Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 09:33 PM JST

PDB ID	:	7WUE
Title	:	Crystal structure of SARS-CoV-2 Receptor Binding Domain in complex with the monoclonal antibody m31A7
Authors	:	Mohapatra, A.
Deposited on	:	2022-02-08
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

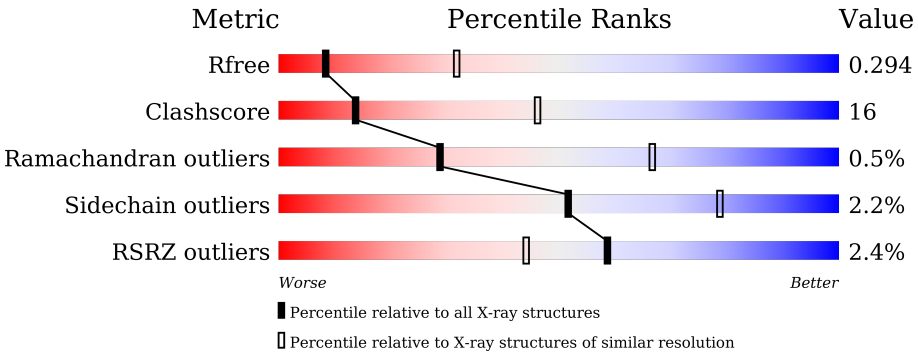
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	195	2% 66% 34%
1	B	195	3% 67% 31%
2	C	239	59% 30% 9%
2	E	239	6% 59% 32% 9%
3	D	240	% 58% 32% 9%
3	F	240	% 56% 35% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	3	33% 67%
4	I	3	33% 67%
5	H	4	75% 25%
5	J	4	75% 25%

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
5	BMA	H	3	-	-	-	X
5	NAG	J	2	-	-	-	X
5	BMA	J	3	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9952 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	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			
1	B	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

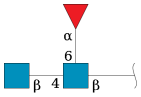
- Molecule 2 is a protein called m31A7 Fab HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	218	Total	C	N	O	S	0	0	0
			1641	1039	265	331	6			
2	E	218	Total	C	N	O	S	0	0	0
			1641	1039	265	331	6			

- Molecule 3 is a protein called m31A7 Fab LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	219	Total	C	N	O	S	0	0	0
			1705	1073	283	343	6			
3	F	219	Total	C	N	O	S	0	0	0
			1705	1073	283	343	6			

- Molecule 4 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.



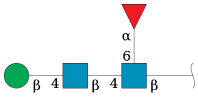
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

Continued on next page...

Continued from previous page...

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

- Molecule 5 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.



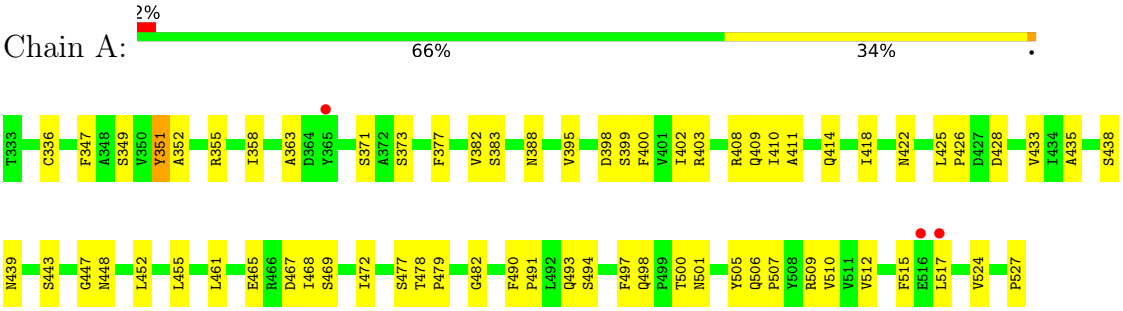
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	4	Total C N O 49 28 2 19	0	0	0
5	J	4	Total C N O 49 28 2 19	0	0	0

3 Residue-property plots (i)

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

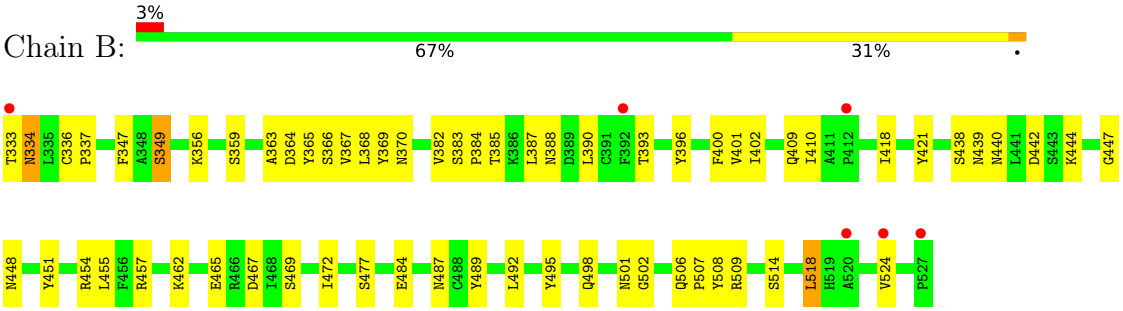
• Molecule 1: Spike protein S1

Chain A:



