



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:04 AM EDT

PDB ID : 7YCK / pdb_00007yck
Title : Crystal structure of SARS-CoV-2 Spike RBD in complex with FP-12A Fab
Authors : Nguyen, V.H.T.; Chen, X.
Deposited on : 2022-07-01
Resolution : 2.60 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:

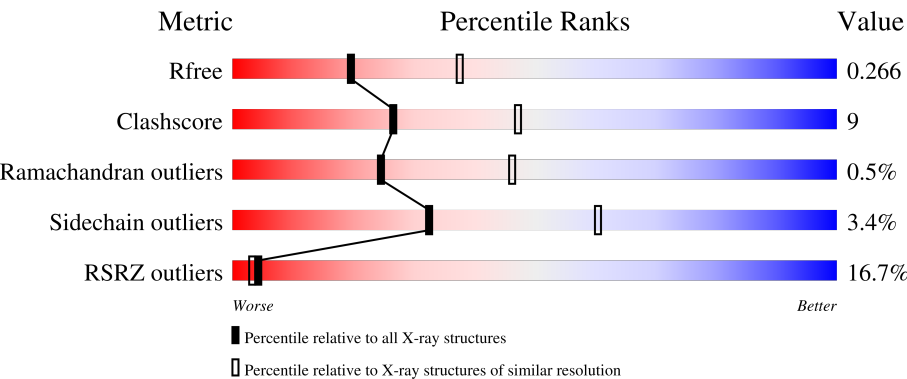
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	204	88% 9%
1	B	204	88% 9%
2	C	224	28% 66% 29%
2	E	224	11% 43% 10% 46%
3	D	216	27% 68% 25% 5%

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Mol	Chain	Length	Quality of chain
3	F	216	
4	G	4	
5	H	3	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8315 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 protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1567	1004	262	293	8			
1	B	199	Total	C	N	O	S	0	0	0
			1577	1010	265	294	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
B	531	HIS	-	expression tag	UNP P0DTC2
B	532	HIS	-	expression tag	UNP P0DTC2
B	533	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2

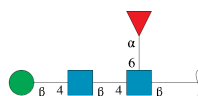
- Molecule 2 is a protein called FP-12A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1623	1027	269	320	7			
2	E	120	Total	C	N	O	S	0	0	0
			932	590	157	180	5			

- Molecule 3 is a protein called FP-12A Fab light chain.

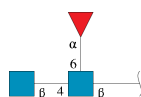
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	210	Total	C	N	O	S	0	0	0
			1579	982	262	330	5			
3	F	109	Total	C	N	O	S	0	0	0
			823	506	138	176	3			

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

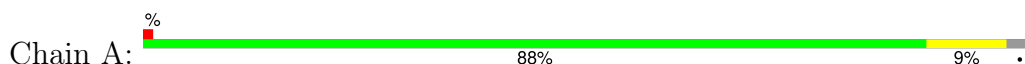
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	C	7	Total	O	0	0
			7	7		
6	D	16	Total	O	0	0
			16	16		
6	B	44	Total	O	0	0
			44	44		
6	E	5	Total	O	0	0
			5	5		
6	F	11	Total	O	0	0
			11	11		

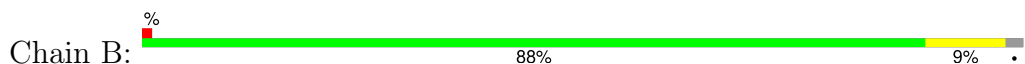
3 Residue-property plots [i](#)

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.

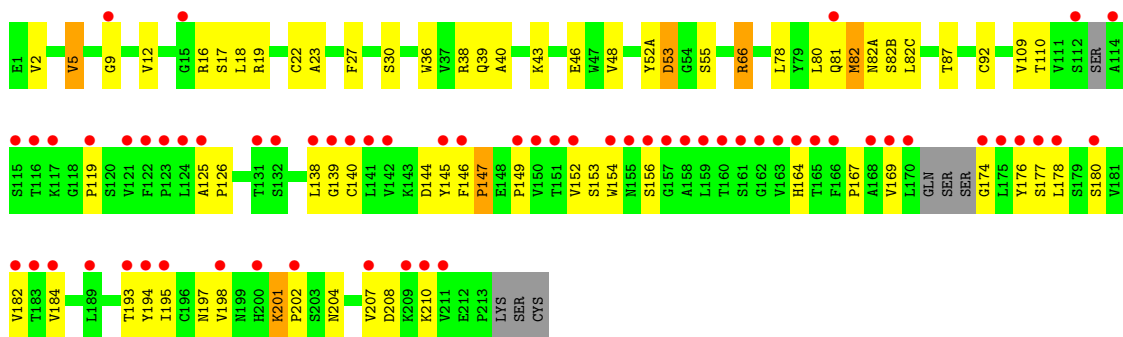
- Molecule 1: Spike protein S1



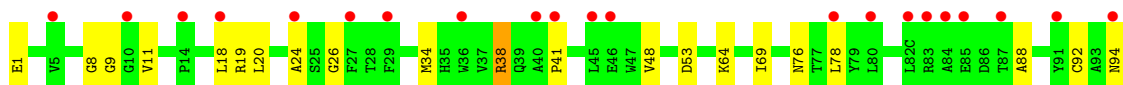
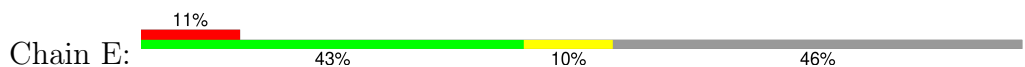
- Molecule 1: Spike protein S1



