCC
R_{free} test set	2750 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10429	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUL, MAN, PG4, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/1562	0.47	0/2124
1	B	0.31	0/1609	0.49	0/2189
1	C	0.28	0/1551	0.45	0/2108
1	D	0.33	0/1519	0.49	0/2064
2	E	0.28	0/1026	0.47	0/1387
2	F	0.30	0/1011	0.47	0/1368
2	G	0.27	0/1031	0.47	0/1395
2	H	0.28	0/1014	0.47	0/1372
All	All	0.30	0/10323	0.47	0/14007

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	A	1520	0	1430	17	0
1	B	1567	0	1486	24	0
1	C	1510	0	1425	12	0
1	D	1478	0	1397	17	0
2	E	1002	0	942	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	987	0	924	9	0
2	G	1006	0	938	7	0
2	H	990	0	927	15	0
3	I	49	0	43	1	0
3	K	49	0	43	6	0
4	J	74	0	64	4	0
5	A	11	0	10	0	0
6	D	14	0	13	1	0
7	E	8	0	8	2	0
8	A	19	0	0	2	0
8	B	19	0	0	0	0
8	C	31	0	0	0	0
8	D	17	0	0	0	0
8	E	19	0	0	0	0
8	F	18	0	0	1	0
8	G	28	0	0	1	0
8	H	13	0	0	0	0
All	All	10429	0	9650	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (111) 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:D:517:LEU:HD22	1:D:517:LEU:O	1.48	1.11
1:D:336:CYS:SG	1:D:363:ALA:HB2	2.03	0.97
1:A:393:THR:HB	1:A:516:GLU:HG3	1.65	0.77
1:A:465:GLU:OE2	3:K:4:FUL:H5	1.88	0.73
2:H:84:PRO:HA	2:H:124:VAL:CG2	2.19	0.72
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.73	0.70
1:A:457:ARG:NH2	3:K:4:FUL:H4	2.08	0.69
2:H:87:THR:HG23	2:H:123:THR:HA	1.73	0.69
2:F:39:GLN:HB2	2:F:45:ARG:HG2	1.74	0.68
1:A:480:CYS:O	1:A:482:GLY:N	2.26	0.68
2:F:73:ASN:ND2	8:F:201:HOH:O	2.23	0.68
1:B:384:PRO:HA	1:B:387:LEU:HD12	1.76	0.68
1:D:517:LEU:O	1:D:517:LEU:CD2	2.37	0.65
1:B:382:VAL:HG23	1:B:387:LEU:CD2	2.27	0.64
2:H:83:LYS:O	2:H:124:VAL:HG21	1.98	0.64
2:H:84:PRO:HA	2:H:124:VAL:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:NH2	8:A:701:HOH:O	2.27	0.62
1:D:393:THR:OG1	1:D:516:GLU:HB3	2.00	0.61
1:A:457:ARG:HH22	3:K:4:FUL:H4	1.65	0.61
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.83	0.60
1:D:517:LEU:N	1:D:517:LEU:CD1	2.64	0.60
1:D:517:LEU:N	1:D:517:LEU:HD13	2.15	0.60
1:B:369:TYR:CD2	1:B:384:PRO:HG2	2.38	0.58
1:D:411:ALA:HB3	1:D:414:GLN:HG2	1.87	0.56
4:J:4:MAN:O2	4:J:4:MAN:H61	2.05	0.56
1:A:334:ASN:O	1:A:362:VAL:N	2.37	0.56
6:D:600:NAG:H83	6:D:600:NAG:H3	1.87	0.55
1:C:417:LYS:HD2	1:C:455:LEU:HD12	1.89	0.55
1:B:331:ASN:ND2	1:A:346:ARG:HH22	2.05	0.54
2:G:118:LYS:NZ	8:G:202:HOH:O	2.38	0.54
1:B:382:VAL:HG23	1:B:387:LEU:HD23	1.89	0.54
3:K:1:NAG:O6	3:K:4:FUL:H63	2.08	0.53
1:A:378:LYS:NZ	1:A:380:TYR:OH	2.38	0.53
2:F:101:SER:O	2:F:101:SER:OG	2.26	0.53
3:K:2:NAG:O3	3:K:3:BMA:O5	2.17	0.52
1:D:364:ASP:O	1:D:367:VAL:HG12	2.11	0.51
1:B:455[A]:LEU:HD12	1:B:456:PHE:CZ	2.45	0.51
1:A:393:THR:CB	1:A:516:GLU:HG3	2.36	0.51
2:H:124:VAL:HG23	2:H:124:VAL:O	2.10	0.51
4:J:5:NAG:O7	4:J:5:NAG:H3	2.11	0.50
4:J:1:NAG:O6	4:J:6:FUL:H63	2.11	0.50
2:F:4:LEU:HD23	2:F:24:VAL:HG22	1.93	0.50
1:C:394:ASN:OD1	1:C:394:ASN:N	2.44	0.49
3:I:1:NAG:H62	3:I:2:NAG:C1	2.42	0.49
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.94	0.49
1:B:476:GLY:H	1:B:487:ASN:HD22	1.60	0.49
1:A:357:ARG:HB2	1:C:335:LEU:HD11	1.96	0.48
2:H:83:LYS:C	2:H:124:VAL:HG21	2.32	0.48
1:C:336:CYS:SG	1:C:363:ALA:HB2	2.53	0.48
2:E:99:TYR:OH	2:E:102:GLY:HA2	2.14	0.48
1:D:485:GLY:H	1:D:488:CYS:HB2	1.79	0.47
2:E:12:VAL:HG22	7:E:201:PG4:H41	1.95	0.47
2:F:40:ALA:HB3	2:F:43:LYS:HG3	1.95	0.47
2:G:90:TYR:O	2:G:119:GLY:HA2	2.15	0.47
3:K:1:NAG:O4	3:K:2:NAG:O7	2.32	0.47