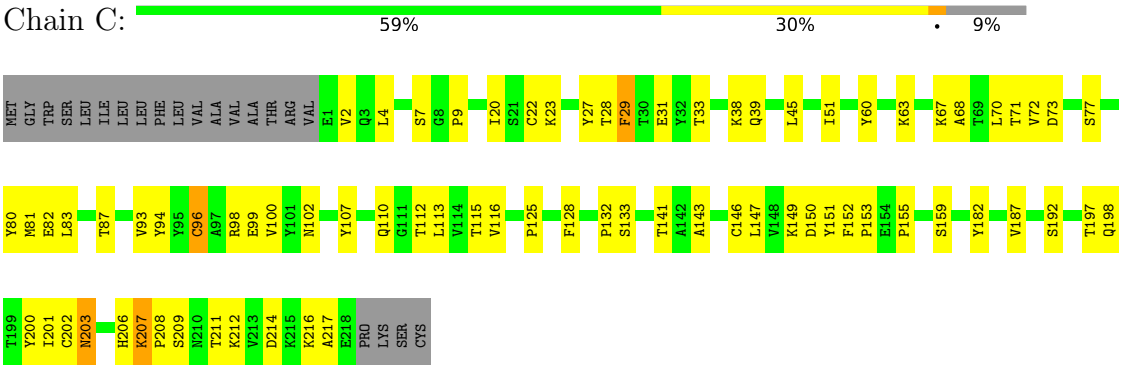
• Molecule 1: Spike protein S1

Chain B:



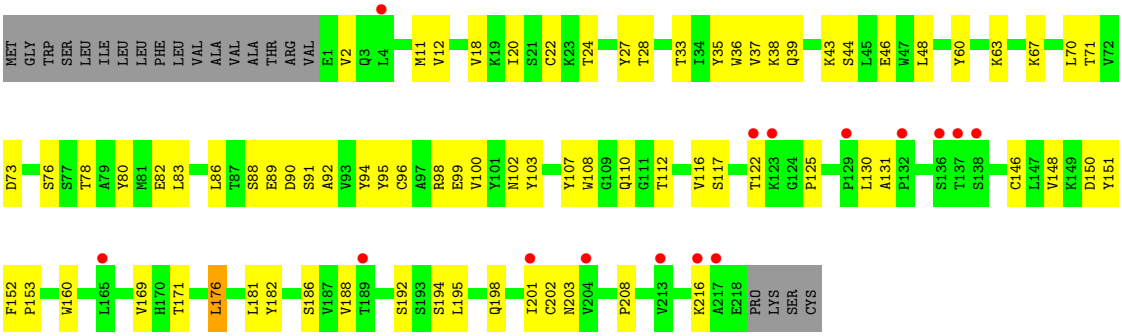
• Molecule 2: m31A7 Fab HEAVY CHAIN

Chain C:



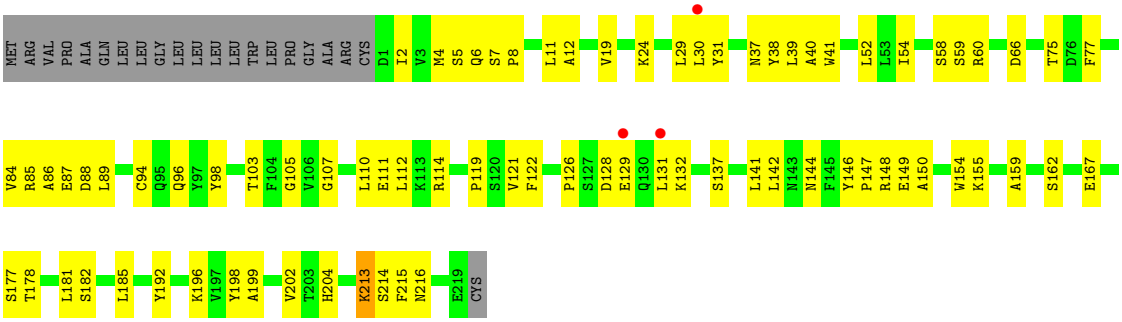
• Molecule 2: m31A7 Fab HEAVY CHAIN

Chain E:



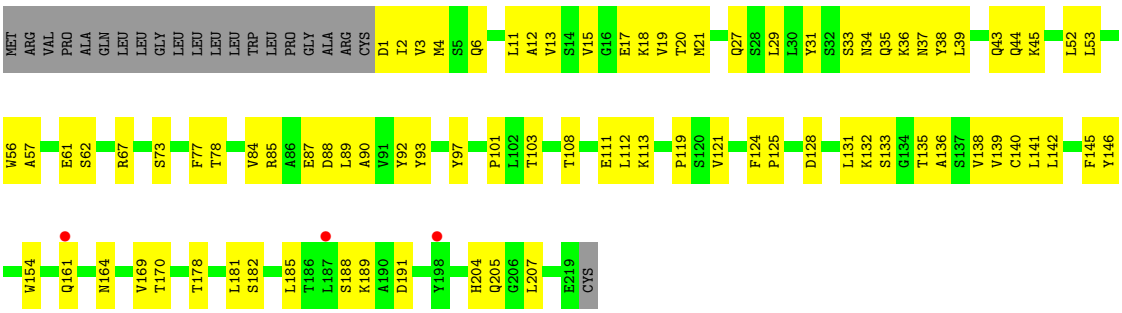
• Molecule 3: m31A7 Fab LIGHT CHAIN

Chain D:



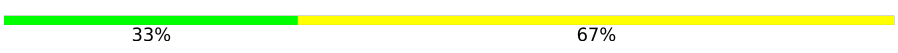
• Molecule 3: m31A7 Fab LIGHT CHAIN

Chain F:



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

Chain G:

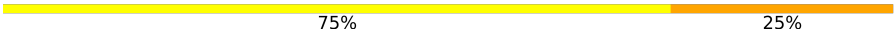


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 5: 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

Chain H:



• Molecule 5: 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

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.46Å 258.12Å 141.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 3.20 47.61 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.61-3.20) 99.0 (47.61-3.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.228 , 0.295 0.229 , 0.294	Depositor DCC
R_{free} test set	1647 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9952	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FUC, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.59	0/1587	0.74	0/2161
1	B	0.57	0/1587	0.71	0/2161
2	C	0.56	0/1681	0.75	0/2292
2	E	0.50	0/1681	0.71	0/2292
3	D	0.52	0/1741	0.75	0/2361
3	F	0.46	0/1741	0.70	0/2361
All	All	0.53	0/10018	0.73	0/13628

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1543	0	1459	55	0
1	B	1543	0	1459	49	0
2	C	1641	0	1603	53	0
2	E	1641	0	1603	53	0
3	D	1705	0	1669	58	0
3	F	1705	0	1669	56	0
4	G	38	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	38	0	34	1	0
5	H	49	0	43	1	0
5	J	49	0	43	1	0
All	All	9952	0	9616	312	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 16.