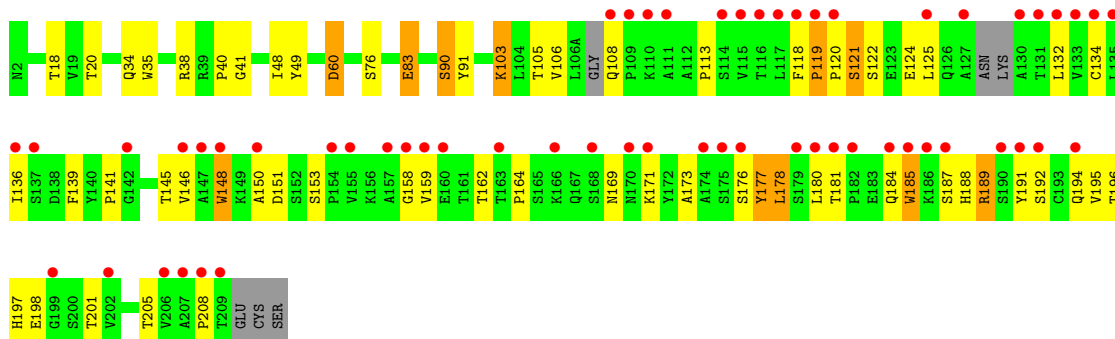
- Molecule 2: FP-12A Fab heavy chain



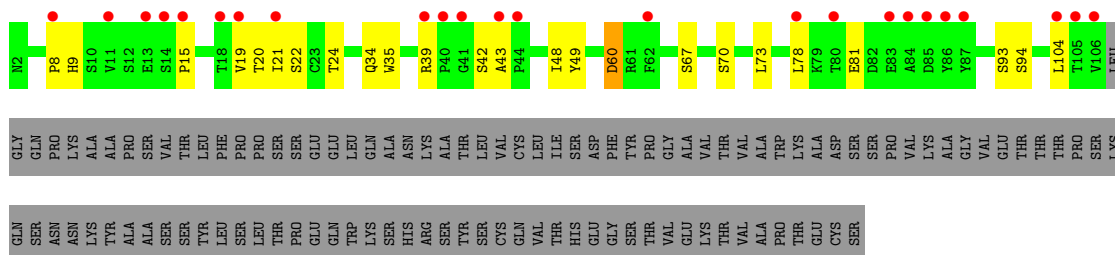
- Molecule 2: FP-12A Fab heavy chain



- Molecule 3: FP-12A Fab light chain



- Molecule 3: FP-12A Fab light chain



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



- Molecule 5: 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	Depositor
Cell constants a, b, c, α , β , γ	58.83Å 79.12Å 92.54Å 76.26° 81.16° 71.13°	Depositor
Resolution (Å)	32.25 – 2.60 32.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (32.25-2.60) 97.7 (32.25-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.264 0.231 , 0.266	Depositor DCC
R_{free} test set	2624 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8315	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, FUC, 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	0.12	0/1611	0.34	0/2191
1	B	0.15	0/1622	0.37	0/2206
2	C	0.16	0/1661	0.40	0/2261
2	E	0.11	0/955	0.36	0/1294
3	D	0.21	0/1617	0.43	0/2208
3	F	0.19	0/842	0.37	0/1147
All	All	0.16	0/8308	0.38	0/11307

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	1567	0	1490	10	0
1	B	1577	0	1497	13	0
2	C	1623	0	1570	51	0
2	E	932	0	876	13	0
3	D	1579	0	1497	52	0
3	F	823	0	764	14	0
4	G	49	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	38	0	34	0	0
6	A	44	0	0	1	0
6	B	44	0	0	1	0
6	C	7	0	0	1	0
6	D	16	0	0	3	0
6	E	5	0	0	0	0
6	F	11	0	0	2	0
All	All	8315	0	7771	148	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 9.