1:B:474:GLN:O	1:B:474:GLN:HG3	2.15	0.46
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD23	1:D:336:CYS:O	2.16	0.46
1:B:396:TYR:O	1:B:513:LEU:HA	2.16	0.46
2:F:1:GLN:HA	2:F:115:TYR:CZ	2.51	0.46
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.97	0.46
2:F:99:TYR:CZ	2:F:102:GLY:HA2	2.51	0.46
1:B:384:PRO:HA	1:B:387:LEU:CD1	2.46	0.45
1:C:461:LEU:HD22	1:C:465:GLU:HB3	1.97	0.45
1:B:331:ASN:N	1:C:359:SER:O	2.49	0.45
1:A:454:ARG:NH1	8:A:704:HOH:O	2.46	0.45
1:C:371:SER:OG	1:C:373:SER:OG	2.23	0.45
2:H:90:TYR:O	2:H:119:GLY:HA2	2.17	0.45
2:F:51:ILE:HG13	2:F:57:THR:HG22	1.99	0.45
2:H:11:LEU:HD22	2:H:12:VAL:H	1.82	0.45
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.57	0.45
1:B:382:VAL:HG23	1:B:387:LEU:HD21	1.98	0.45
1:A:360:ASN:H	1:A:523:THR:HB	1.82	0.45
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.99	0.45
1:B:455[A]:LEU:HD12	1:B:456:PHE:CE2	2.52	0.44
1:B:462:LYS:HE3	1:B:462:LYS:HB2	1.69	0.44
1:C:419:ALA:O	1:C:424:LYS:HB2	2.18	0.44
2:G:83:LYS:HG3	2:G:85:GLU:HG2	1.99	0.44
2:H:18:LEU:HD23	2:H:18:LEU:HA	1.81	0.44
2:H:13:GLN:HG2	2:H:14:PRO:HD2	2.00	0.44
1:D:338:PHE:HE1	1:D:358:ILE:HD13	1.83	0.43
2:G:12:VAL:HG23	2:G:124:VAL:HG22	1.99	0.43
1:D:480:CYS:O	1:D:482:GLY:N	2.51	0.43
2:G:101:SER:O	2:G:101:SER:OG	2.30	0.43
1:B:458:LYS:HD2	2:H:44:GLU:OE2	2.18	0.43
2:H:121:GLN:HE21	2:H:123:THR:HG22	1.83	0.43
1:B:388:ASN:HB3	1:B:527:PRO:HD2	2.01	0.43
2:F:90:TYR:O	2:F:119:GLY:HA2	2.19	0.43
2:H:71:ARG:NH2	2:H:76:ASN:OD1	2.52	0.42
4:J:2:NAG:HO3	4:J:3:MAN:C1	2.33	0.42
2:G:87:THR:HG23	2:G:123:THR:HA	2.00	0.42
1:B:346:ARG:HH21	1:B:346:ARG:HG3	1.85	0.42
2:E:17:SER:OG	7:E:201:PG4:H61	2.20	0.42
2:E:75:LYS:HB2	2:E:75:LYS:HE3	1.73	0.41
2:G:82(C):LEU:HB3	2:G:124:VAL:HG21	2.03	0.41
1:B:453:TYR:CE2	1:B:455[A]:LEU:HD23	2.56	0.41
1:A:379:CYS:HA	1:A:432:CYS:HA	2.02	0.41
1:D:338:PHE:CE1	1:D:358:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:SER:HA	1:A:510:VAL:O	2.21	0.41
1:D:457:ARG:NE	1:D:467:ASP:OD2	2.35	0.41
1:B:471:GLU:O	1:B:491:PRO:HG3	2.20	0.41
2:E:56:ASN:O	2:E:58:LYS:NZ	2.52	0.41
2:H:11:LEU:HD22	2:H:12:VAL:N	2.36	0.41
1:C:379:CYS:HA	1:C:432:CYS:HA	2.03	0.40
1:D:412:PRO:HB3	1:D:426:PRO:O	2.21	0.40
2:E:64:LYS:NZ	2:E:64:LYS:HB3	2.37	0.40
1:D:364:ASP:HA	1:D:388:ASN:OD1	2.22	0.40
1:B:374:PHE:HA	1:B:436:TRP:HB3	2.03	0.40
1:A:359:SER:O	1:C:331:ASN:N	2.54	0.40
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.57	0.40
1:D:444:LYS:HD3	1:D:444:LYS:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/199 (95%)	177 (94%)	10 (5%)	2 (1%)	14	13
1	B	195/199 (98%)	185 (95%)	10 (5%)	0	100	100
1	C	187/199 (94%)	178 (95%)	9 (5%)	0	100	100
1	D	183/199 (92%)	171 (93%)	10 (6%)	2 (1%)	14	13
2	E	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
2	F	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
2	G	130/131 (99%)	128 (98%)	2 (2%)	0	100	100
2	H	128/131 (98%)	127 (99%)	1 (1%)	0	100	100
All	All	1269/1320 (96%)	1219 (96%)	46 (4%)	4 (0%)	41	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	481	ASN
1	D	481	ASN
1	A	482	GLY
1	D	360	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/171 (96%)	162 (98%)	3 (2%)	59	70
1	B	171/171 (100%)	166 (97%)	5 (3%)	42	52
1	C	164/171 (96%)	160 (98%)	4 (2%)	49	59
1	D	160/171 (94%)	159 (99%)	1 (1%)	86	93
2	E	104/104 (100%)	100 (96%)	4 (4%)	33	41
2	F	102/104 (98%)	99 (97%)	3 (3%)	42	52
2	G	104/104 (100%)	103 (99%)	1 (1%)	76	85
2	H	102/104 (98%)	101 (99%)	1 (1%)	76	85
All	All	1072/1100 (98%)	1050 (98%)	22 (2%)	55	65

