



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2022 – 04:13 PM JST

PDB ID : 7VN9  
Title : Crystal structure of human coronavirus 229E spike protein receptor-binding domain in complex with C04 Fab  
Authors : Xiang, J.C.; Yang, B.  
Deposited on : 2021-10-10  
Resolution : 4.49 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

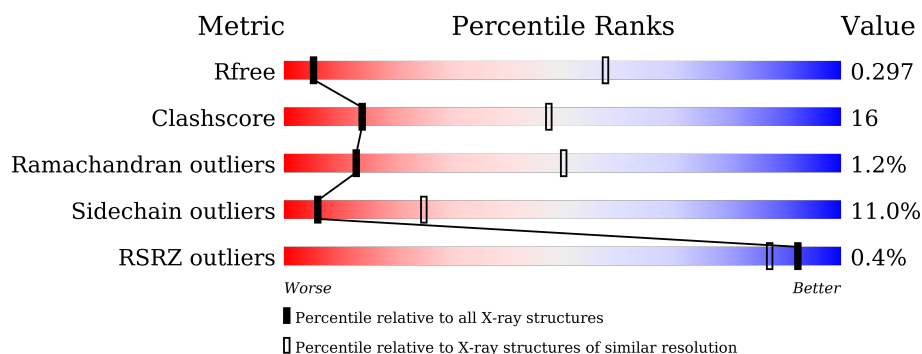
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.49 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.




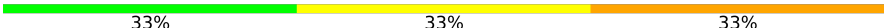
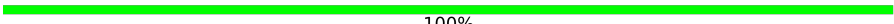
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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  $\geq 3$ , 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	231	<div> <div>%</div> <div> <div>52%</div> <div>35%</div> <div>5%</div> <div>7%</div> </div> </div>
1	H	231	<div> <div>68%</div> <div>24%</div> <div>• 6%</div> </div>
2	B	215	<div> <div>61%</div> <div>27%</div> <div>• 8%</div> </div>
2	L	215	<div> <div>65%</div> <div>31%</div> <div>• •</div> </div>
3	C	148	<div> <div>%</div> <div>53%</div> <div>34%</div> <div>• 9%</div> </div>
3	E	148	<div> <div>%</div> <div>47%</div> <div>39%</div> <div>5%</div> <div>9%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	D	3	 33% 67%
4	G	3	 33% 33% 33%
5	F	2	 100%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8541 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 C04 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1617	1027	269	316	5			
1	A	215	Total	C	N	O	S	0	0	0
			1590	1009	265	311	5			

- Molecule 2 is a protein called C04 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1630	1021	274	330	5			
2	B	198	Total	C	N	O	S	0	0	0
			1515	950	253	307	5			

- Molecule 3 is a protein called Spike glycoprotein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	134	Total	C	N	O	S	0	0	0
			1036	677	165	187	7			
3	C	135	Total	C	N	O	S	0	0	0
			1033	671	168	187	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLU	-	expression tag	UNP P15423
E	437	ASN	-	expression tag	UNP P15423
E	438	LEU	-	expression tag	UNP P15423
E	439	TYR	-	expression tag	UNP P15423
E	440	PHE	-	expression tag	UNP P15423
E	441	GLN	-	expression tag	UNP P15423
C	436	GLU	-	expression tag	UNP P15423
C	437	ASN	-	expression tag	UNP P15423

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	438	LEU	-	expression tag	UNP P15423
C	439	TYR	-	expression tag	UNP P15423
C	440	PHE	-	expression tag	UNP P15423
C	441	GLN	-	expression tag	UNP P15423

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



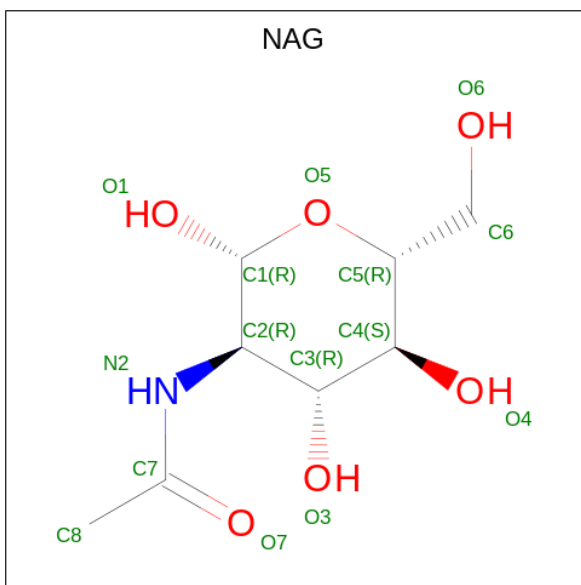
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