All (312) 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)
2:E:20:ILE:HG21	2:E:112:THR:HG21	1.51	0.91
2:C:9:PRO:HB3	2:C:113:LEU:HB3	1.64	0.80
1:A:438:SER:HB3	1:A:507:PRO:HB2	1.62	0.79
1:B:359:SER:HA	1:B:524:VAL:HG22	1.63	0.79
1:B:487:ASN:HD21	2:E:33:THR:HG21	1.45	0.79
2:C:100:VAL:HG12	2:C:102:ASN:H	1.49	0.78
2:C:113:LEU:HD23	2:C:155:PRO:HD3	1.66	0.77
1:B:477:SER:N	2:E:99:GLU:OE2	2.18	0.77
2:E:12:VAL:HG11	2:E:86:LEU:HD12	1.67	0.75
1:A:472:ILE:HD12	1:A:472:ILE:H	1.50	0.74
1:A:411:ALA:HB3	1:A:414:GLN:HG2	1.70	0.74
3:F:161:GLN:HB3	3:F:164:ASN:HD21	1.53	0.74
1:B:438:SER:HB2	1:B:507:PRO:HB2	1.71	0.73
2:C:71:THR:HG23	2:C:80:TYR:HB2	1.70	0.73
1:A:355:ARG:NE	1:A:398:ASP:OD1	2.19	0.73
2:E:192:SER:HA	2:E:195:LEU:HD13	1.70	0.72
3:D:39:LEU:HD22	3:D:77:PHE:CD2	2.25	0.72
1:A:388:ASN:HB2	1:A:527:PRO:HD2	1.73	0.71
3:D:167:GLU:HB2	3:D:181:LEU:HD21	1.70	0.70
2:C:125:PRO:HB3	2:C:151:TYR:HB3	1.72	0.70
2:C:27:TYR:CE2	2:C:98:ARG:HD2	2.28	0.69
1:B:444:LYS:HB3	1:B:448:ASN:HB2	1.75	0.69
2:E:125:PRO:HB3	2:E:151:TYR:HB3	1.76	0.68
1:A:447:GLY:HA2	1:A:498:GLN:HG2	1.75	0.67
3:D:129:GLU:HA	3:D:132:LYS:HE3	1.75	0.67
3:D:199:ALA:HB2	3:D:214:SER:HB2	1.77	0.67
2:C:159:SER:OG	2:C:203:ASN:OD1	2.13	0.67
1:A:439:ASN:HD21	1:A:506:GLN:CD	1.99	0.66
3:F:131:LEU:HB3	3:F:189:LYS:HE2	1.79	0.65
3:D:19:VAL:HG23	3:D:84:VAL:HG11	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:SER:O	2:C:112:THR:HG22	1.97	0.65
3:D:24:LYS:HA	3:D:75:THR:O	1.97	0.65
3:D:38:TYR:HB2	3:D:98:TYR:HB2	1.80	0.64
1:A:477:SER:OG	2:C:100:VAL:O	2.16	0.64
3:F:29:LEU:O	3:F:37:ASN:HA	1.97	0.63
2:E:94:TYR:O	2:E:112:THR:HG22	1.98	0.63
3:F:21:MET:HG2	3:F:108:THR:HG21	1.80	0.63
3:D:58:SER:OG	3:D:58:SER:O	2.15	0.63
1:B:364:ASP:OD1	1:B:364:ASP:N	2.30	0.63
3:F:37:ASN:HD21	3:F:73:SER:HB2	1.63	0.63
2:E:37:VAL:HG11	2:E:108:TRP:HZ3	1.64	0.62
1:B:487:ASN:ND2	2:E:33:THR:HG21	2.15	0.61
3:D:196:LYS:HE2	3:D:216:ASN:ND2	2.15	0.61
3:F:124:PHE:HB2	3:F:139:VAL:HB	1.81	0.61
1:B:337:PRO:HG2	1:B:356:LYS:HE2	1.83	0.61
3:F:4:MET:HE1	3:F:29:LEU:HD11	1.82	0.61
2:C:98:ARG:HG2	2:C:99:GLU:H	1.67	0.60
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.83	0.60
3:D:144:ASN:HA	3:D:178:THR:HB	1.84	0.60
1:B:439:ASN:HA	1:B:507:PRO:HG2	1.84	0.60
3:F:119:PRO:HD2	3:F:207:LEU:HD21	1.83	0.60
1:A:479:PRO:HD3	3:D:38:TYR:CE1	2.37	0.59
3:D:154:TRP:CG	3:D:185:LEU:HD13	2.37	0.59
2:E:46:GLU:OE2	2:E:63:LYS:NZ	2.22	0.59
2:E:160:TRP:CD1	2:E:169:VAL:HG21	2.38	0.59
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.85	0.59
1:A:433:VAL:HG22	1:A:512:VAL:HG13	1.83	0.59
1:A:402:ILE:HD11	1:A:418:ILE:HG21	1.85	0.59
3:F:13:VAL:HG21	3:F:19:VAL:HG22	1.85	0.58
2:E:169:VAL:HA	2:E:188:VAL:HA	1.85	0.58
2:E:130:LEU:HB3	3:F:124:PHE:CD2	2.38	0.58
2:E:71:THR:OG1	2:E:80:TYR:HB2	2.04	0.57
3:F:20:THR:HG23	3:F:78:THR:HG23	1.86	0.57
2:E:122:THR:HG22	2:E:153:PRO:HD3	1.85	0.57
3:F:112:LEU:HD23	3:F:113:LYS:N	2.19	0.57
3:F:13:VAL:HG11	3:F:19:VAL:HG21	1.87	0.57
3:F:67:ARG:HD3	3:F:85:ARG:HH21	1.68	0.57
1:A:400:PHE:HZ	1:A:410:ILE:HD13	1.70	0.57
2:C:152:PHE:CE1	2:C:182:TYR:HE1	2.23	0.57
3:F:43:GLN:HE22	3:F:45:LYS:HE2	1.70	0.56
1:A:402:ILE:HD12	1:A:410:ILE:HD11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:43:GLN:HG3	3:F:92:TYR:CZ	2.40	0.56
1:A:478:THR:HG22	1:A:479:PRO:O	2.06	0.56
3:F:128:ASP:O	3:F:132:LYS:HG3	2.06	0.56
3:D:192:TYR:O	3:D:198:TYR:OH	2.23	0.56
1:A:439:ASN:HD21	1:A:506:GLN:CG	2.20	0.55
2:C:27:TYR:CZ	2:C:98:ARG:HD2	2.41	0.55
2:E:18:VAL:HG12	2:E:83:LEU:HB2	1.88	0.55
2:C:187:VAL:HG21	3:D:141:LEU:HD22	1.88	0.55
1:A:472:ILE:HD13	1:A:482:GLY:HA2	1.86	0.55
1:B:365:TYR:CD2	1:B:388:ASN:HA	2.42	0.55