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

Mol	Chain	Res	Type
1	B	385	THR
1	B	455[A]	LEU
1	B	455[B]	LEU
1	B	479	PRO
1	B	480	CYS
1	A	346	ARG
1	A	359	SER
1	A	516	GLU
1	C	338	PHE
1	C	369	TYR

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Mol	Chain	Res	Type
1	C	377	PHE
1	C	391	CYS
1	D	517	LEU
2	E	17	SER
2	E	25	SER
2	E	101	SER
2	E	111	ASP
2	F	7	SER
2	F	17	SER
2	F	61	ASP
2	G	43	LYS
2	H	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	331	ASN
1	A	481	ASN
1	D	354	ASN
1	D	360	ASN
2	H	5	GLN

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 ⓘ

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	I	1	3,1	14,14,15	1.05	1 (7%)	17,19,21	1.01	1 (5%)
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.95	1 (5%)
3	BMA	I	3	3	11,11,12	0.29	0	15,15,17	0.64	0
3	FUL	I	4	3	10,10,11	0.30	0	14,14,16	0.79	0
4	NAG	J	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	1.21	1 (5%)
4	NAG	J	2	4	14,14,15	0.20	0	17,19,21	0.38	0
4	MAN	J	3	4	11,11,12	0.32	0	15,15,17	1.18	3 (20%)
4	MAN	J	4	4	11,11,12	0.24	0	15,15,17	1.51	3 (20%)
4	NAG	J	5	4	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
4	FUL	J	6	4	10,10,11	0.41	0	14,14,16	1.15	2 (14%)
3	NAG	K	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	K	2	3	14,14,15	0.38	0	17,19,21	1.09	2 (11%)
3	BMA	K	3	3	11,11,12	0.25	0	15,15,17	0.91	1 (6%)
3	FUL	K	4	3	10,10,11	0.40	0	14,14,16	1.37	2 (14%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C1-C2	3.52	1.57	1.52
3	K	1	NAG	C1-C2	2.92	1.56	1.52
4	J	1	NAG	C1-C2	2.53	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	4	MAN	C1-O5-C5	3.58	117.05	112.19
3	K	4	FUL	C1-C2-C3	3.49	113.96	109.67
3	K	1	NAG	C1-O5-C5	2.99	116.24	112.19
4	J	1	NAG	C1-O5-C5	2.91	116.14	112.19
4	J	3	MAN	C1-O5-C5	2.90	116.13	112.19
3	I	1	NAG	O4-C4-C3	-2.69	104.12	110.35
3	K	2	NAG	O5-C1-C2	-2.63	107.14	111.29
4	J	4	MAN	O5-C1-C2	2.62	114.81	110.77
4	J	4	MAN	C3-C4-C5	2.59	114.86	110.24
3	K	4	FUL	C3-C4-C5	2.52	113.70	109.77
3	K	2	NAG	C2-N2-C7	-2.46	119.40	122.90
4	J	6	FUL	C3-C4-C5	2.43	113.56	109.77
4	J	3	MAN	O5-C1-C2	2.38	114.45	110.77
3	I	2	NAG	C2-N2-C7	-2.32	119.61	122.90
4	J	6	FUL	C1-C2-C3	2.30	112.49	109.67
3	K	3	BMA	O5-C1-C2	-2.29	107.23	110.77
4	J	5	NAG	O5-C1-C2	-2.23	107.77	111.29
4	J	3	MAN	C3-C4-C5	2.07	113.93	110.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	5	NAG	C3-C2-N2-C7
4	J	5	NAG	C8-C7-N2-C2
4	J	5	NAG	O7-C7-N2-C2
3	K	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
4	J	3	MAN	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	J	3	MAN	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6