All (148) 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:B:391:CYS:SG	1:B:529:LYS:HD3	2.19	0.83
2:C:126:PRO:HB3	2:C:138:LEU:HD12	1.63	0.80
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.74	0.70
2:E:94:ASN:O	2:E:101:ASP:N	2.25	0.68
3:D:119:PRO:HG3	3:D:132:LEU:HG	1.77	0.66
2:C:154:TRP:NE1	2:C:195:ILE:HB	2.10	0.65
2:E:94:ASN:HB3	2:E:102:VAL:H	1.61	0.65
2:E:8:GLY:HA3	2:E:20:LEU:HD23	1.79	0.65
3:F:60:ASP:N	3:F:60:ASP:OD1	2.30	0.65
3:F:21:ILE:HD12	3:F:73:LEU:HD23	1.78	0.64
3:F:35:TRP:HB2	3:F:48:ILE:HB	1.79	0.64
2:C:22:CYS:HB3	2:C:78:LEU:HB3	1.79	0.64
3:D:35:TRP:HB2	3:D:48:ILE:HB	1.79	0.64
1:B:529:LYS:O	1:B:529:LYS:HG3	1.98	0.63
3:D:103:LYS:NZ	6:D:305:HOH:O	2.31	0.63
3:D:194:GLN:HA	3:D:205:THR:HB	1.80	0.63
3:F:34:GLN:HG3	3:F:49:TYR:HA	1.79	0.62
3:D:151:ASP:OD1	3:D:187:SER:OG	2.18	0.62
3:D:105:THR:HG21	3:D:141:PRO:HB3	1.82	0.60
1:B:340:GLU:N	1:B:340:GLU:OE1	2.35	0.60
2:C:184:VAL:HG21	2:C:194:TYR:CZ	2.38	0.59
3:D:118:PHE:CD2	3:D:120:PRO:HG3	2.37	0.59
3:D:176:SER:C	3:D:177:TYR:HD1	2.10	0.59
2:C:126:PRO:CB	2:C:138:LEU:HD12	2.31	0.59
2:E:24:ALA:HB3	2:E:76:ASN:HB3	1.85	0.59
3:F:15:PRO:HA	3:F:78:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:PHE:C	3:D:120:PRO:HD3	2.28	0.58
3:D:60:ASP:OD1	3:D:60:ASP:N	2.32	0.58
3:D:150:ALA:HA	3:D:191:TYR:CE1	2.39	0.58
2:C:154:TRP:CD1	2:C:195:ILE:HB	2.40	0.57
3:F:93:SER:OG	3:F:94:SER:N	2.38	0.56
1:A:359:SER:OG	1:A:394:ASN:OD1	2.22	0.56
1:A:376:THR:HG22	1:A:435:ALA:HB3	1.87	0.56
3:D:191:TYR:HB3	3:D:208:PRO:HG2	1.88	0.56
2:C:152:VAL:HG22	2:C:198:VAL:HG13	1.88	0.56
3:D:18:THR:HG22	3:D:76:SER:HA	1.87	0.56
2:C:9:GLY:HA3	2:C:18:LEU:HD21	1.88	0.55
2:C:12:VAL:HG21	2:C:18:LEU:HD22	1.88	0.55
2:C:5:VAL:HG13	2:C:23:ALA:HB3	1.89	0.55
2:C:39:GLN:NE2	6:C:302:HOH:O	2.39	0.55
3:D:146:VAL:HG22	3:D:195:VAL:HG22	1.88	0.55
2:C:82:MET:HE1	2:C:109:VAL:HG21	1.89	0.55
2:C:40:ALA:HB3	2:C:43:LYS:HE3	1.89	0.54
2:C:193:THR:HG23	2:C:210:LYS:HE3	1.90	0.54
2:C:201:LYS:HB3	2:C:202:PRO:HD3	1.90	0.54
3:F:67:SER:N	6:F:302:HOH:O	2.41	0.53
1:B:391:CYS:SG	1:B:529:LYS:CD	2.95	0.53
3:F:8:PRO:HD3	3:F:22:SER:HB2	1.91	0.52
3:F:43:ALA:N	6:F:304:HOH:O	2.41	0.52
2:C:154:TRP:HE1	2:C:195:ILE:HB	1.73	0.52
3:D:120:PRO:O	3:D:122:SER:N	2.42	0.52
1:A:460:ASN:HB3	6:A:624:HOH:O	2.10	0.52
1:A:340:GLU:N	1:A:340:GLU:OE1	2.41	0.52
2:C:125:ALA:HB3	3:D:120:PRO:HG2	1.92	0.52
2:E:41:PRO:HD3	2:E:88:ALA:HA	1.92	0.52
3:D:192:SER:HA	3:D:208:PRO:HD2	1.93	0.51
3:D:196:THR:HG23	3:D:201:THR:HG21	1.93	0.51
2:C:169:VAL:HG12	2:C:174:GLY:HA2	1.92	0.51
3:D:145:THR:HG23	3:D:196:THR:HB	1.92	0.51
2:C:144:ASP:N	2:C:176:TYR:O	2.45	0.50
2:C:184:VAL:HG11	2:C:194:TYR:OH	2.13	0.49
2:C:126:PRO:CG	2:C:138:LEU:HD12	2.42	0.49
2:C:138:LEU:O	2:C:182:VAL:N	2.38	0.48
2:C:87:THR:HG23	2:C:110:THR:HA	1.94	0.48
2:C:126:PRO:HG3	2:C:138:LEU:HD12	1.94	0.48
3:D:113:PRO:HB2	3:D:136:ILE:HG23	1.96	0.48
3:D:34:GLN:HG3	3:D:49:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:PRO:HB3	3:D:139:PHE:HB3	1.95	0.48
2:C:169:VAL:HG21	3:D:159:VAL:HG13	1.96	0.48
3:D:178:LEU:HD21	3:D:191:TYR:OH	2.14	0.48
3:D:125:LEU:HD11	3:D:185:TRP:HH2	1.79	0.47
3:D:108:GLN:C	6:D:303:HOH:O	2.57	0.47
3:D:189:ARG:N	3:D:189:ARG:HD3	2.29	0.47
2:E:69:ILE:HD11	2:E:78:LEU:HD11	1.96	0.47
3:D:118:PHE:HD2	3:D:120:PRO:HG3	1.78	0.46
2:E:11:VAL:HA	2:E:110:THR:O	2.16	0.46
2:E:9:GLY:HA3	2:E:18:LEU:HD11	1.97	0.46
2:E:34:MET:HB3	2:E:78:LEU:HD22	1.96	0.46
3:F:24:THR:HG22	3:F:70:SER:HB3	1.98	0.46
2:C:38:ARG:NH2	2:C:46:GLU:OE1	2.49	0.46
1:A:379:CYS:HA	1:A:432:CYS:HA	1.97	0.45
1:A:393:THR:HG21	1:A:518:LEU:HD12	1.98	0.45
3:D:134:CYS:HB2	3:D:148:TRP:CZ2	2.52	0.45
3:D:185:TRP:C	3:D:185:TRP:CD1	2.94	0.45
2:C:125:ALA:H	3:D:120:PRO:HG2	1.81	0.45
3:D:150:ALA:N	3:D:153:SER:O	2.50	0.45
3:D:158:GLY:HA2	3:D:178:LEU:HB2	1.98	0.45
2:C:177:SER:HB2	3:D:177:TYR:HE2	1.82	0.45
1:B:379:CYS:HA	1:B:432:CYS:HA	1.98	0.45
2:C:16:ARG:HD2	2:C:16:ARG:HA	1.66	0.45
2:C:154:TRP:CD2	2:C:156:SER:HB2	2.52	0.45