2:C:68:ALA:HA	2:C:82:GLU:O	2.06	0.55
1:B:454:ARG:HA	1:B:492:LEU:HD23	1.87	0.55
3:F:44:GLN:O	3:F:90:ALA:HB1	2.06	0.55
3:D:2:ILE:HD11	3:D:29:LEU:HD21	1.89	0.55
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.72	0.55
1:B:382:VAL:HG21	1:B:387:LEU:HD13	1.89	0.55
1:B:382:VAL:HG22	1:B:383:SER:H	1.72	0.54
3:D:12:ALA:HB2	3:D:111:GLU:HB2	1.89	0.54
3:D:114:ARG:HG3	3:D:177:SER:HB2	1.89	0.53
1:B:438:SER:OG	1:B:509:ARG:HG3	2.09	0.53
1:A:399:SER:HA	1:A:510:VAL:O	2.08	0.53
2:C:39:GLN:HB2	2:C:45:LEU:HD23	1.90	0.53
2:C:203:ASN:HA	2:C:214:ASP:OD1	2.08	0.53
3:F:3:VAL:HA	3:F:103:THR:HG21	1.90	0.53
1:A:382:VAL:HG22	1:A:383:SER:H	1.72	0.53
1:A:336:CYS:HB2	1:A:363:ALA:HB2	1.89	0.53
3:D:146:TYR:CD1	3:D:147:PRO:HA	2.44	0.53
2:E:73:ASP:OD2	2:E:76:SER:N	2.25	0.53
1:A:402:ILE:HG23	1:A:403:ARG:N	2.23	0.53
3:D:199:ALA:CB	3:D:214:SER:HB2	2.39	0.53
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.44	0.52
1:B:462:LYS:O	1:B:465:GLU:HB3	2.09	0.52
3:F:37:ASN:ND2	3:F:73:SER:HB2	2.24	0.52
3:F:145:PHE:N	3:F:178:THR:HB	2.24	0.52
2:E:194:SER:HB2	2:E:198:GLN:HB2	1.91	0.52
1:A:409:GLN:HA	1:A:414:GLN:HG3	1.91	0.52
1:A:400:PHE:CZ	1:A:410:ILE:HD13	2.45	0.52
2:E:83:LEU:HB3	2:E:86:LEU:HD21	1.91	0.52
3:F:188:SER:O	3:F:191:ASP:N	2.43	0.52
2:E:27:TYR:CE2	2:E:98:ARG:HD2	2.45	0.51
1:B:472:ILE:HD12	1:B:484:GLU:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:201:ILE:HG12	2:C:216:LYS:HG2	1.92	0.51
3:F:33:SER:C	3:F:35:GLN:H	2.14	0.51
4:I:1:NAG:O3	4:I:3:FUC:H5	2.11	0.51
1:A:461:LEU:HD23	1:A:465:GLU:OE1	2.10	0.51
3:F:135:THR:HG22	3:F:136:ALA:H	1.75	0.51
3:F:204:HIS:CG	3:F:205:GLN:N	2.79	0.51
2:C:206:HIS:HB3	2:C:211:THR:HB	1.92	0.51
2:C:133:SER:OG	3:D:122:PHE:HB3	2.10	0.51
2:C:141:THR:O	2:C:192:SER:HB3	2.10	0.50
3:D:114:ARG:HB3	3:D:146:TYR:CD2	2.46	0.50
2:E:11:MET:HE1	2:E:153:PRO:HB3	1.93	0.50
1:B:454:ARG:HH22	1:B:469:SER:N	2.09	0.50
3:F:112:LEU:HD23	3:F:113:LYS:H	1.76	0.50
3:D:5:SER:HB2	3:D:24:LYS:HB3	1.94	0.50
3:D:181:LEU:HD23	3:D:182:SER:N	2.26	0.50
3:D:4:MET:HB2	3:D:105:GLY:HA2	1.93	0.50
1:B:393:THR:HG21	1:B:518:LEU:HB3	1.92	0.50
1:B:347:PHE:CD2	1:B:509:ARG:HD3	2.46	0.50
1:B:400:PHE:HZ	1:B:410:ILE:HD12	1.77	0.50
3:D:54:ILE:HG23	3:D:59:SER:H	1.76	0.50
3:D:88:ASP:O	3:D:110:LEU:HD23	2.11	0.50
1:B:366:SER:O	1:B:370:ASN:ND2	2.45	0.49
2:C:132:PRO:HA	2:C:143:ALA:O	2.13	0.49
1:B:349:SER:OG	1:B:451:TYR:HA	2.12	0.49
3:F:141:LEU:C	3:F:142:LEU:HD12	2.33	0.49
1:B:333:THR:O	1:B:334:ASN:ND2	2.41	0.49
1:A:472:ILE:CD1	1:A:482:GLY:HA2	2.43	0.49
2:C:197:THR:OG1	2:C:198:GLN:N	2.42	0.49
2:E:99:GLU:HG3	2:E:100:VAL:N	2.27	0.49
3:F:56:TRP:HH2	5:J:4:FUC:H3	1.77	0.49
5:H:1:NAG:O3	5:H:2:NAG:N2	2.37	0.49
3:F:2:ILE:HD12	3:F:27:GLN:OE1	2.12	0.49
2:C:125:PRO:HD2	2:C:211:THR:HG21	1.95	0.48
3:F:131:LEU:HD22	3:F:189:LYS:HG3	1.95	0.48
1:A:452:LEU:HD23	1:A:494:SER:HA	1.95	0.48
1:A:349:SER:HB3	1:A:452:LEU:H	1.77	0.48
2:C:33:THR:HB	2:C:99:GLU:OE1	2.13	0.48
3:D:128:ASP:O	3:D:132:LYS:HG2	2.13	0.48
3:D:149:GLU:N	3:D:149:GLU:OE1	2.45	0.48
2:E:18:VAL:O	2:E:82:GLU:HA	2.14	0.48
1:B:365:TYR:HD2	1:B:388:ASN:HA	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:43:GLN:HB2	3:F:53:LEU:HD11	1.94	0.48
3:F:31:TYR:HB2	3:F:38:TYR:HE2	1.78	0.48
3:D:121:VAL:O	3:D:213:LYS:HE3	2.14	0.48
3:F:146:TYR:HB2	3:F:178:THR:HG22	1.96	0.48
3:D:11:LEU:HD12	3:D:11:LEU:HA	1.74	0.48
2:E:176:LEU:HG	2:E:182:TYR:CD1	2.49	0.48
2:C:28:THR:HB	2:C:31:GLU:HG3	1.95	0.47
2:C:99:GLU:HG2	2:C:100:VAL:H	1.79	0.47
1:B:409:GLN:OE1	1:B:418:ILE:HB	2.13	0.47
2:E:171:THR:HG23	2:E:186:SER:HB2	1.95	0.47
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.63	0.47
2:C:99:GLU:HG2	2:C:100:VAL:N	2.29	0.47