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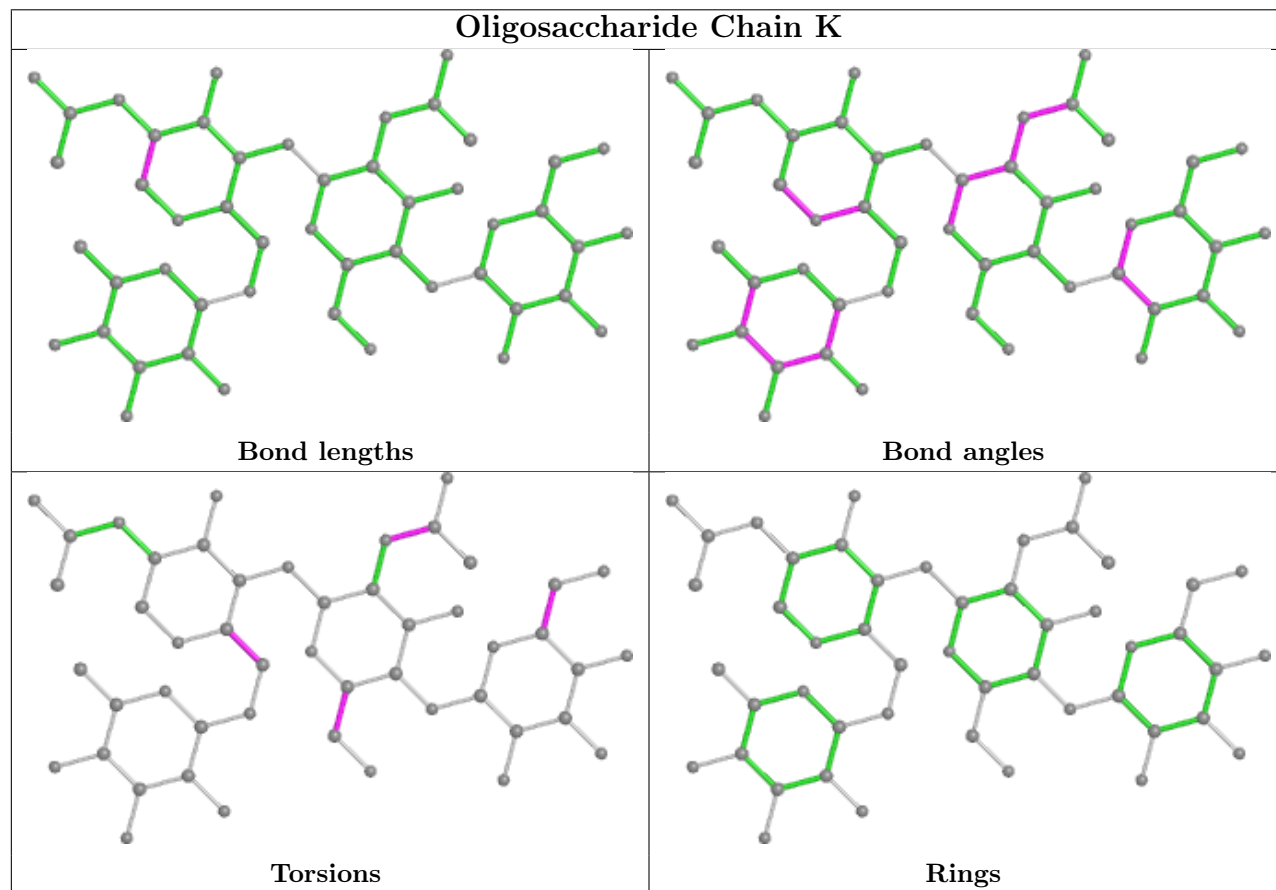
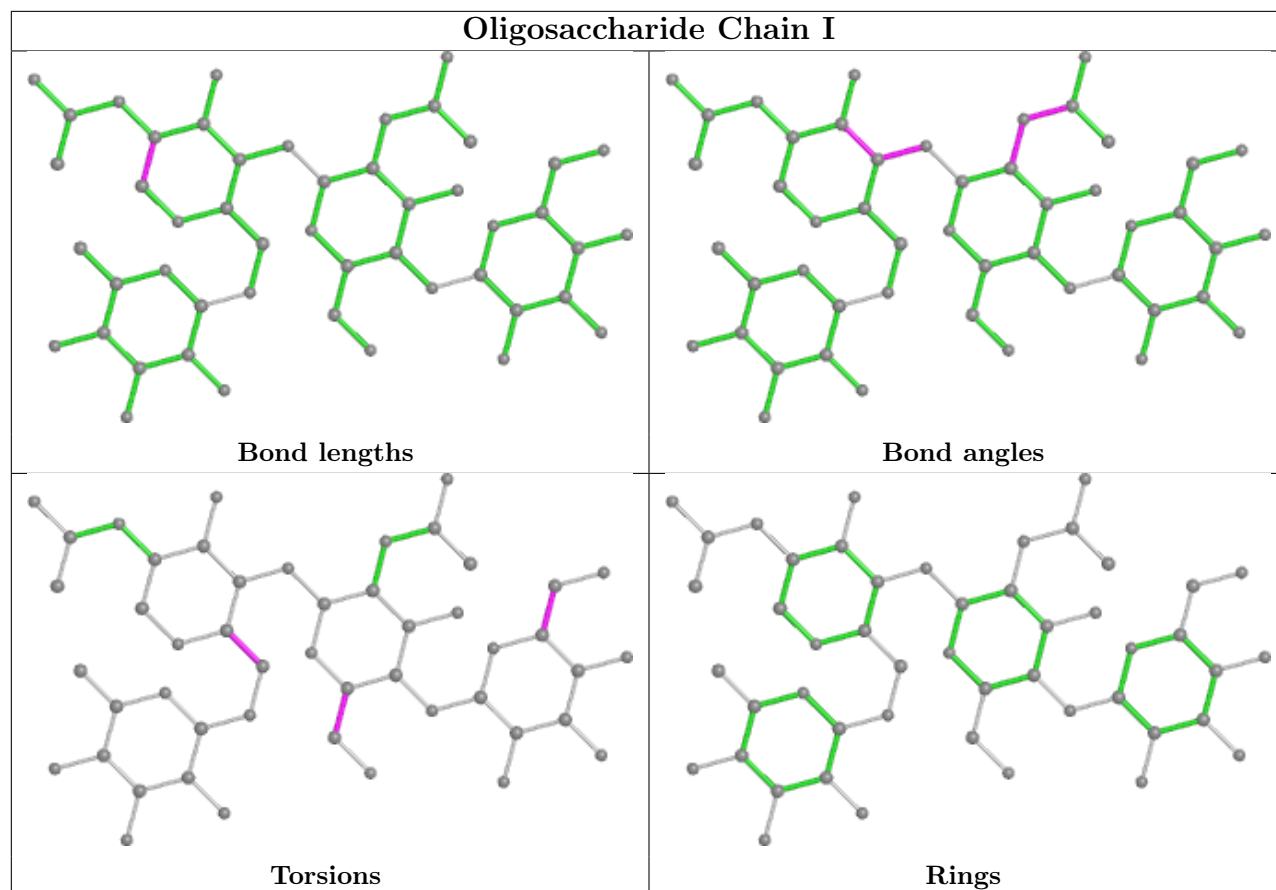
Mol	Chain	Res	Type	Atoms
3	I	3	BMA	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6