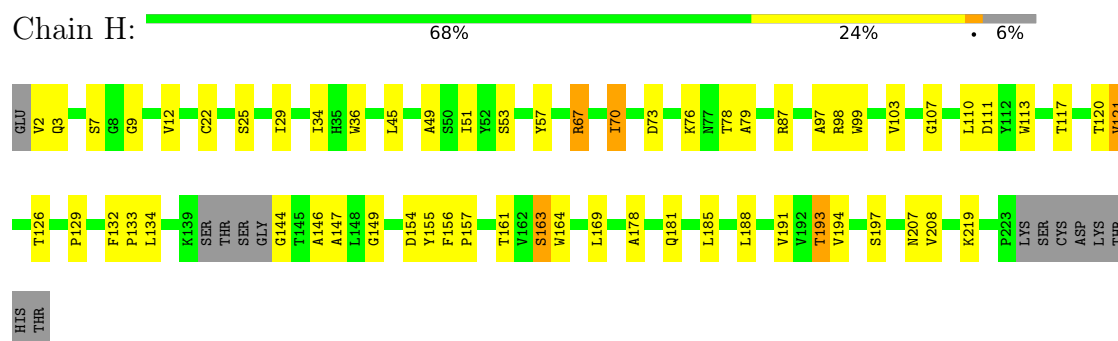


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

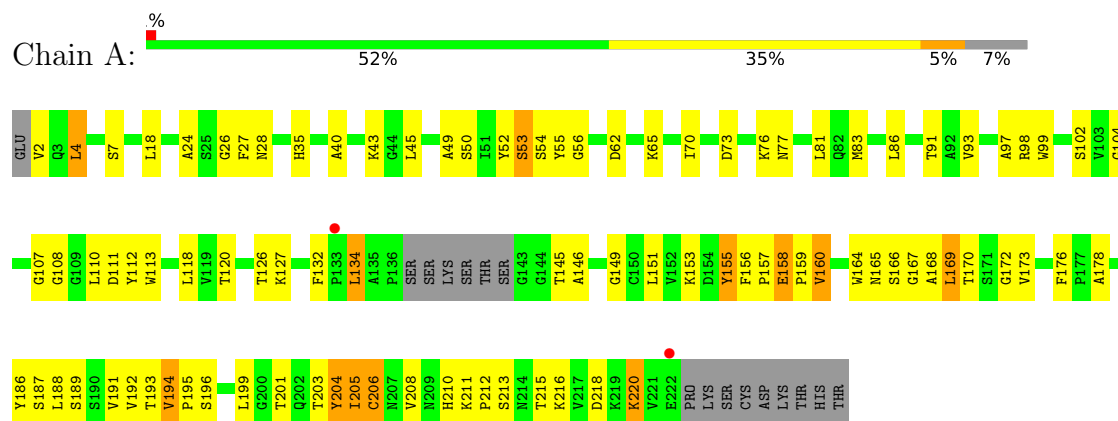
### 3 Residue-property plots

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

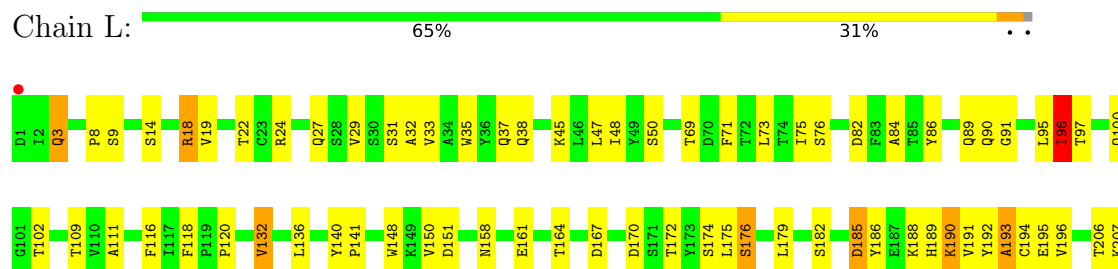
#### • Molecule 1: C04 Fab heavy chain

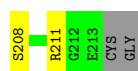


#### • Molecule 1: C04 Fab heavy chain



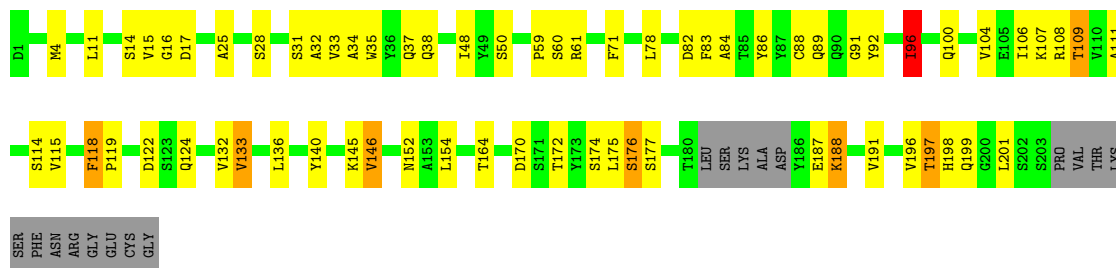
#### • Molecule 2: C04 Fab light chain





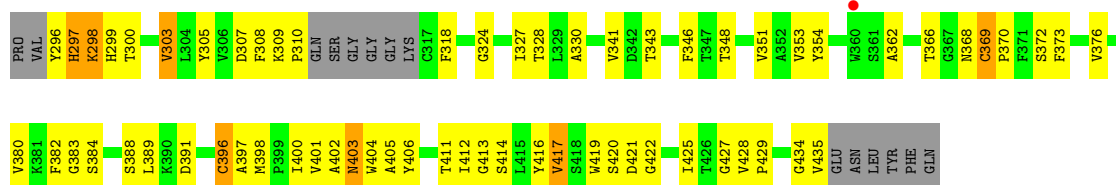
- Molecule 2: C04 Fab light chain

Chain B: 61% 27% 8%



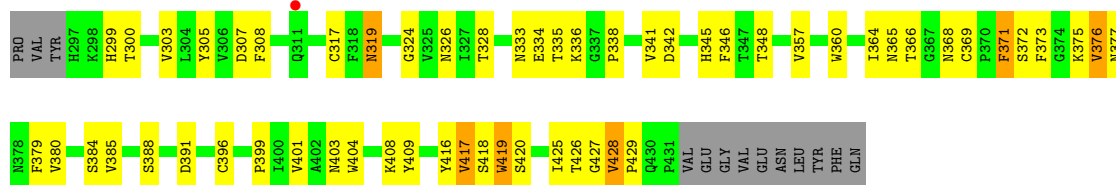
- Molecule 3: Spike glycoprotein S1

Chain E: 47% 39% 5% 9%



- Molecule 3: Spike glycoprotein S1

Chain C: 53% 34% 9%



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

Chain D: 33% 67%



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

Chain G: 33% 33% 33%





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.73Å 183.73Å 255.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.66 – 4.49 42.66 – 4.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.66-4.49) 99.4 (42.66-4.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.273 , 0.288 0.284 , 0.297	Depositor DCC
$R_{free}$ test set	797 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	169.7	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 204.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.40	0/1631	0.67	0/2226
1	H	0.34	0/1659	0.59	1/2264 (0.0%)
2	B	0.43	0/1547	0.70	1/2100 (0.0%)
2	L	0.36	0/1665	0.57	0/2260
3	C	0.61	0/1067	0.93	0/1454
3	E	0.59	0/1070	0.90	0/1460
All	All	0.45	0/8639	0.71	2/11764 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	144	GLY	N-CA-C	-5.62	99.05	113.10
2	B	118	PHE	CB-CA-C	5.14	120.68	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1590	0	1533	74	8
1	H	1617	0	1569	30	0
2	B	1515	0	1474	37	9
2	L	1630	0	1591	46	0
3	C	1033	0	983	41	8
3	E	1036	0	983	45	9
4	D	39	0	34	1	0
4	G	39	0	34	1	0
5	F	28	0	25	0	0
6	C	14	0	13	0	0
All	All	8541	0	8239	264	17

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 16.