3:D:177:TYR:N	3:D:177:TYR:CD1	2.85	0.45
2:C:19:ARG:HG3	2:C:81:GLN:OE1	2.16	0.44
3:D:38:ARG:HH12	3:D:41:GLY:H	1.65	0.44
1:B:341:VAL:HG11	1:B:397:ALA:HB1	1.98	0.44
2:C:30:SER:O	2:C:52(A):TYR:HB2	2.17	0.44
2:E:18:LEU:HD12	2:E:19:ARG:H	1.83	0.44
3:D:40:PRO:O	6:D:301:HOH:O	2.21	0.44
3:D:180:LEU:HG	3:D:181:THR:O	2.18	0.44
3:D:187:SER:OG	3:D:188:HIS:N	2.50	0.44
1:B:368:LEU:HD22	1:B:377:PHE:HE1	1.82	0.44
1:A:403:ARG:NH1	1:A:405:ASP:OD2	2.50	0.44
2:C:38:ARG:HG2	2:C:48:VAL:HG22	1.99	0.44
2:C:201:LYS:HD2	2:C:201:LYS:HA	1.69	0.44
3:F:78:LEU:HD11	3:F:104:LEU:HD21	2.00	0.43
3:D:132:LEU:HD22	3:D:191:TYR:CE2	2.54	0.43
2:C:154:TRP:CD1	2:C:154:TRP:O	2.72	0.43
3:D:176:SER:C	3:D:177:TYR:CD1	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:SER:HA	1:B:369:TYR:CD2	2.54	0.43
2:C:16:ARG:HG3	2:C:17:SER:H	1.84	0.43
3:D:90:SER:OG	3:D:91:TYR:N	2.49	0.43
3:D:164:PRO:HD2	3:D:173:ALA:O	2.19	0.43
3:D:197:HIS:CE1	3:D:198:GLU:HG2	2.53	0.43
2:C:53:ASP:HB3	2:C:55:SER:H	1.83	0.42
2:C:153:SER:O	2:C:197:ASN:N	2.51	0.42
2:E:1:GLU:O	2:E:26:GLY:HA3	2.18	0.42
3:F:8:PRO:CD	3:F:22:SER:HB2	2.49	0.42
2:C:147:PRO:HD2	2:C:202:PRO:CG	2.48	0.42
3:D:180:LEU:HD13	3:D:191:TYR:OH	2.18	0.42
2:C:167:PRO:HD2	2:C:177:SER:O	2.19	0.42
1:B:393:THR:O	1:B:523:THR:OG1	2.36	0.42
2:C:36:TRP:NE1	2:C:80:LEU:HB2	2.35	0.42
2:E:38:ARG:HG3	2:E:48:VAL:HG21	2.01	0.42
1:A:354:ASN:O	1:A:398:ASP:HA	2.20	0.41
1:B:417:LYS:HG2	6:B:622:HOH:O	2.20	0.41
2:C:177:SER:HB2	3:D:177:TYR:CE2	2.55	0.41
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.56	0.41
2:C:139:GLY:HA3	2:C:180:SER:O	2.19	0.41
2:C:154:TRP:CE3	2:C:156:SER:HB2	2.55	0.41
3:D:180:LEU:HD22	3:D:191:TYR:CE2	2.56	0.41
3:D:180:LEU:HG	3:D:181:THR:N	2.35	0.41
2:C:146:PHE:HA	2:C:147:PRO:HA	1.82	0.41
2:C:164:HIS:O	2:C:178:LEU:HD11	2.21	0.41
2:C:207:VAL:HG12	2:C:208:ASP:N	2.36	0.41
1:B:408:ARG:HE	1:B:408:ARG:HB3	1.49	0.41
2:E:64:LYS:HE3	2:E:64:LYS:HB2	1.89	0.41
1:A:444:LYS:O	1:A:499:PRO:HD3	2.21	0.41
2:C:153:SER:HB3	2:C:154:TRP:H	1.72	0.41
3:D:169:ASN:C	3:D:171:LYS:H	2.29	0.41
1:B:406:GLU:HB3	1:B:418:ILE:HG13	2.02	0.41
3:D:121:SER:O	3:D:124:GLU:HB3	2.21	0.40
3:D:197:HIS:ND1	3:D:198:GLU:HG2	2.36	0.40
3:F:20:THR:HA	3:F:73:LEU:O	2.21	0.40
2:C:2:VAL:HG13	2:C:27:PHE:CD1	2.57	0.40
3:D:83:GLU:OE2	3:D:106:VAL:N	2.53	0.40
3:F:39:ARG:HB2	3:F:42:SER:HB3	2.04	0.40
2:C:66:ARG:H	2:C:66:ARG:HG2	1.53	0.40
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.57	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	196/204 (96%)	186 (95%)	10 (5%)	0	100	100
1	B	197/204 (97%)	188 (95%)	9 (5%)	0	100	100
2	C	211/224 (94%)	181 (86%)	27 (13%)	3 (1%)	9	19
2	E	118/224 (53%)	108 (92%)	10 (8%)	0	100	100
3	D	204/216 (94%)	181 (89%)	21 (10%)	2 (1%)	12	28
3	F	107/216 (50%)	101 (94%)	6 (6%)	0	100	100
All	All	1033/1288 (80%)	945 (92%)	83 (8%)	5 (0%)	24	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	119	PRO
2	C	201	LYS
3	D	121	SER
2	C	147	PRO
2	C	149	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	A	171/177 (97%)	171 (100%)	0	100	100
1	B	172/177 (97%)	171 (99%)	1 (1%)	78	91
2	C	178/187 (95%)	168 (94%)	10 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	96/187 (51%)	93 (97%)	3 (3%)	35	63
3	D	181/187 (97%)	169 (93%)	12 (7%)	15	34
3	F	95/187 (51%)	91 (96%)	4 (4%)	26	52
All	All	893/1102 (81%)	863 (97%)	30 (3%)	32	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	5	VAL
2	C	53	ASP
2	C	66	ARG
2	C	82	MET
2	C	82(A)	ASN
2	C	82(B)	SER
2	C	82(C)	LEU
2	C	92	CYS
2	C	140	CYS
2	C	204	ASN
3	D	20	THR
3	D	60	ASP
3	D	83	GLU
3	D	90	SER
3	D	103	LYS
3	D	148	TRP
3	D	162	THR
3	D	177	TYR
3	D	178	LEU
3	D	184	GLN
3	D	185	TRP
3	D	189	ARG
1	B	529	LYS
2	E	38	ARG
2	E	53	ASP
2	E	92	CYS
3	F	9	HIS
3	F	19	VAL
3	F	60	ASP
3	F	81	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	81	GLN
2	C	82(A)	ASN
2	C	197	ASN
3	D	169	ASN
3	D	184	GLN
1	B	360	ASN
1	B	531	HIS
2	E	3	GLN
2	E	56	ASN
2	E	76	ASN
3	F	53	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 ⓘ