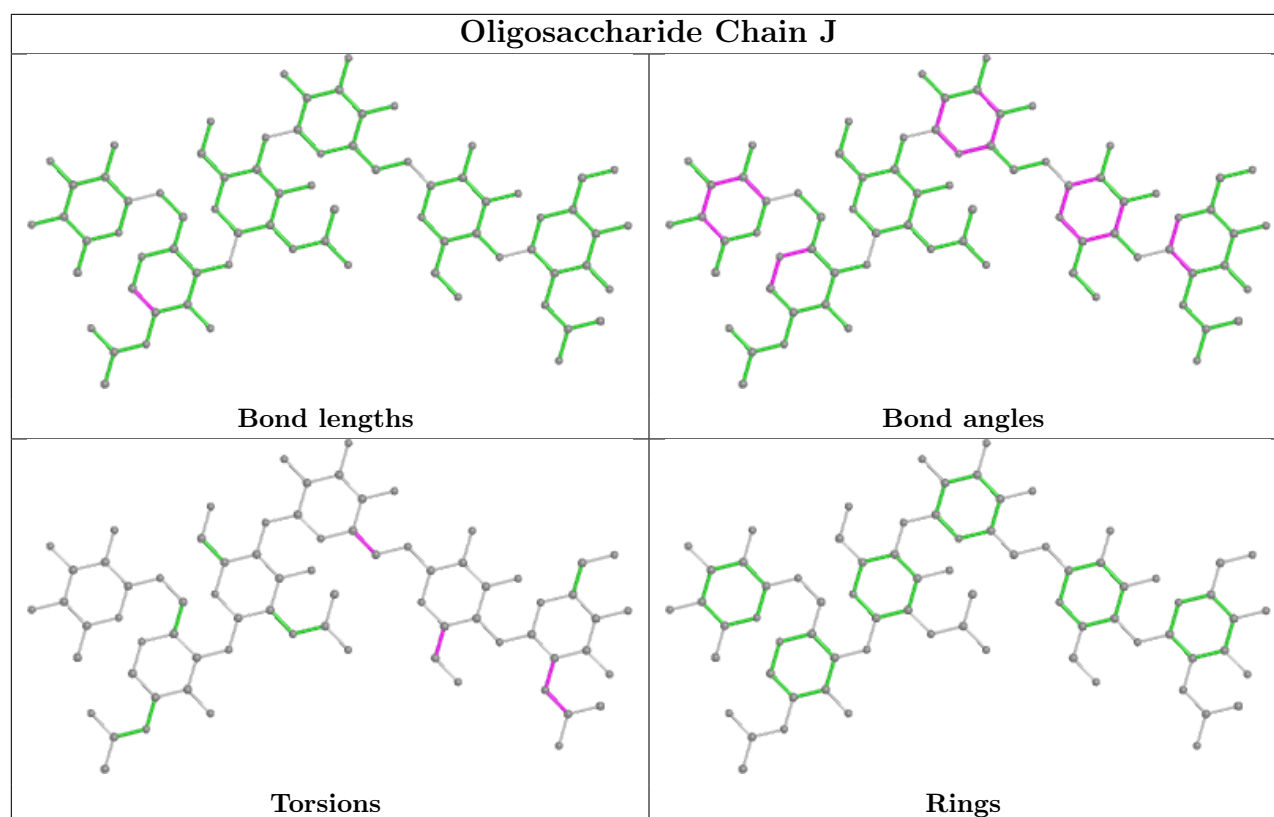
There are no ring outliers.