All (264) 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)
3:C:333:ASN:HB2	3:C:336:LYS:HB2	1.44	1.00
1:A:93:VAL:HG13	1:A:118:LEU:HD23	1.50	0.94
1:H:97:ALA:HB1	1:H:110:LEU:HD21	1.54	0.89
1:A:203:THR:HG21	1:A:220:LYS:HG3	1.54	0.88
3:E:307:ASP:HB2	3:E:353:VAL:HB	1.58	0.86
3:E:368:ASN:HB2	3:E:397:ALA:H	1.39	0.85
2:B:82:ASP:O	2:B:86:TYR:OH	1.94	0.85
1:H:129:PRO:HB3	1:H:155:TYR:HB3	1.64	0.79
1:A:93:VAL:HG13	1:A:118:LEU:CD2	2.13	0.79
1:A:169:LEU:HD23	1:A:204:TYR:HB2	1.65	0.78
1:A:208:VAL:O	1:A:216:LYS:HA	1.84	0.77
2:B:28:SER:HB3	3:C:342:ASP:HB3	1.67	0.77
3:E:380:VAL:H	3:E:427:GLY:HA3	1.52	0.75
1:A:164:TRP:HA	1:A:205:ILE:O	1.88	0.74
1:A:203:THR:OG1	1:A:220:LYS:NZ	2.20	0.74
2:L:150:VAL:HA	2:L:192:TYR:HB2	1.71	0.72
1:A:127:LYS:HB2	1:A:156:PHE:HB3	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:360:TRP:HA	3:C:404:TRP:HA	1.71	0.71
1:A:93:VAL:HG22	1:A:118:LEU:CD2	2.20	0.71
3:E:369:CYS:HB3	3:E:419:TRP:HZ2	1.55	0.70
1:A:24:ALA:O	1:A:77:ASN:ND2	2.25	0.70
3:E:391:ASP:HA	3:E:416:TYR:CG	2.27	0.70
1:A:73:ASP:HB3	1:A:76:LYS:HB2	1.73	0.70
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.74	0.70
1:H:156:PHE:HB2	1:H:185:LEU:HD23	1.75	0.69
3:E:370:PRO:HD3	3:C:379:PHE:HB2	1.74	0.69
1:A:91:THR:HG23	1:A:120:THR:HA	1.73	0.68
3:E:308:PHE:HA	3:E:324:GLY:O	1.96	0.66
1:H:73:ASP:HB3	1:H:76:LYS:HB2	1.77	0.66
2:L:91:GLY:HA3	2:L:96:ILE:HG22	1.78	0.65
3:E:297:HIS:O	3:E:298:LYS:HB2	1.96	0.65
3:C:391:ASP:HA	3:C:416:TYR:CG	2.32	0.64
1:A:70:ILE:HD13	1:A:81:LEU:HD13	1.80	0.64
1:A:160:VAL:HG21	1:A:188:LEU:HD21	1.79	0.64
2:L:8:PRO:O	2:L:102:THR:OG1	2.10	0.64
3:E:307:ASP:OD1	3:E:354:TYR:HA	1.98	0.64
3:C:419:TRP:HA	3:C:419:TRP:CE3	2.32	0.64
1:A:206:CYS:H	1:A:220:LYS:HE3	1.62	0.63
1:A:194:VAL:HG12	1:A:195:PRO:HD2	1.81	0.63
3:C:369:CYS:HB3	3:C:371:PHE:HD1	1.64	0.63
2:L:164:THR:HG1	2:L:174:SER:H	1.45	0.63
2:B:28:SER:CB	3:C:342:ASP:HB3	2.28	0.63
1:H:178:ALA:HA	1:H:188:LEU:HB3	1.81	0.62
2:L:136:LEU:HD13	2:L:175:LEU:HB3	1.79	0.62
2:B:146:VAL:HG21	2:B:197:THR:H	1.64	0.62
3:C:360:TRP:CE2	3:C:404:TRP:HB2	2.34	0.62
3:C:403:ASN:HB3	3:C:409:TYR:HA	1.80	0.62
1:H:98:ARG:NH2	1:H:111:ASP:OD2	2.25	0.62
3:C:384:SER:HB3	3:C:420:SER:HB3	1.80	0.62
3:E:396:CYS:HB3	3:E:417:VAL:HG22	1.81	0.61
1:A:149:GLY:HA3	1:A:191:VAL:HG12	1.82	0.61
1:A:62:ASP:HA	1:A:65:LYS:HB2	1.82	0.61
2:L:150:VAL:HA	2:L:192:TYR:CB	2.30	0.61
2:B:164:THR:HG1	2:B:174:SER:H	1.49	0.61
2:B:59:PRO:HB2	2:B:61:ARG:HG2	1.84	0.60
2:L:193:ALA:HB3	2:L:208:SER:HA	1.83	0.60
3:E:382:PHE:HB2	3:E:425:ILE:HB	1.83	0.60
2:L:35:TRP:CE2	2:L:73:LEU:HB2	2.36	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:120:PRO:HD3	2:L:132:VAL:HG13	1.84	0.60
2:L:38:GLN:O	2:L:84:ALA:HB1	2.03	0.59
2:B:146:VAL:CG2	2:B:197:THR:H	2.16	0.59
2:B:164:THR:HG21	2:B:174:SER:HB2	1.84	0.59
3:E:401:VAL:HG12	3:E:411:THR:HA	1.84	0.59
2:B:119:PRO:HA	2:B:132:VAL:HG13	1.85	0.59
3:C:299:HIS:HA	3:C:345:HIS:HB2	1.84	0.59
1:A:102:SER:HB2	1:A:107:GLY:HA3	1.84	0.59
1:A:206:CYS:H	1:A:220:LYS:CE	2.15	0.59
1:A:167:GLY:O	1:A:204:TYR:HB3	2.02	0.59
3:E:305:TYR:HA	3:E:351:VAL:HB	1.84	0.58
2:B:170:ASP:O	2:B:172:THR:HG23	2.03	0.58
3:C:307:ASP:HB3	3:C:326:ASN:HB3	1.84	0.58
1:A:99:TRP:NE1	1:A:108:GLY:HA2	2.21	0.56
1:A:166:SER:HB2	1:A:205:ILE:HG21	1.86	0.56
3:C:365:ASN:O	3:C:399:PRO:HD2	2.06	0.56
1:A:169:LEU:HD12	1:A:170:THR:N	2.21	0.56
1:H:29:ILE:HB	1:H:34:ILE:HD11	1.88	0.56
3:E:341:VAL:HG12	3:E:343:THR:H	1.72	0.55
2:L:29:VAL:HG21	2:L:90:GLN:HG3	1.88	0.55
1:A:4:LEU:HD11	1:A:97:ALA:HA	1.87	0.55
1:A:206:CYS:H	1:A:220:LYS:NZ	2.05	0.55
3:E:303:VAL:HG23	3:E:330:ALA:HB2	1.88	0.54
3:E:307:ASP:HB2	3:E:353:VAL:CB	2.34	0.54
1:A:155:TYR:O	1:A:186:TYR:HB2	2.08	0.54
1:H:146:ALA:HA	2:L:116:PHE:CE1	2.43	0.54
1:A:178:ALA:HA	1:A:188:LEU:HB3	1.90	0.54
3:C:371:PHE:CD1	3:C:419:TRP:HZ2	2.26	0.54
1:H:2:VAL:HA	1:H:25:SER:O	2.08	0.53
3:E:348:THR:HB	3:E:373:PHE:CZ	2.42	0.53
4:G:1:NAG:H4	4:G:2:NAG:C7	2.38	0.53
3:C:384:SER:HB3	3:C:420:SER:CB	2.39	0.53
2:L:186:TYR:CE1	2:L:211:ARG:HD3	2.43	0.53
1:A:98:ARG:HG2	1:A:99:TRP:H	1.73	0.53
1:H:49:ALA:HB3	1:H:70:ILE:HD11	1.91	0.52
2:B:136:LEU:HD13	2:B:175:LEU:HB3	1.91	0.52
3:C:319:ASN:HB2	3:C:408:LYS:HD3	1.90	0.52
1:H:110:LEU:HD22	1:H:113:TRP:NE1	2.24	0.52
1:H:134:LEU:HB3	2:L:118:PHE:CD2	2.44	0.52
3:E:370:PRO:HD2	3:E:419:TRP:CZ2	2.45	0.52
1:A:98:ARG:HG2	1:A:99:TRP:N	2.24	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:372:SER:O	3:E:376:VAL:HG23	2.10	0.52
1:A:134:LEU:HD22	1:A:151:LEU:HB2	1.91	0.52
1:H:163:SER:HB3	1:H:207:ASN:HB2	1.92	0.52
2:L:164:THR:HG21	2:L:174:SER:HB2	1.91	0.51
3:E:400:ILE:HB	3:E:413:GLY:HA3	1.90	0.51
1:A:210:HIS:HB3	1:A:213:SER:OG	2.10	0.51
2:L:31:SER:H	3:E:384:SER:HB2	1.75	0.51
3:E:383:GLY:HA3	3:E:422:GLY:HA3	1.91	0.51
1:A:52:TYR:CE2	1:A:54:SER:HB3	2.45	0.51
2:B:34:ALA:HA	2:B:48:ILE:O	2.11	0.51
3:C:428:VAL:HG12	3:C:429:PRO:HD2	1.93	0.51
3:E:307:ASP:HA	3:E:354:TYR:N	2.26	0.51
1:A:203:THR:CG2	1:A:220:LYS:HG3	2.35	0.51
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.45	0.51
3:C:419:TRP:HA	3:C:419:TRP:HE3	1.73	0.51
2:L:19:VAL:CG2	2:L:75:ILE:HB	2.41	0.51
3:C:369:CYS:N	3:C:396:CYS:HB2	2.26	0.51
1:H:12:VAL:O	1:H:121:VAL:HA	2.11	0.51
3:E:309:LYS:HD2	3:E:310:PRO:HD2	1.93	0.51
1:A:104:GLY:HA3	3:C:419:TRP:O	2.11	0.50
1:A:93:VAL:CG1	1:A:118:LEU:HD23	2.33	0.50
2:L:193:ALA:CB	2:L:208:SER:HA	2.41	0.50
2:L:190:LYS:HG3	2:L:191:VAL:HG23	1.92	0.50
1:A:145:THR:HG22	1:A:146:ALA:H	1.76	0.50
2:L:148:TRP:CD2	2:L:179:LEU:HD22	2.47	0.49
1:A:93:VAL:HG22	1:A:118:LEU:HD22	1.94	0.49
2:B:114:SER:O	2:B:136:LEU:HA	2.12	0.49
2:B:32:ALA:HB1	2:B:91:GLY:O	2.12	0.49
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.47	0.49
1:H:163:SER:N	1:H:207:ASN:O	2.44	0.49
1:A:169:LEU:HD12	1:A:170:THR:H	1.76	0.49
3:E:384:SER:O	3:E:420:SER:HB3	2.12	0.48
1:A:4:LEU:N	1:A:4:LEU:HD23	2.27	0.48
3:E:383:GLY:CA	3:E:422:GLY:HA3	2.43	0.48
3:E:434:GLY:O	3:E:435:VAL:C	2.51	0.48
2:L:35:TRP:O	2:L:47:LEU:HB2	2.13	0.48
2:B:108:ARG:HH21	2:B:109:THR:HB	1.79	0.48
1:H:161:THR:O	1:H:208:VAL:HA	2.13	0.48
1:A:99:TRP:HE1	1:A:108:GLY:HA2	1.78	0.48
1:A:176:PHE:HB2	1:A:189:SER:O	2.14	0.48
2:L:193:ALA:HB3	2:L:207:LYS:O	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:400:ILE:HB	3:E:413:GLY:CA	2.44	0.48
3:E:404:TRP:O	3:E:405:ALA:C	2.53	0.48