1:B:447:GLY:HA2	1:B:498:GLN:HG2	1.96	0.47
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.96	0.47
3:D:29:LEU:O	3:D:37:ASN:HA	2.15	0.47
3:F:169:VAL:HG12	3:F:170:THR:H	1.79	0.47
1:A:371:SER:C	1:A:373:SER:H	2.18	0.47
2:C:198:GLN:HB3	2:C:200:TYR:CE1	2.49	0.47
2:E:2:VAL:HB	2:E:107:TYR:CD1	2.49	0.47
3:D:85:ARG:HG3	3:D:86:ALA:H	1.79	0.47
3:D:6:GLN:OE1	3:D:107:GLY:N	2.42	0.47
2:E:201:ILE:HG12	2:E:216:LYS:HB2	1.97	0.47
3:F:181:LEU:HD23	3:F:182:SER:N	2.30	0.47
2:E:88:SER:O	2:E:91:SER:OG	2.32	0.46
3:D:7:SER:HA	3:D:8:PRO:HA	1.72	0.46
2:E:37:VAL:HG11	2:E:108:TRP:CZ3	2.47	0.46
1:A:351:TYR:HE1	1:A:468:ILE:HD12	1.81	0.46
1:A:467:ASP:OD1	1:A:469:SER:HB2	2.15	0.46
2:C:29:PHE:CD2	2:C:77:SER:HA	2.50	0.46
1:A:479:PRO:HB3	3:D:31:TYR:CD2	2.51	0.46
1:B:442:ASP:HB3	1:B:451:TYR:CE2	2.51	0.46
2:E:176:LEU:HG	2:E:182:TYR:CE1	2.51	0.46
1:B:502:GLY:O	1:B:506:GLN:HG3	2.15	0.46
1:A:395:VAL:HG22	1:A:515:PHE:CD1	2.50	0.46
2:E:38:LYS:HB2	2:E:94:TYR:CE1	2.50	0.46
2:E:20:ILE:CG2	2:E:112:THR:HG21	2.35	0.46
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.98	0.46
2:C:2:VAL:HB	2:C:107:TYR:CE2	2.51	0.46
2:E:100:VAL:HG12	2:E:102:ASN:H	1.81	0.46
3:D:19:VAL:HG21	3:D:110:LEU:HD11	1.98	0.45
2:C:20:ILE:HD12	2:C:81:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HB3	1:B:498:GLN:HE22	1.80	0.45
3:D:41:TRP:CZ3	3:D:94:CYS:HB3	2.50	0.45
1:B:455:LEU:O	1:B:455:LEU:HD23	2.16	0.45
3:F:52:LEU:HG	3:F:53:LEU:N	2.30	0.45
1:A:395:VAL:CG2	1:A:524:VAL:HG21	2.47	0.45
1:B:367:VAL:HA	1:B:370:ASN:ND2	2.31	0.45
1:B:384:PRO:HA	1:B:387:LEU:HD22	1.98	0.45
2:E:125:PRO:HB2	2:E:148:VAL:HG12	1.98	0.45
1:B:336:CYS:HB2	1:B:363:ALA:HB2	1.97	0.45
1:A:472:ILE:HD12	1:A:472:ILE:N	2.27	0.45
3:D:85:ARG:HB3	3:D:87:GLU:HG2	1.99	0.45
3:D:148:ARG:O	3:D:148:ARG:HG2	2.17	0.45
3:D:96:GLN:HE21	3:D:103:THR:H	1.64	0.45
2:E:60:TYR:OH	2:E:70:LEU:N	2.29	0.45
1:A:351:TYR:CE1	1:A:352:ALA:HB2	2.51	0.45
1:A:433:VAL:CG2	1:A:512:VAL:HG13	2.47	0.45
1:B:347:PHE:CE2	1:B:509:ARG:HB3	2.52	0.45
1:B:454:ARG:NH2	1:B:467:ASP:OD1	2.50	0.45
1:A:498:GLN:O	1:A:501:ASN:HB2	2.16	0.45
2:C:187:VAL:HG11	3:D:141:LEU:HD13	1.99	0.45
2:E:131:ALA:O	3:F:125:PRO:HD2	2.17	0.45
3:F:17:GLU:HB3	3:F:18:LYS:H	1.41	0.45
2:C:149:LYS:HD2	2:C:150:ASP:OD2	2.17	0.44
2:C:207:LYS:O	2:C:209:SER:N	2.50	0.44
3:F:11:LEU:HA	3:F:11:LEU:HD12	1.56	0.44
1:A:472:ILE:H	1:A:472:ILE:CD1	2.24	0.44
2:C:20:ILE:HD12	2:C:81:MET:CE	2.47	0.44
3:D:87:GLU:HG2	3:D:87:GLU:H	1.61	0.44
1:A:347:PHE:CD2	1:A:509:ARG:HD3	2.52	0.44
3:D:60:ARG:HD3	3:D:66:ASP:HA	1.99	0.44
1:B:438:SER:O	1:B:440:ASN:N	2.50	0.44
2:E:22:CYS:O	2:E:78:THR:HA	2.18	0.44
2:C:93:VAL:HG22	2:C:113:LEU:HD13	1.99	0.44
3:D:126:PRO:HB3	3:D:137:SER:O	2.18	0.44
2:E:150:ASP:HB3	2:E:181:LEU:HD13	1.99	0.44
3:F:43:GLN:NE2	3:F:45:LYS:HE2	2.32	0.44
1:A:358:ILE:HB	1:A:395:VAL:HG12	2.00	0.44
2:C:216:LYS:HB3	2:C:217:ALA:H	1.58	0.44
2:E:110:GLN:H	2:E:110:GLN:HG3	1.53	0.44
2:C:60:TYR:HE1	2:C:70:LEU:HG	1.83	0.44
3:D:112:LEU:HD12	3:D:112:LEU:HA	1.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:VAL:HB	2:C:107:TYR:CD2	2.53	0.44
2:C:212:LYS:HE3	2:C:212:LYS:HB3	1.78	0.44
3:D:147:PRO:HB2	3:D:149:GLU:OE1	2.18	0.44
2:C:128:PHE:HD2	2:C:147:LEU:HD23	1.83	0.43
3:F:33:SER:O	3:F:35:GLN:N	2.51	0.43
1:B:401:VAL:HA	1:B:508:TYR:O	2.18	0.43
3:F:39:LEU:HD22	3:F:77:PHE:CG	2.53	0.43
1:A:402:ILE:HD11	1:A:418:ILE:HG13	1.99	0.43
1:A:402:ILE:CD1	1:A:418:ILE:HG21	2.47	0.43
3:D:150:ALA:HB2	3:D:204:HIS:HD2	1.83	0.43
3:D:192:TYR:CD1	3:D:198:TYR:CZ	3.06	0.43
1:B:498:GLN:HB2	1:B:501:ASN:OD1	2.18	0.43
2:E:67:LYS:NZ	2:E:90:ASP:OD2	2.39	0.43
3:D:40:ALA:HB1	3:D:52:LEU:HD11	2.00	0.43