12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0
3	K	4	FUL	4	0
3	K	3	BMA	1	0
4	J	2	NAG	1	0
4	J	4	MAN	1	0
3	K	2	NAG	2	0
4	J	6	FUL	1	0
4	J	3	MAN	1	0
4	J	5	NAG	1	0
3	I	2	NAG	1	0
4	J	1	NAG	1	0
3	K	1	NAG	2	0

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





5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	MAN	A	601	-	11,11,12	1.09	1 (9%)	15,15,17	1.83	5 (33%)
6	NAG	D	600	-	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
7	PG4	E	201	-	7,7,12	0.44	0	6,6,11	0.29	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
5	MAN	A	601	-	-	1/2/19/22	0/1/1/1
6	NAG	D	600	-	-	5/6/23/26	0/1/1/1
7	PG4	E	201	-	-	1/5/5/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	MAN	C1-C2	2.66	1.58	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	NAG	C2-N2-C7	4.36	129.11	122.90
5	A	601	MAN	C1-O5-C5	3.94	117.54	112.19
5	A	601	MAN	O5-C1-C2	3.40	116.02	110.77
5	A	601	MAN	C3-C4-C5	-2.42	105.92	110.24
5	A	601	MAN	O2-C2-C3	-2.21	105.72	110.14
5	A	601	MAN	C1-C2-C3	2.07	112.21	109.67
6	D	600	NAG	C1-C2-N2	2.06	114.01	110.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	600	NAG	O5-C5-C6-O6
6	D	600	NAG	C4-C5-C6-O6
6	D	600	NAG	C8-C7-N2-C2
6	D	600	NAG	O7-C7-N2-C2
7	E	201	PG4	O2-C3-C4-O3
5	A	601	MAN	C4-C5-C6-O6
6	D	600	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	NAG	1	0
7	E	201	PG4	2	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	A	193/199 (96%)	0.16	3 (1%)	72	80	37, 54, 80, 91	0
1	B	198/199 (99%)	0.14	6 (3%)	50	61	44, 60, 89, 101	0
1	C	191/199 (95%)	0.24	9 (4%)	31	44	40, 54, 91, 111	0
1	D	184/199 (92%)	0.62	20 (10%)	5	9	44, 60, 96, 115	0
2	E	130/131 (99%)	0.02	3 (2%)	60	70	39, 50, 73, 81	0
2	F	130/131 (99%)	0.15	3 (2%)	60	70	42, 53, 70, 82	0
2	G	131/131 (100%)	-0.02	1 (0%)	86	91	42, 55, 73, 96	0
2	H	130/131 (99%)	0.53	7 (5%)	25	37	46, 62, 81, 101	0
All	All	1287/1320 (97%)	0.24	52 (4%)	38	51	37, 56, 89, 115	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	5.2
1	D	368	LEU	5.1
2	H	27	PHE	4.1
1	B	529	SER	4.1
1	B	521	PRO	4.1
1	D	372	ALA	4.1
1	D	369	TYR	4.1
2	F	27	PHE	3.9
1	D	391	CYS	3.8
1	B	387	LEU	3.6
2	H	125	SER	3.6
1	D	362	VAL	3.5
1	D	517	LEU	3.5
1	D	371	SER	3.5
1	C	365	TYR	3.5
1	D	392	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	518	LEU	3.2
2	H	14	PRO	3.1
2	E	27	PHE	3.1
1	C	372	ALA	3.0
1	C	392	PHE	3.0
1	D	365	TYR	2.9
2	F	42	GLY	2.9
2	H	1	GLN	2.9
1	D	338	PHE	2.8
1	D	481	ASN	2.8
2	E	1	GLN	2.7
1	C	369	TYR	2.7
1	D	370	ASN	2.7
1	D	367	VAL	2.6
1	D	335	LEU	2.6
1	A	393	THR	2.5
1	D	364	ASP	2.5
1	D	363	ALA	2.4
1	D	390	LEU	2.4
1	C	529	SER	2.4
2	H	88	ALA	2.4
1	A	369	TYR	2.3
2	E	99	TYR	2.3
1	C	527	PRO	2.3
1	C	390	LEU	2.3
2	G	127	HIS	2.3
1	B	382	VAL	2.2
2	H	84	PRO	2.2
1	C	332	ILE	2.2
1	C	362	VAL	2.2
1	D	466[A]	ARG	2.1
1	A	529	SER	2.1
1	D	334	ASN	2.1
1	D	360	ASN	2.1
1	B	528	GLY	2.1
2	F	41	PRO	2.1