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.95	0.47
2:L:170:ASP:O	2:L:172:THR:HG23	2.13	0.47
2:B:38:GLN:O	2:B:84:ALA:HB1	2.14	0.47
1:H:98:ARG:HG2	1:H:99:TRP:N	2.29	0.47
1:H:22:CYS:HB2	1:H:36:TRP:CZ2	2.50	0.47
1:A:153:LYS:HA	1:A:187:SER:HB2	1.96	0.47
2:L:3:GLN:HA	2:L:97:THR:HG21	1.95	0.47
2:B:25:ALA:HB1	2:B:28:SER:O	2.15	0.47
3:C:333:ASN:HB3	3:C:336:LYS:H	1.80	0.47
2:B:146:VAL:HG23	2:B:196:VAL:HB	1.97	0.47
3:C:376:VAL:HG12	3:C:380:VAL:HG21	1.96	0.46
2:L:9:SER:O	2:L:102:THR:HA	2.16	0.46
3:E:403:ASN:HB2	3:E:406:TYR:HA	1.96	0.46
2:L:148:TRP:CE2	2:L:179:LEU:HB2	2.51	0.46
2:L:161:GLU:HA	2:L:176:SER:O	2.15	0.46
1:A:49:ALA:HB3	1:A:70:ILE:HD11	1.96	0.46
2:B:31:SER:O	2:B:50:SER:HA	2.16	0.46
2:B:83:PHE:HB2	2:B:106:ILE:HD11	1.97	0.46
1:A:110:LEU:HD12	1:A:113:TRP:CZ2	2.51	0.46
3:C:384:SER:HA	3:C:425:ILE:HD12	1.96	0.46
2:B:111:ALA:HB3	2:B:140:TYR:N	2.31	0.46
3:E:369:CYS:CA	3:E:396:CYS:HB2	2.39	0.46
1:A:111:ASP:OD1	1:A:112:TYR:N	2.48	0.46
1:A:210:HIS:O	1:A:213:SER:N	2.49	0.46
2:B:188:LYS:HD2	2:B:188:LYS:HA	1.67	0.46
3:C:377:ASN:HB3	3:C:429:PRO:HA	1.98	0.46
2:L:32:ALA:HB1	2:L:91:GLY:O	2.15	0.45
2:B:198:HIS:CG	2:B:199:GLN:H	2.34	0.45
2:B:92:TYR:N	2:B:96:ILE:HG22	2.31	0.45
3:C:372:SER:HB3	3:C:375:LYS:HB2	1.98	0.45
3:C:305:TYR:HB2	3:C:328:THR:HB	1.99	0.45
2:L:185:ASP:HA	2:L:188:LYS:HD2	1.98	0.45
2:B:133:VAL:HA	2:B:177:SER:O	2.16	0.45
2:L:132:VAL:HG23	2:L:179:LEU:HB3	1.99	0.45
1:A:97:ALA:HB3	1:A:110:LEU:HD13	1.97	0.45
1:A:164:TRP:O	1:A:168:ALA:HA	2.16	0.45
1:A:166:SER:HB2	1:A:205:ILE:CG2	2.45	0.45
2:B:198:HIS:CG	2:B:199:GLN:N	2.84	0.45
1:H:154:ASP:OD1	1:H:181:GLN:NE2	2.42	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:362:ALA:HA	3:E:402:ALA:HA	1.98	0.45
1:A:134:LEU:HB3	2:B:118:PHE:CE2	2.52	0.45
1:A:156:PHE:HA	1:A:157:PRO:HA	1.52	0.45
1:A:204:TYR:HD1	1:A:204:TYR:HA	1.75	0.45
1:A:102:SER:CB	1:A:107:GLY:HA3	2.47	0.45
1:A:166:SER:HB2	1:A:205:ILE:CB	2.47	0.45
2:L:195:GLU:HG2	2:L:196:VAL:N	2.32	0.44
2:L:37:GLN:O	2:L:45:LYS:N	2.43	0.44
1:A:170:THR:O	1:A:172:GLY:N	2.50	0.44
3:C:338:PRO:HA	3:C:388:SER:HB2	1.99	0.44
1:A:157:PRO:HD2	1:A:212:PRO:HG2	2.00	0.44
2:B:132:VAL:HG12	2:B:133:VAL:H	1.83	0.44
1:A:132:PHE:CG	2:B:124:GLN:HG3	2.52	0.44
2:L:148:TRP:CE3	2:L:179:LEU:HD22	2.53	0.44
3:E:391:ASP:HA	3:E:416:TYR:CD1	2.53	0.44
2:L:95:LEU:O	2:L:96:ILE:HG12	2.17	0.44
1:A:35:HIS:ND1	1:A:50:SER:HB3	2.32	0.44
1:A:153:LYS:HA	1:A:187:SER:CB	2.48	0.44
1:A:210:HIS:CE1	1:A:212:PRO:HB2	2.53	0.44
1:H:98:ARG:HG2	1:H:99:TRP:H	1.82	0.44
1:A:40:ALA:HB3	1:A:43:LYS:HB2	2.00	0.44
1:A:213:SER:C	1:A:215:THR:N	2.71	0.44
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.48	0.44
1:A:27:PHE:CE1	1:A:98:ARG:HD2	2.53	0.43
3:C:348:THR:HB	3:C:373:PHE:CZ	2.53	0.43
3:E:300:THR:O	3:E:346:PHE:HA	2.18	0.43
3:E:369:CYS:HB3	3:E:396:CYS:HB2	1.61	0.43
1:A:2:VAL:HG13	1:A:26:GLY:HA3	1.99	0.43
3:C:371:PHE:CG	3:C:419:TRP:HZ2	2.36	0.43
1:A:165:ASN:O	1:A:168:ALA:N	2.51	0.43
1:H:67:ARG:NH2	1:H:87:ARG:HD3	2.33	0.43
2:L:111:ALA:HB3	2:L:140:TYR:N	2.34	0.43
1:H:51:ILE:HA	1:H:57:TYR:O	2.19	0.43
1:A:99:TRP:CE2	1:A:108:GLY:HA2	2.54	0.43
3:C:346:PHE:O	3:C:427:GLY:HA2	2.19	0.43
3:E:369:CYS:HB3	3:E:419:TRP:CZ2	2.45	0.42
1:H:147:ALA:HB2	1:H:193:THR:HA	2.00	0.42
2:L:82:ASP:O	2:L:86:TYR:OH	2.26	0.42
3:E:368:ASN:HB2	3:E:397:ALA:N	2.19	0.42
3:C:360:TRP:CD2	3:C:404:TRP:HB2	2.54	0.42
1:H:9:GLY:HA3	1:H:117:THR:OG1	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:CYS:HB3	1:H:79:ALA:HB3	2.02	0.42
1:H:132:PHE:HA	1:H:133:PRO:HD3	1.84	0.42
2:L:18:ARG:HG3	2:L:76:SER:O	2.20	0.42
2:L:22:THR:HA	2:L:71:PHE:O	2.20	0.42
3:C:308:PHE:HA	3:C:324:GLY:O	2.20	0.42
1:H:149:GLY:HA3	1:H:191:VAL:HG12	2.02	0.42
2:L:140:TYR:CG	2:L:141:PRO:HA	2.55	0.42
3:E:384:SER:HB3	3:E:420:SER:CB	2.49	0.42
1:A:166:SER:O	1:A:205:ILE:HB	2.19	0.42
1:A:220:LYS:HE2	1:A:220:LYS:HB3	1.73	0.42
3:C:396:CYS:SG	3:C:417:VAL:HG13	2.59	0.42
3:E:305:TYR:HB3	3:E:353:VAL:HG21	2.01	0.42
3:C:300:THR:HG21	3:C:341:VAL:HG13	2.01	0.42
1:H:164:TRP:HB3	1:H:169:LEU:HD22	2.01	0.41
3:C:300:THR:N	3:C:345:HIS:O	2.53	0.41
3:C:333:ASN:CB	3:C:336:LYS:H	2.32	0.41
4:D:1:NAG:H61	4:D:2:NAG:HN2	1.85	0.41
2:B:107:LYS:HA	2:B:140:TYR:OH	2.19	0.41
1:H:103:VAL:HG11	3:E:421:ASP:H	1.86	0.41
3:E:414:SER:HB2	3:E:416:TYR:CE1	2.54	0.41
1:A:134:LEU:HB2	1:A:149:GLY:O	2.19	0.41
2:L:90:GLN:O	2:L:96:ILE:HA	2.19	0.41
3:E:300:THR:HB	3:E:343:THR:OG1	2.21	0.41
2:B:33:VAL:HG21	2:B:71:PHE:CD1	2.56	0.41
3:C:334:GLU:HG2	3:C:335:THR:N	2.36	0.41
1:A:98:ARG:O	1:A:110:LEU:HD22	2.20	0.41
1:A:153:LYS:HB3	1:A:153:LYS:HE2	1.78	0.41
2:L:33:VAL:O	2:L:50:SER:N	2.49	0.41
3:E:307:ASP:CB	3:E:353:VAL:HB	2.40	0.41
2:B:91:GLY:HA3	2:B:96:ILE:HA	2.02	0.41
2:B:175:LEU:HD23	2:B:176:SER:N	2.35	0.41
3:E:384:SER:HB3	3:E:420:SER:HB3	2.03	0.41
1:A:158:GLU:HB3	1:A:160:VAL:HG22	2.02	0.40
1:H:156:PHE:HA	1:H:157:PRO:HA	1.94	0.40
2:L:151:ASP:CG	2:L:189:HIS:HB3	2.42	0.40
3:E:389:LEU:HD12	3:E:389:LEU:HA	1.89	0.40
3:C:371:PHE:HB3	3:C:419:TRP:CZ2	2.56	0.40
2:L:167:ASP:HB3	2:L:170:ASP:HB2	2.03	0.40
2:L:194:CYS:O	2:L:206:THR:HG23	2.21	0.40
2:B:16:GLY:H	2:B:78:LEU:HB3	1.86	0.40
2:B:28:SER:OG	3:C:342:ASP:HB3	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:368:ASN:HB3	3:C:396:CYS:HB2	2.04	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:299:HIS:CD2	2:B:15:VAL:O[4_665]	1.10	1.10
3:E:299:HIS:NE2	2:B:15:VAL:N[4_665]	1.39	0.81
3:E:299:HIS:CG	2:B:15:VAL:O[4_665]	1.41	0.79
1:A:56:GLY:N	3:C:409:TYR:OH[7_555]	1.51	0.69
1:A:56:GLY:N	3:C:409:TYR:CZ[7_555]	1.58	0.62
1:A:53:SER:O	3:C:409:TYR:OH[7_555]	1.67	0.53
3:E:299:HIS:NE2	2:B:14:SER:C[4_665]	1.74	0.46
3:E:299:HIS:CD2	2:B:15:VAL:C[4_665]	1.85	0.35
3:E:299:HIS:ND1	2:B:17:ASP:N[4_665]	1.88	0.32
1:A:55:TYR:C	3:C:409:TYR:CZ[7_555]	1.88	0.32
1:A:55:TYR:C	3:C:409:TYR:CE2[7_555]	1.96	0.24
1:A:56:GLY:CA	3:C:409:TYR:CE1[7_555]	1.97	0.23
1:A:55:TYR:CA	3:C:409:TYR:CE2[7_555]	1.98	0.22
3:E:299:HIS:NE2	2:B:15:VAL:C[4_665]	2.01	0.19
3:E:299:HIS:NE2	2:B:15:VAL:CA[4_665]	2.03	0.17
3:E:299:HIS:NE2	2:B:15:VAL:O[4_665]	2.05	0.15
1:A:54:SER:OG	3:C:365:ASN:ND2[7_555]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/231 (91%)	190 (90%)	18 (8%)	3 (1%)	11	47
1	H	214/231 (93%)	201 (94%)	12 (6%)	1 (0%)	29	68
2	B	194/215 (90%)	169 (87%)	22 (11%)	3 (2%)	10	46