3:F:119:PRO:O	3:F:121:VAL:HG23	2.18	0.43
2:E:35:TYR:CE2	2:E:99:GLU:OE1	2.70	0.43
1:A:403:ARG:NH1	1:A:505:TYR:HD1	2.16	0.43
1:A:490:PHE:CD2	1:A:491:PRO:HD2	2.54	0.43
1:B:492:LEU:HD23	1:B:492:LEU:HA	1.80	0.43
2:E:39:GLN:O	2:E:92:ALA:HB1	2.19	0.43
3:F:140:CYS:HB2	3:F:154:TRP:CH2	2.53	0.43
1:A:500:THR:HG21	1:B:489:TYR:HB3	2.01	0.43
3:D:89:LEU:HD12	3:D:110:LEU:O	2.19	0.43
2:E:103:TYR:HA	3:F:97:TYR:CZ	2.54	0.43
1:A:349:SER:CB	1:A:452:LEU:H	2.32	0.43
1:A:426:PRO:HB2	1:A:428:ASP:OD1	2.19	0.43
2:E:89:GLU:H	2:E:89:GLU:HG2	1.64	0.43
3:F:34:ASN:HB3	3:F:36:LYS:HG2	2.01	0.43
1:B:359:SER:HA	1:B:524:VAL:CG2	2.43	0.42
3:D:19:VAL:CG2	3:D:84:VAL:HG11	2.48	0.42
2:E:91:SER:HB3	2:E:116:VAL:H	1.84	0.42
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.54	0.42
2:C:4:LEU:HD23	2:C:96:CYS:SG	2.60	0.42
2:C:72:VAL:HG22	2:C:73:ASP:N	2.33	0.42
3:F:38:TYR:HD1	3:F:97:TYR:CE1	2.37	0.42
3:F:39:LEU:HB3	3:F:57:ALA:HB2	2.00	0.42
1:B:438:SER:C	1:B:440:ASN:H	2.22	0.42
2:C:115:THR:HG21	2:C:153:PRO:HB3	2.02	0.42
3:D:39:LEU:HD22	3:D:77:PHE:CG	2.53	0.42
3:D:155:LYS:HA	3:D:159:ALA:O	2.20	0.42
3:F:1:ASP:HB3	3:F:101:PRO:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:LEU:HD23	2:C:155:PRO:CD	2.42	0.42
2:E:117:SER:HB3	2:E:152:PHE:CZ	2.55	0.42
2:E:86:LEU:HD23	2:E:86:LEU:HA	1.76	0.42
3:F:12:ALA:HA	3:F:111:GLU:O	2.19	0.42
3:F:138:VAL:HB	3:F:185:LEU:HB3	2.02	0.42
3:F:139:VAL:HG12	3:F:140:CYS:N	2.35	0.41
2:E:24:THR:HB	2:E:27:TYR:HE1	1.85	0.41
2:E:60:TYR:CE1	2:E:70:LEU:HG	2.55	0.41
2:C:23:LYS:HE3	2:C:23:LYS:HB3	1.63	0.41
3:D:214:SER:OG	3:D:215:PHE:N	2.54	0.41
3:D:30:LEU:HD23	3:D:30:LEU:HA	1.74	0.41
2:E:43:LYS:HG3	2:E:44:SER:H	1.84	0.41
2:C:38:LYS:HG3	2:C:94:TYR:HE1	1.85	0.41
1:B:367:VAL:HA	1:B:370:ASN:HD21	1.85	0.41
3:F:15:VAL:HA	3:F:84:VAL:HG13	2.03	0.41
3:F:87:GLU:C	3:F:89:LEU:H	2.24	0.41
1:A:455:LEU:HA	1:A:455:LEU:HD23	1.86	0.41
2:C:33:THR:HG23	2:C:51:ILE:O	2.20	0.41
2:C:149:LYS:O	2:C:182:TYR:O	2.38	0.41
2:E:153:PRO:HD2	2:E:208:PRO:CB	2.50	0.41
1:A:349:SER:HB3	1:A:452:LEU:O	2.21	0.41
2:C:67:LYS:O	2:C:83:LEU:HA	2.21	0.41
3:D:142:LEU:HD21	3:D:202:VAL:HG13	2.02	0.41
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.78	0.41
2:C:207:LYS:HB2	2:C:208:PRO:HD3	2.02	0.41
1:B:387:LEU:HA	1:B:390:LEU:HD12	2.03	0.41
2:E:36:TRP:HB2	2:E:48:LEU:HD11	2.03	0.41
2:E:37:VAL:HG13	2:E:95:TYR:HB2	2.03	0.41
3:F:6:GLN:OE1	3:F:93:TYR:HA	2.21	0.41
2:C:87:THR:O	2:C:116:VAL:HG11	2.21	0.40
2:C:110:GLN:H	2:C:110:GLN:HG2	1.50	0.40
1:B:347:PHE:CE2	1:B:509:ARG:HD3	2.56	0.40
3:F:61:GLU:HG3	3:F:62:SER:N	2.36	0.40
3:D:128:ASP:HA	3:D:131:LEU:HB2	2.03	0.40
3:D:198:TYR:HB2	3:D:215:PHE:CE2	2.57	0.40
1:B:385:THR:H	1:B:385:THR:HG23	1.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	193/195 (99%)	162 (84%)	30 (16%)	1 (0%)	29 67
1	B	193/195 (99%)	166 (86%)	25 (13%)	2 (1%)	15 54
2	C	216/239 (90%)	187 (87%)	29 (13%)	0	100 100
2	E	216/239 (90%)	186 (86%)	29 (13%)	1 (0%)	29 67
3	D	217/240 (90%)	181 (83%)	35 (16%)	1 (0%)	29 67
3	F	217/240 (90%)	186 (86%)	30 (14%)	1 (0%)	29 67
All	All	1252/1348 (93%)	1068 (85%)	178 (14%)	6 (0%)	29 67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	LEU
3	F	88	ASP
2	E	28	THR
1	B	402	ILE
1	A	443	SER
3	D	119	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	168/168 (100%)	164 (98%)	4 (2%)	49 77
1	B	168/168 (100%)	164 (98%)	4 (2%)	49 77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	186/204 (91%)	178 (96%)	8 (4%)	29 64
2	E	186/204 (91%)	181 (97%)	5 (3%)	44 75
3	D	195/212 (92%)	193 (99%)	2 (1%)	76 90
3	F	195/212 (92%)	194 (100%)	1 (0%)	88 95
All	All	1098/1168 (94%)	1074 (98%)	24 (2%)	52 79