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	1	1,4	14,14,15	0.45	0	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.27	0	17,19,21	0.49	0
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	0.71	0
4	FUC	G	4	4	10,10,11	1.01	0	14,14,16	1.32	2 (14%)
5	NAG	H	1	1,5	14,14,15	0.52	0	17,19,21	0.59	0
5	NAG	H	2	5	14,14,15	0.29	0	17,19,21	0.48	0
5	FUC	H	3	5	10,10,11	0.93	0	14,14,16	1.89	3 (21%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	FUC	O5-C5-C4	4.32	117.33	109.55
5	H	3	FUC	C1-O5-C5	4.07	122.56	112.97
4	G	4	FUC	C1-C2-C3	2.76	113.67	109.64
4	G	4	FUC	O5-C5-C4	2.74	114.48	109.55
5	H	3	FUC	C3-C4-C5	2.61	113.77	109.81

There are no chirality outliers.

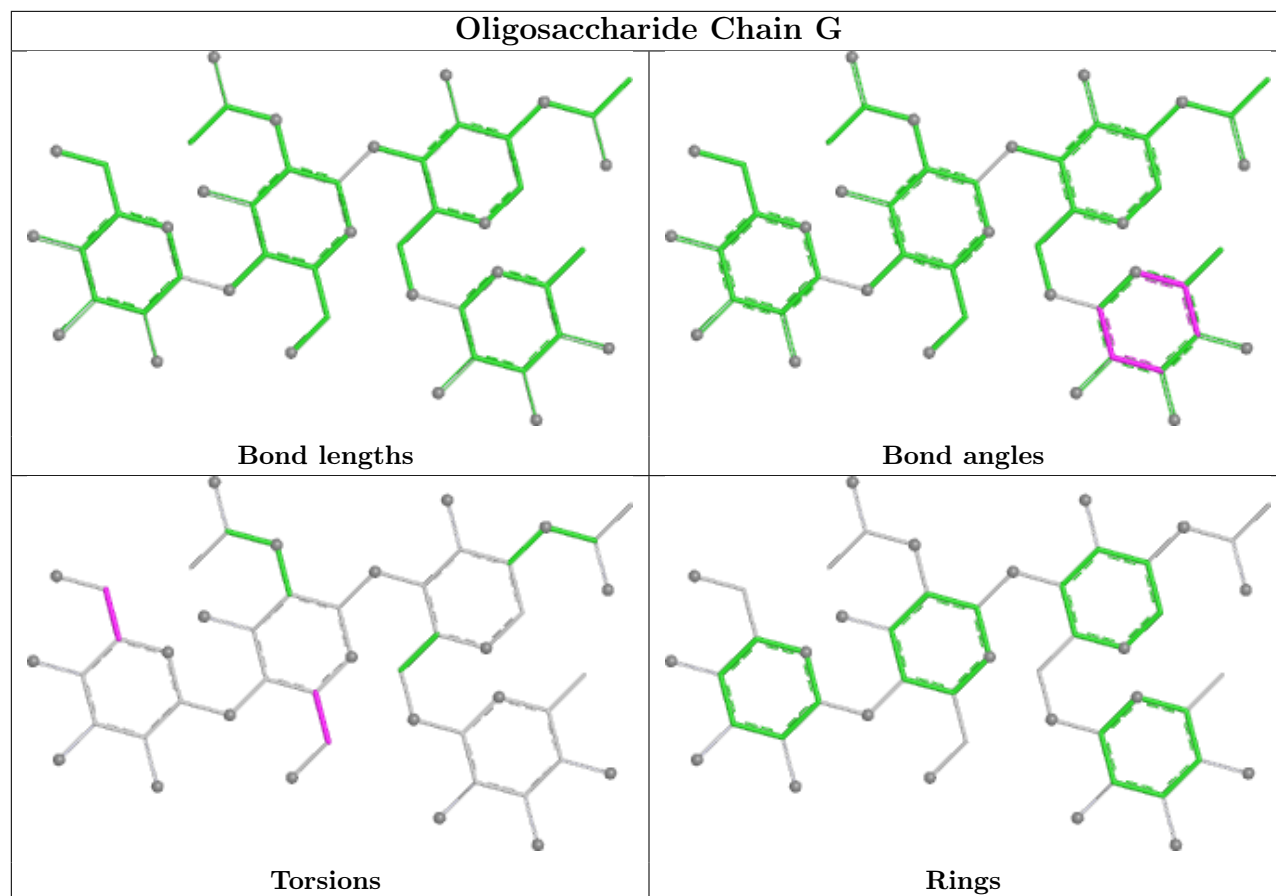
All (6) torsion outliers are listed below:

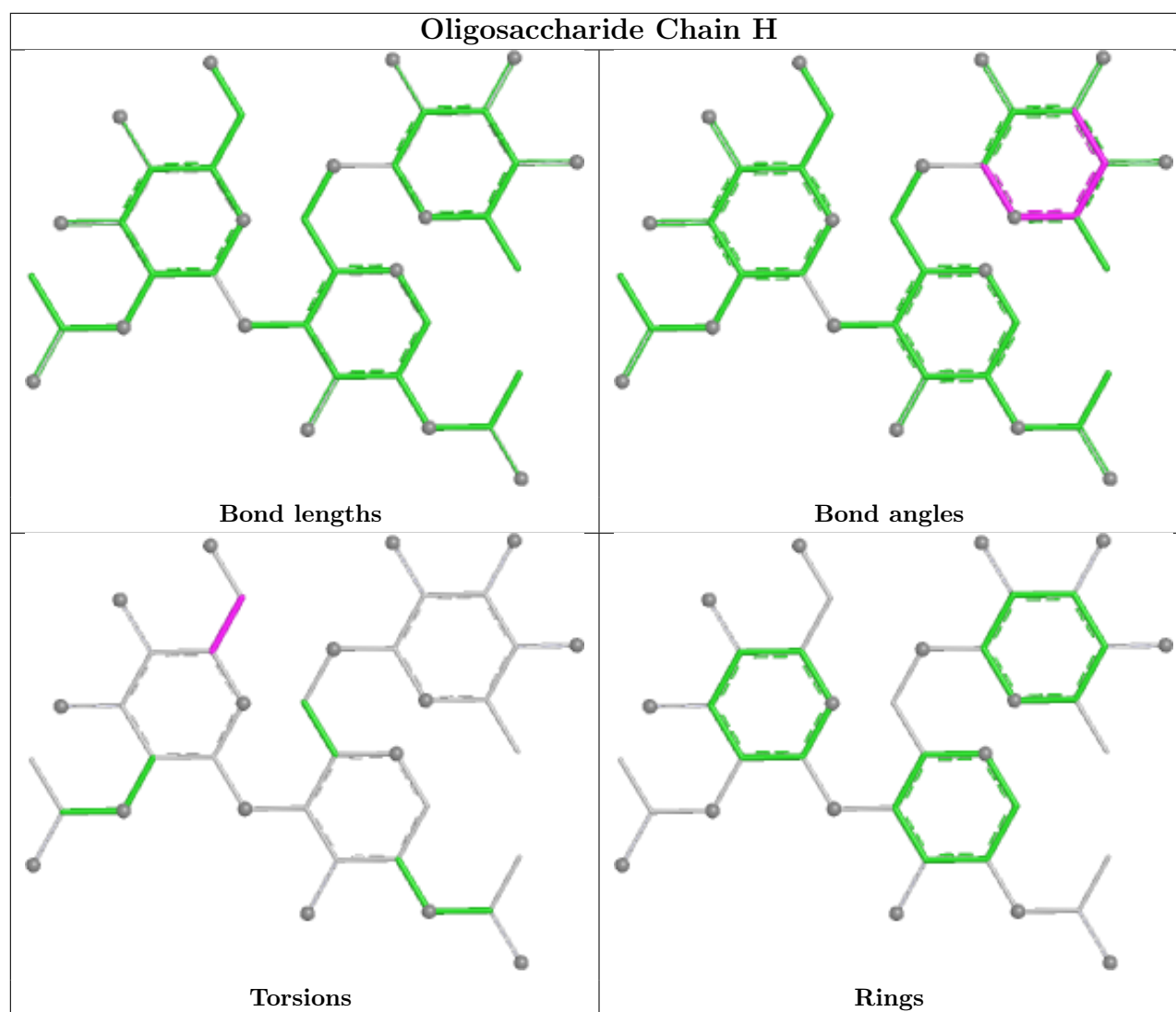
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	198/204 (97%)	-0.02	3 (1%) 72 68	32, 44, 73, 98	0
1	B	199/204 (97%)	-0.06	3 (1%) 72 68	29, 43, 64, 93	0
2	C	217/224 (96%)	1.30	63 (29%) 1 1	38, 91, 139, 161	0
2	E	120/224 (53%)	1.33	25 (20%) 2 2	40, 91, 130, 134	0
3	D	210/216 (97%)	1.19	58 (27%) 1 1	40, 75, 151, 160	0
3	F	109/216 (50%)	1.28	24 (22%) 2 2	42, 77, 111, 121	0
All	All	1053/1288 (81%)	0.77	176 (16%) 4 3	29, 62, 136, 161	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	158	ALA	7.5
3	D	208	PRO	5.3
3	D	191	TYR	5.2
3	D	209	THR	5.1
3	D	206	VAL	4.8
2	C	175	LEU	4.8
2	C	142	VAL	4.7
2	C	121	VAL	4.4
2	C	202	PRO	4.2
3	D	146	VAL	4.2
2	E	82(C)	LEU	4.1
1	B	531	HIS	3.9
2	C	161	SER	3.9
3	D	118	PHE	3.9
2	E	111	VAL	3.9
2	E	10	GLY	3.9
3	F	106	VAL	3.9
1	A	333	THR	3.9
3	D	127	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	194	TYR	3.8
3	D	160	GLU	3.8
2	C	159	LEU	3.8
3	F	39	ARG	3.8
3	D	131	THR	3.7
2	E	84	ALA	3.7
3	D	130	ALA	3.7
2	C	141	LEU	3.6
2	C	157	GLY	3.6
3	D	109	PRO	3.6
3	D	119	PRO	3.6
3	D	115	VAL	3.6
2	C	119	PRO	3.4
3	D	207	ALA	3.4
3	F	11	VAL	3.4
2	C	195	ILE	3.4
2	C	180	SER	3.4
3	D	181	THR	3.3
2	C	154	TRP	3.3
3	F	104	LEU	3.3
2	C	182	VAL	3.3
3	D	185	TRP	3.3
3	F	85	ASP	3.3
3	D	182	PRO	3.3
2	C	200	HIS	3.3
3	D	134	CYS	3.2
3	F	105	THR	3.2
1	B	333	THR	3.2
2	C	152	VAL	3.2
2	C	183	THR	3.2
3	D	180	LEU	3.1
3	D	179	SER	3.1
2	C	176	TYR	3.1
3	F	83	GLU	3.1
3	D	120	PRO	3.1
2	C	193	THR	3.1
2	C	168	ALA	3.1
3	F	43	ALA	3.1
3	D	202	VAL	3.1
3	D	132	LEU	3.0
2	C	155	ASN	3.0
3	D	174	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	122	PHE	3.0
3	D	147	ALA	3.0
2	C	150	VAL	3.0
3	D	168	SER	3.0
2	C	140	CYS	3.0
2	C	114	ALA	3.0
2	C	170	LEU	2.9
3	F	21	ILE	2.9
3	D	117	LEU	2.9
2	C	151	THR	2.9
2	C	211	VAL	2.9
2	E	5	VAL	2.9
2	C	145	TYR	2.8
3	D	158	GLY	2.8
3	D	135	LEU	2.8
3	D	148	TRP	2.8
2	C	112	SER	2.8
2	C	117	LYS	2.8
3	D	190	SER	2.8
3	D	155	VAL	2.8
3	F	41	GLY	2.8
2	C	116	THR	2.8
3	D	176	SER	2.7
3	D	133	VAL	2.7
3	F	15	PRO	2.7
3	D	108	GLN	2.7
3	D	125	LEU	2.7
2	E	87	THR	2.7
3	D	163	THR	2.7
3	F	40	PRO	2.7
3	D	142	GLY	2.7
2	C	156	SER	2.7
2	E	14	PRO	2.7
2	E	41	PRO	2.6
2	C	198	VAL	2.6
2	C	160	THR	2.6
3	D	194	GLN	2.6
2	C	138	LEU	2.6
3	D	150	ALA	2.6
3	F	78	LEU	2.5
2	E	103	TRP	2.5
2	C	162	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	44	PRO	2.5
3	D	157	ALA	2.5
3	F	84	ALA	2.5
3	D	136	ILE	2.4
1	A	530	SER	2.4
2	C	209	LYS	2.4
2	E	109	VAL	2.4
2	C	125	ALA	2.4
3	D	187	SER	2.4
2	C	123	PRO	2.4
3	F	86	TYR	2.4
2	E	80	LEU	2.4
2	E	94	ASN	2.4
3	D	114	SER	2.4
2	C	174	GLY	2.4
3	D	116	THR	2.3
3	D	192	SER	2.3
3	F	14	SER	2.3
3	F	8	PRO	2.3
2	C	184	VAL	2.3
2	E	45	LEU	2.3
3	D	175	SER	2.3
2	E	46	GLU	2.3
3	D	137	SER	2.3
2	E	36	TRP	2.3
2	C	146	PHE	2.3
2	C	189	LEU	2.3
1	A	519	HIS	2.3
2	C	131	THR	2.3
3	D	110	LYS	2.3
3	D	171	LYS	2.3
2	E	91	TYR	2.3
2	C	139	GLY	2.3
2	E	18	LEU	2.3
1	B	370	ASN	2.2
3	D	154	PRO	2.2
2	C	9	GLY	2.2
3	D	111	ALA	2.2
2	C	177	SER	2.2
2	E	27	PHE	2.2
2	E	24	ALA	2.2
3	F	18	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	83	ARG	2.2
2	C	124	LEU	2.2
2	C	178	LEU	2.2
2	C	81	GLN	2.2
3	F	13	GLU	2.1
3	D	199	GLY	2.1
2	C	149	PRO	2.1
3	D	166	LYS	2.1
2	C	15	GLY	2.1
3	F	80	THR	2.1
2	C	210	LYS	2.1
3	D	170	ASN	2.1
2	C	164	HIS	2.1
3	F	87	TYR	2.1
2	C	207	VAL	2.1
3	F	19	VAL	2.1
2	E	29	PHE	2.1
3	F	62	PHE	2.1
2	E	78	LEU	2.1
2	C	163	VAL	2.1
2	C	169	VAL	2.1
2	C	166	PHE	2.1
2	E	85	GLU	2.0
2	C	115	SER	2.0
2	C	132	SER	2.0
3	D	186	LYS	2.0
2	C	165	THR	2.0
3	D	184	GLN	2.0
2	E	95	GLY	2.0
2	E	40	ALA	2.0
3	D	159	VAL	2.0