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	211/215 (98%)	194 (92%)	14 (7%)	3 (1%)	11	47
3	C	133/148 (90%)	128 (96%)	5 (4%)	0	100	100
3	E	130/148 (88%)	122 (94%)	5 (4%)	3 (2%)	6	37
All	All	1093/1188 (92%)	1004 (92%)	76 (7%)	13 (1%)	13	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	ILE
2	L	96	ILE
2	L	193	ALA
3	E	297	HIS
3	E	298	LYS
1	A	205	ILE
2	L	27	GLN
1	A	196	SER
2	B	188	LYS
3	E	429	PRO
2	B	187	GLU
1	H	107	GLY
1	A	159	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	171/188 (91%)	149 (87%)	22 (13%)	4	20
1	H	176/188 (94%)	161 (92%)	15 (8%)	10	36
2	B	173/187 (92%)	153 (88%)	20 (12%)	5	23
2	L	186/187 (100%)	170 (91%)	16 (9%)	10	35
3	C	112/124 (90%)	97 (87%)	15 (13%)	4	20
3	E	113/124 (91%)	99 (88%)	14 (12%)	4	22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	931/998 (93%)	829 (89%)	102 (11%)	6 25

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	7	SER
1	H	45	LEU
1	H	53	SER
1	H	67	ARG
1	H	70	ILE
1	H	78	THR
1	H	120	THR
1	H	121	VAL
1	H	126	THR
1	H	163	SER
1	H	193	THR
1	H	194	VAL
1	H	197	SER
1	H	219	LYS
2	L	3	GLN
2	L	14	SER
2	L	18	ARG
2	L	24	ARG
2	L	48	ILE
2	L	69	THR
2	L	89	GLN
2	L	96	ILE
2	L	100	GLN
2	L	109	THR
2	L	132	VAL
2	L	158	ASN
2	L	176	SER
2	L	182	SER
2	L	185	ASP
2	L	190	LYS
3	E	296	TYR
3	E	303	VAL
3	E	318	PHE
3	E	327	ILE
3	E	328	THR
3	E	366	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	E	369	CYS
3	E	388	SER
3	E	396	CYS
3	E	398	MET
3	E	403	ASN
3	E	412	ILE
3	E	417	VAL
3	E	428	VAL
1	A	4	LEU
1	A	7	SER
1	A	18	LEU
1	A	28	ASN
1	A	45	LEU
1	A	53	SER
1	A	126	THR
1	A	134	LEU
1	A	155	TYR
1	A	160	VAL
1	A	169	LEU
1	A	173	VAL
1	A	192	VAL
1	A	193	THR
1	A	194	VAL
1	A	199	LEU
1	A	201	THR
1	A	204	TYR
1	A	206	CYS
1	A	211	LYS
1	A	218	ASP
1	A	220	LYS
2	B	4	MET
2	B	11	LEU
2	B	37	GLN
2	B	60	SER
2	B	89	GLN
2	B	96	ILE
2	B	100	GLN
2	B	104	VAL
2	B	109	THR
2	B	115	VAL
2	B	122	ASP
2	B	133	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	145	LYS
2	B	146	VAL
2	B	152	ASN
2	B	154	LEU
2	B	176	SER
2	B	191	VAL
2	B	197	THR
2	B	201	LEU
3	C	303	VAL
3	C	317	CYS
3	C	319	ASN
3	C	357	VAL
3	C	364	ILE
3	C	366	THR
3	C	371	PHE
3	C	376	VAL
3	C	385	VAL
3	C	401	VAL
3	C	417	VAL
3	C	418	SER
3	C	419	TRP
3	C	426	THR
3	C	428	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	137	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 ⓘ