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	TYR
1	A	377	PHE
1	A	408	ARG
1	A	517	LEU
2	C	22	CYS
2	C	29	PHE
2	C	63	LYS
2	C	96	CYS
2	C	146	CYS
2	C	202	CYS
2	C	203	ASN
2	C	207	LYS
3	D	162	SER
3	D	213	LYS
1	B	334	ASN
1	B	349	SER
1	B	369	TYR
1	B	495	TYR
2	E	96	CYS
2	E	146	CYS
2	E	176	LEU
2	E	202	CYS
2	E	203	ASN
3	F	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
2	C	177	GLN
3	D	96	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	216	ASN
1	B	487	ASN
2	E	52	ASN
3	F	37	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	0.74	0	17,19,21	0.81	0
4	NAG	G	2	4	14,14,15	0.68	1 (7%)	17,19,21	1.01	1 (5%)
4	FUC	G	3	4	10,10,11	1.75	3 (30%)	14,14,16	1.03	1 (7%)
5	NAG	H	1	5,2	14,14,15	0.35	0	17,19,21	0.75	0
5	NAG	H	2	5	14,14,15	0.66	0	17,19,21	1.65	3 (17%)
5	BMA	H	3	5	11,11,12	1.82	4 (36%)	15,15,17	1.19	2 (13%)
5	FUC	H	4	5	10,10,11	1.55	2 (20%)	14,14,16	2.14	4 (28%)
4	NAG	I	1	1,4	14,14,15	0.61	0	17,19,21	1.77	4 (23%)
4	NAG	I	2	4	14,14,15	0.86	1 (7%)	17,19,21	0.97	1 (5%)
4	FUC	I	3	4	10,10,11	1.64	3 (30%)	14,14,16	1.16	1 (7%)
5	NAG	J	1	5,2	14,14,15	0.87	2 (14%)	17,19,21	0.52	0
5	NAG	J	2	5	14,14,15	0.88	2 (14%)	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMA	J	3	5	11,11,12	1.21	1 (9%)	15,15,17	0.89	0
5	FUC	J	4	5	10,10,11	1.61	2 (20%)	14,14,16	1.17	1 (7%)