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

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

6.3 Carbohydrates ⓘ

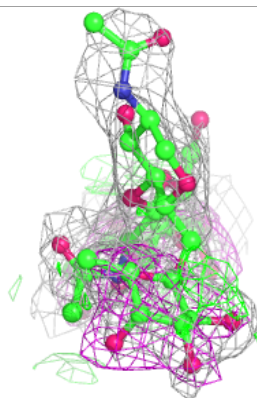
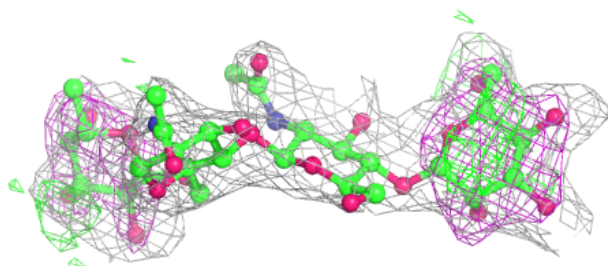
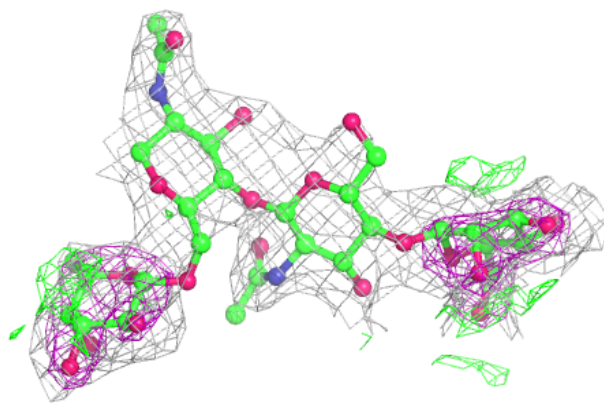
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	5	14/15	0.47	0.30	84,111,116,118	0
3	BMA	I	3	11/12	0.54	0.42	30,30,30,30	0
4	MAN	J	3	11/12	0.64	0.31	100,109,115,116	0
4	MAN	J	4	11/12	0.68	0.19	107,115,117,121	0
3	BMA	K	3	11/12	0.68	0.32	30,30,30,30	0
4	NAG	J	2	14/15	0.71	0.30	104,112,117,119	0
4	NAG	J	1	14/15	0.71	0.22	66,93,102,105	0
4	FUL	J	6	10/11	0.73	0.42	30,30,30,30	0
3	NAG	K	2	14/15	0.78	0.26	102,107,113,117	0
3	FUL	I	4	10/11	0.78	0.36	30,30,30,30	0
3	NAG	I	1	14/15	0.84	0.15	79,97,106,111	0
3	NAG	I	2	14/15	0.85	0.19	91,100,103,104	0
3	FUL	K	4	10/11	0.85	0.38	30,30,30,30	0
3	NAG	K	1	14/15	0.88	0.13	55,81,90,100	0

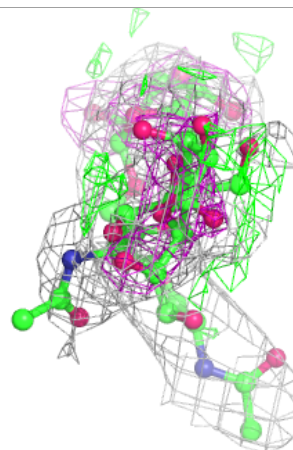
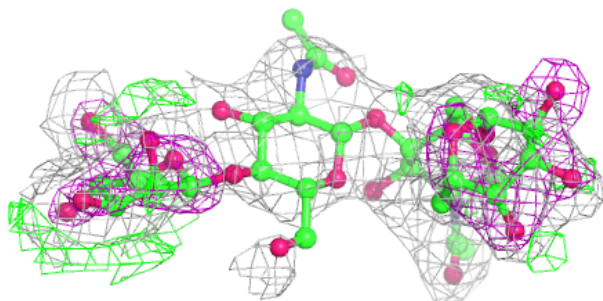
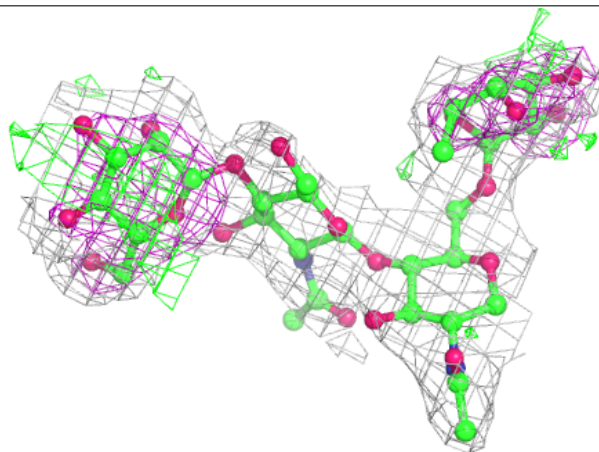
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