8 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	D	1	3,4	14,14,15	0.59	0	17,19,21	1.01	1 (5%)
4	NAG	D	2	4	14,14,15	0.43	0	17,19,21	1.03	1 (5%)
4	BMA	D	3	4	11,11,12	0.27	0	15,15,17	0.86	0
5	NAG	F	1	3,5	14,14,15	0.37	0	17,19,21	0.62	0
5	NAG	F	2	5	14,14,15	0.35	0	17,19,21	0.43	0
4	NAG	G	1	3,4	14,14,15	0.47	0	17,19,21	1.11	0
4	NAG	G	2	4	14,14,15	0.48	0	17,19,21	1.64	2 (11%)
4	BMA	G	3	4	11,11,12	0.25	0	15,15,17	0.73	0

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C1-O5-C5	5.36	119.46	112.19
4	D	2	NAG	C2-N2-C7	2.65	126.68	122.90
4	D	1	NAG	C2-N2-C7	2.52	126.49	122.90
4	G	2	NAG	C4-C3-C2	2.41	114.55	111.02



There are no chirality outliers.

All (17) torsion outliers are listed below:

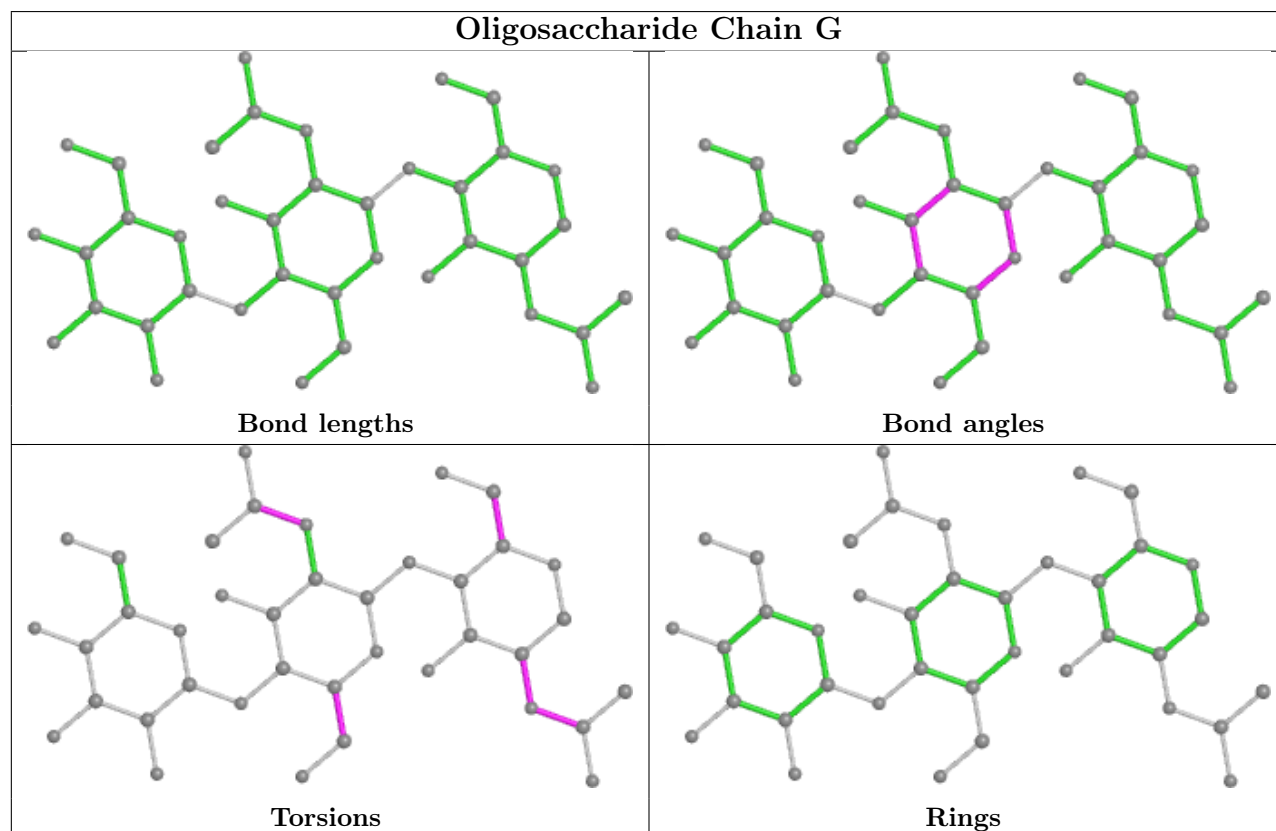
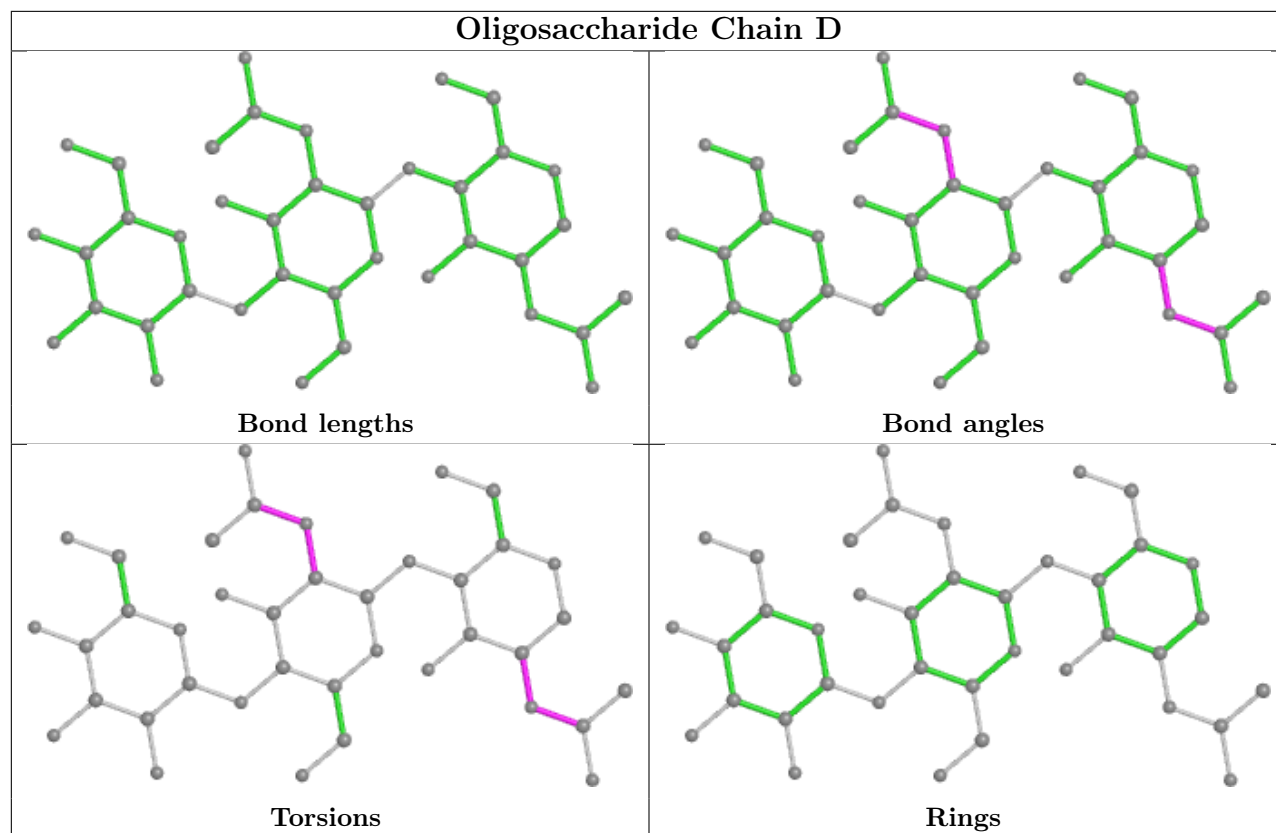
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C1-C2-N2-C7
5	F	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7
4	G	2	NAG	O5-C5-C6-O6