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

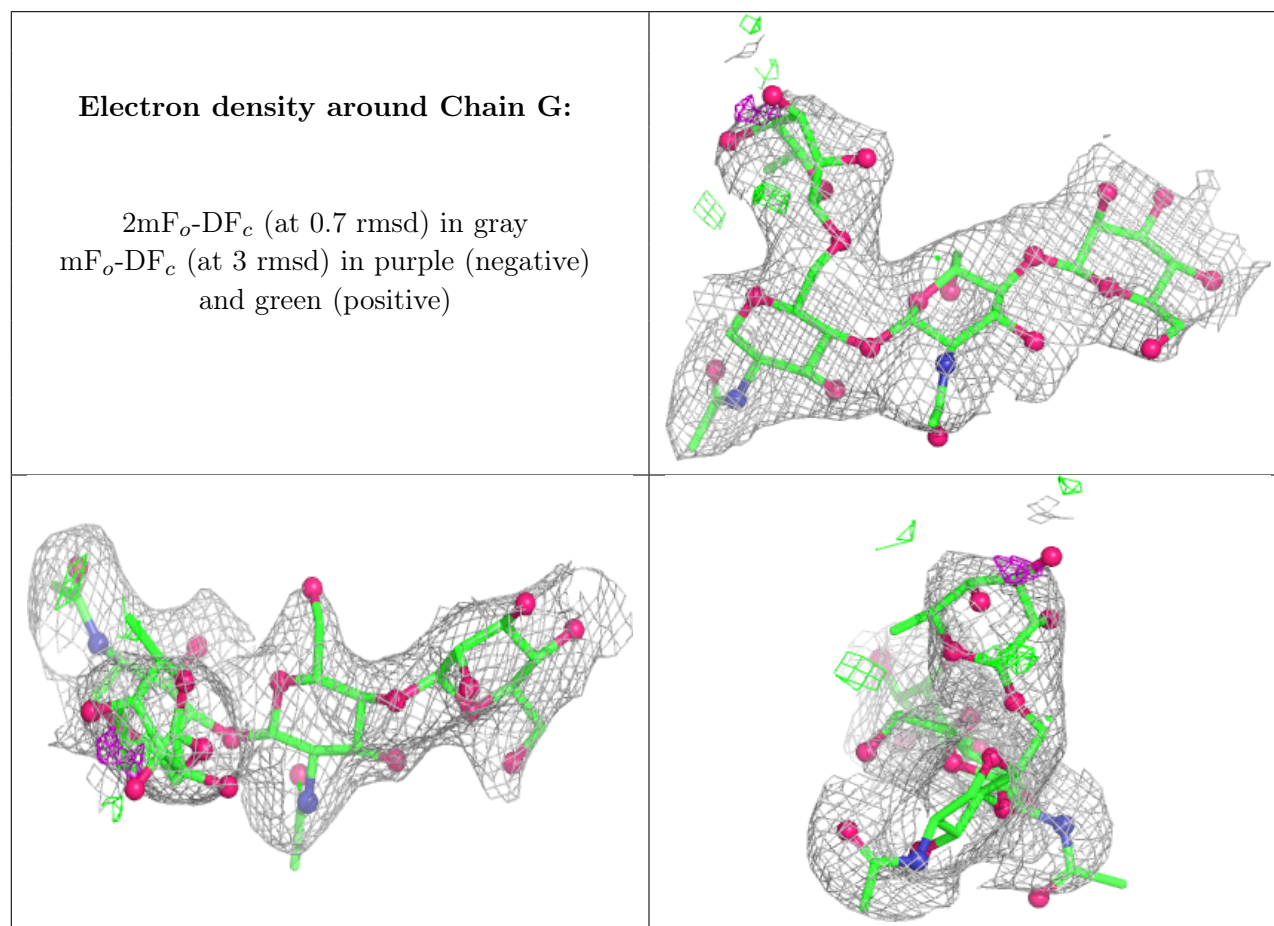
There are no non-standard protein/DNA/RNA residues in this entry.