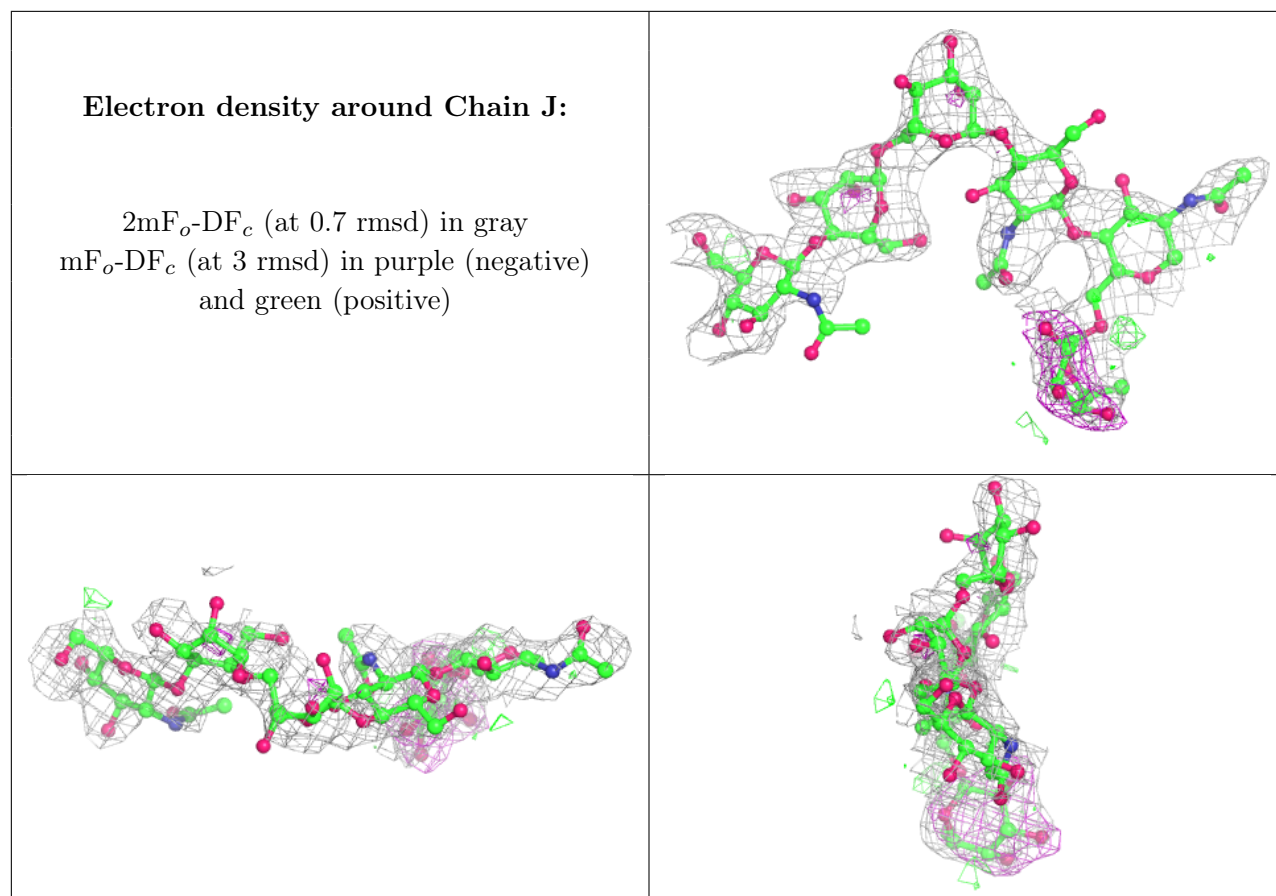
Electron density around Chain I:

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

**Electron density around Chain K:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	A	601	11/12	0.72	0.33	93,99,105,110	0
6	NAG	D	600	14/15	0.75	0.30	81,100,108,112	0
7	PG4	E	201	8/13	0.82	0.32	39,52,56,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.