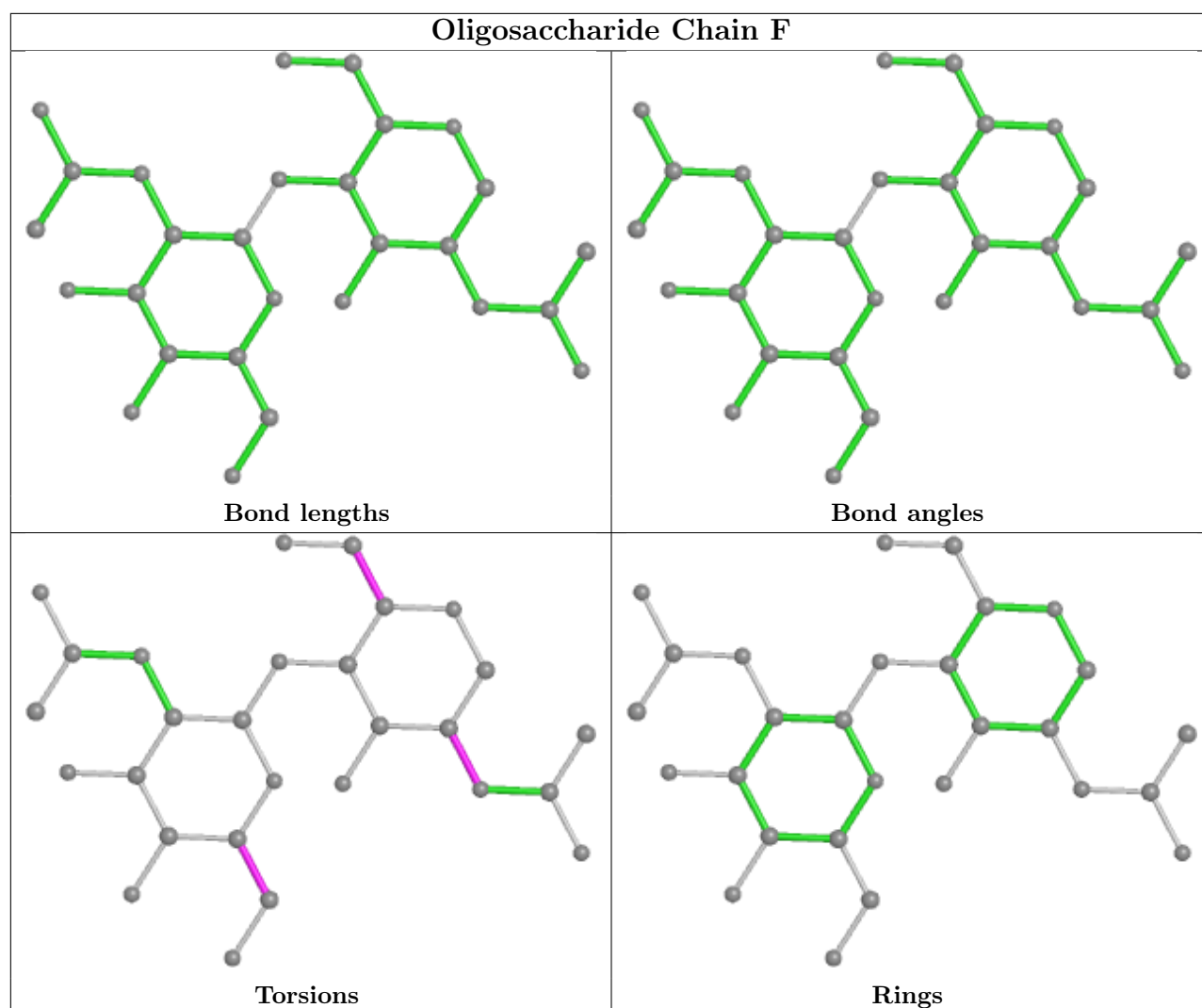
There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0
4	D	2	NAG	1	0
4	G	2	NAG	1	0
4	D	1	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 ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	C	501	3	14,14,15	1.01	1 (7%)	17,19,21	0.66	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
6	NAG	C	501	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	501	NAG	O5-C1	3.37	1.49	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/231 (93%)	-0.15	2 (0%) 84 77	158, 200, 231, 263	0
1	H	218/231 (94%)	-0.26	0 100 100	169, 202, 230, 251	0
2	B	198/215 (92%)	-0.15	0 100 100	153, 192, 227, 241	0
2	L	213/215 (99%)	-0.23	1 (0%) 91 85	157, 192, 226, 259	0
3	C	135/148 (91%)	-0.13	1 (0%) 87 82	119, 196, 244, 272	0
3	E	134/148 (90%)	-0.08	1 (0%) 87 82	123, 190, 232, 274	0
All	All	1113/1188 (93%)	-0.18	5 (0%) 92 87	119, 197, 231, 274	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	1	ASP	3.7
1	A	222	GLU	2.9
1	A	133	PRO	2.4
3	C	311	GLN	2.3
3	E	360	TRP	2.1

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

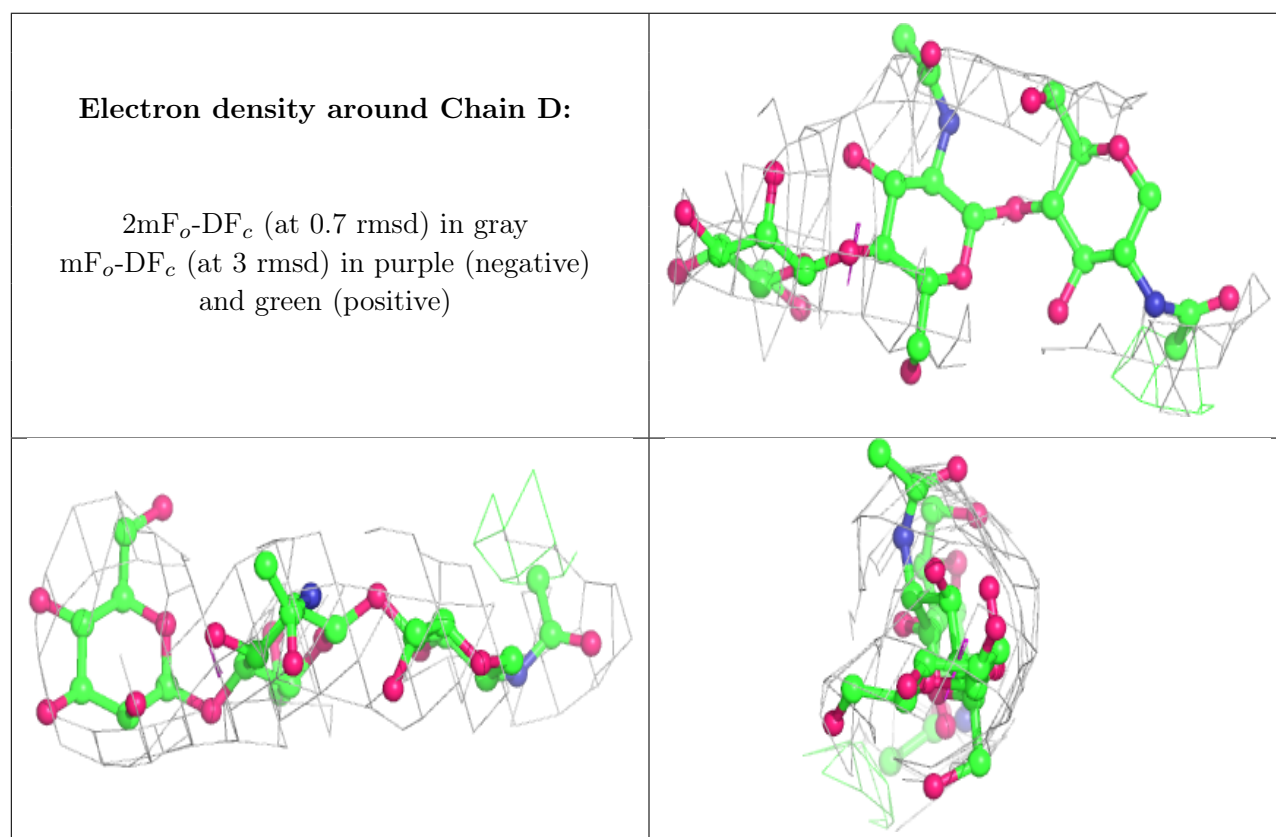
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 95<sup>th</sup> 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.