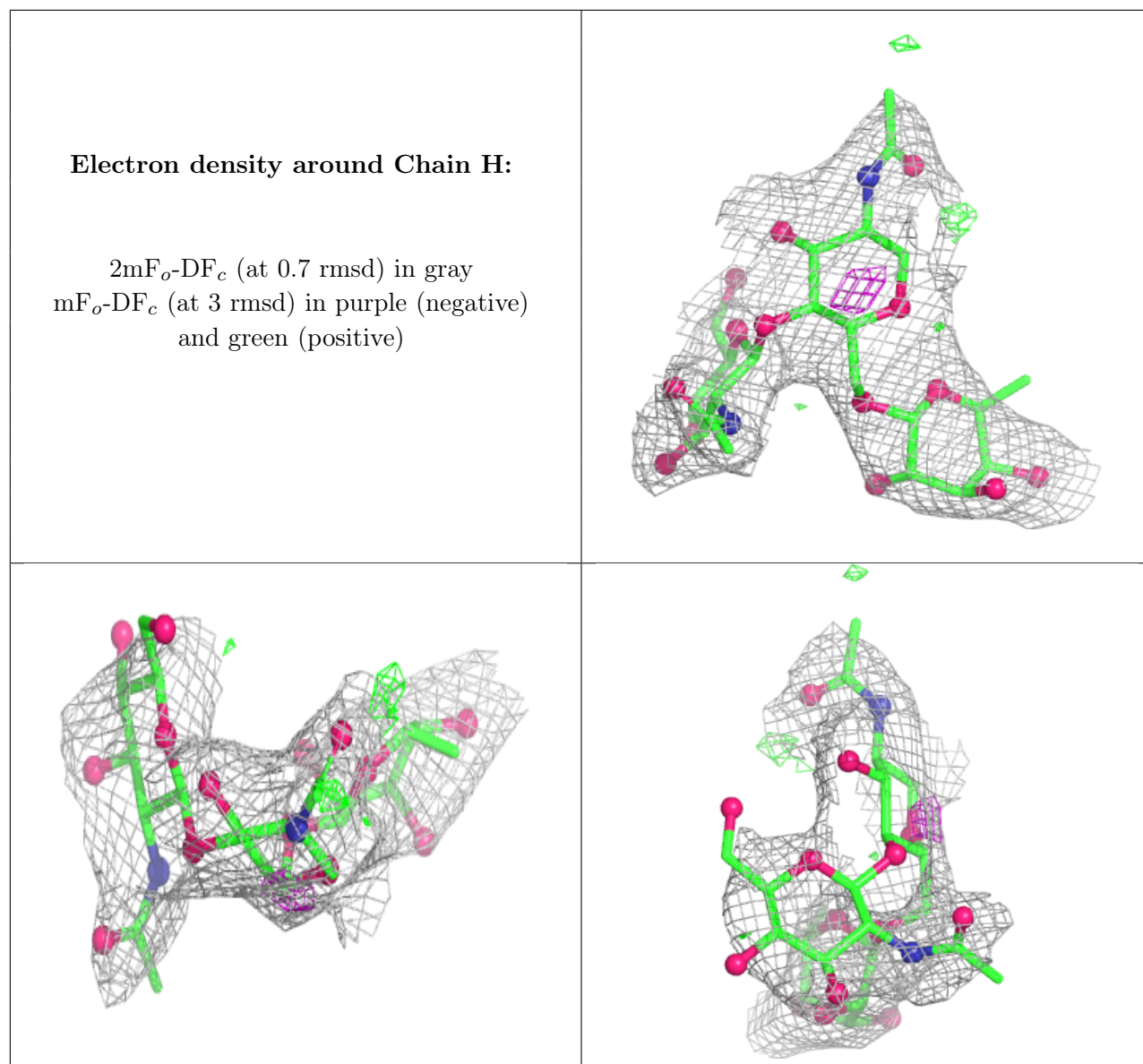
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
4	BMA	G	3	11/12	0.50	0.11	114,120,123,123	0
5	NAG	H	2	14/15	0.64	0.12	98,106,113,118	0
4	FUC	G	4	10/11	0.73	0.20	72,83,90,93	0
5	NAG	H	1	14/15	0.75	0.13	69,80,96,96	0
4	NAG	G	2	14/15	0.76	0.12	100,105,112,113	0
4	NAG	G	1	14/15	0.83	0.11	71,78,88,96	0
5	FUC	H	3	10/11	0.84	0.16	75,87,92,95	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.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.