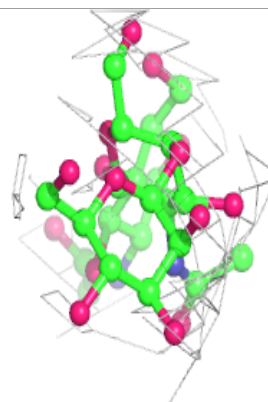
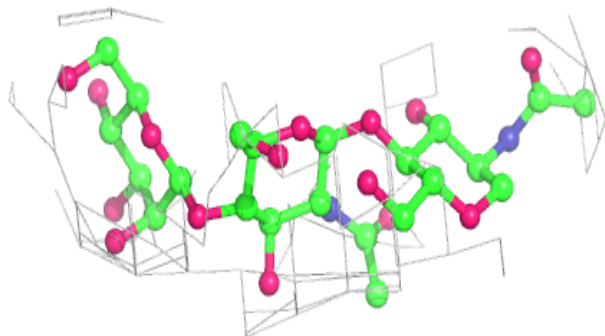
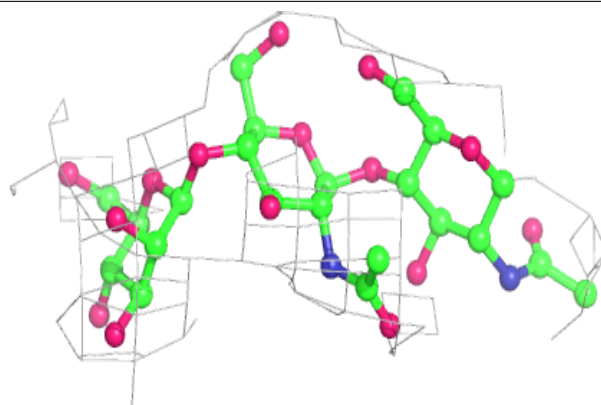
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	D	3	11/12	0.78	0.40	266,267,267,268	0
4	BMA	G	3	11/12	0.81	0.27	250,252,254,254	0
4	NAG	D	1	14/15	0.85	0.18	236,237,238,238	0
5	NAG	F	1	14/15	0.86	0.25	240,241,245,245	0
4	NAG	G	2	14/15	0.88	0.25	242,245,246,247	0
5	NAG	F	2	14/15	0.89	0.22	247,249,251,251	0
4	NAG	G	1	14/15	0.92	0.13	207,219,220,220	0
4	NAG	D	2	14/15	0.93	0.23	254,257,260,260	0

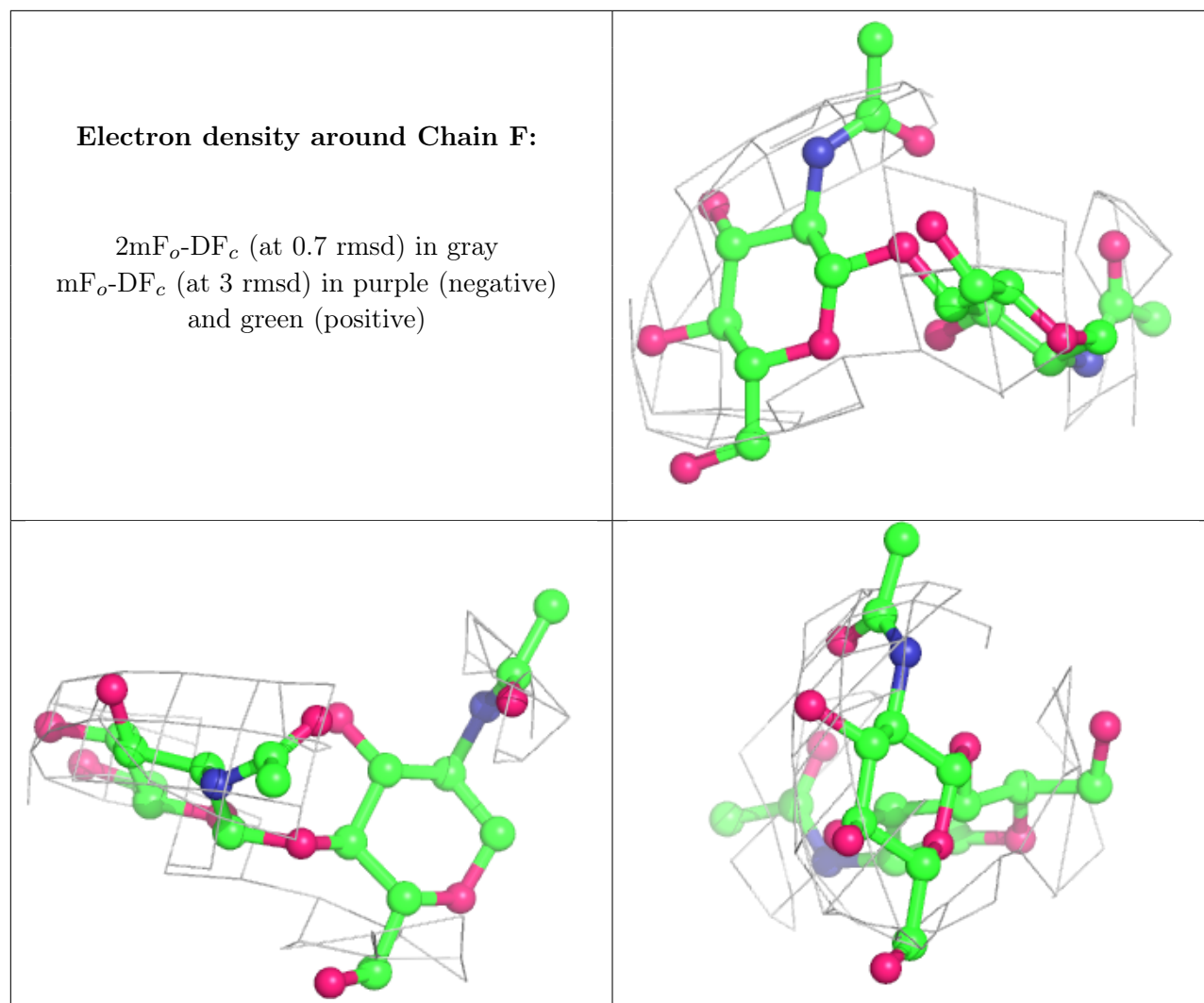
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 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, 95<sup>th</sup> 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
6	NAG	C	501	14/15	0.77	0.30	230,231,233,233	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.