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	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1
5	NAG	H	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	FUC	H	4	5	-	-	0/1/1/1
4	NAG	I	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	FUC	I	3	4	-	-	0/1/1/1
5	NAG	J	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
5	FUC	J	4	5	-	-	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	FUC	C4-C3	3.44	1.61	1.52
5	J	4	FUC	C2-C3	3.28	1.57	1.52
5	H	3	BMA	O5-C5	3.28	1.50	1.43
4	I	3	FUC	O5-C5	3.11	1.50	1.43
5	H	4	FUC	O5-C1	2.98	1.48	1.43
5	H	3	BMA	C2-C3	2.88	1.56	1.52
5	H	3	BMA	O5-C1	2.75	1.48	1.43
4	I	2	NAG	O5-C1	2.74	1.48	1.43
5	J	3	BMA	C4-C5	2.42	1.58	1.53
5	J	1	NAG	C1-C2	2.41	1.55	1.52
4	G	3	FUC	C1-C2	2.40	1.57	1.52
5	H	4	FUC	O5-C5	2.39	1.48	1.43
4	G	2	NAG	O5-C1	-2.38	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	FUC	C4-C5	2.35	1.58	1.52
4	I	3	FUC	O5-C1	2.33	1.47	1.43
5	J	2	NAG	O5-C1	2.22	1.47	1.43
5	H	3	BMA	C1-C2	2.18	1.57	1.52
5	J	2	NAG	C1-C2	2.16	1.55	1.52
4	I	3	FUC	C1-C2	2.13	1.57	1.52
5	J	4	FUC	C1-C2	2.12	1.57	1.52
5	J	1	NAG	O5-C1	2.01	1.46	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	1	NAG	C1-O5-C5	4.99	118.95	112.19
5	H	2	NAG	C3-C4-C5	4.60	118.44	110.24
5	H	4	FUC	O5-C1-C2	4.18	117.23	110.77
5	H	4	FUC	C1-O5-C5	4.08	122.02	112.78
4	G	2	NAG	C1-O5-C5	3.73	117.24	112.19
5	H	4	FUC	C1-C2-C3	3.60	114.10	109.67
5	H	2	NAG	C1-O5-C5	3.28	116.63	112.19
5	H	3	BMA	C1-O5-C5	2.95	116.18	112.19
5	J	4	FUC	C1-O5-C5	2.78	119.08	112.78
4	I	1	NAG	C4-C3-C2	2.71	114.99	111.02
4	I	2	NAG	C3-C4-C5	2.70	115.05	110.24
5	H	4	FUC	C3-C4-C5	-2.67	105.62	109.77
4	G	3	FUC	O2-C2-C1	2.64	114.56	109.15
4	I	1	NAG	C3-C4-C5	2.56	114.81	110.24
4	I	3	FUC	C1-O5-C5	2.48	118.40	112.78
4	I	1	NAG	C1-C2-N2	2.27	114.37	110.49
5	H	3	BMA	O3-C3-C2	2.22	114.25	109.99
5	H	2	NAG	O5-C5-C4	2.17	116.10	110.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7
5	J	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C1-C2-N2-C7
5	J	3	BMA	O5-C5-C6-O6

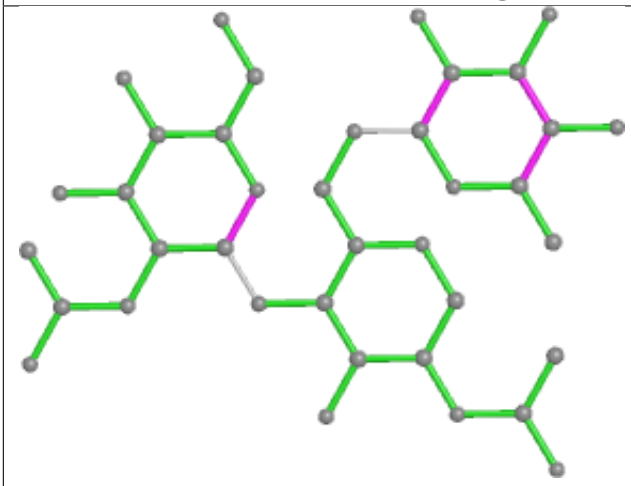
There are no ring outliers.

5 monomers are involved in 3 short contacts:

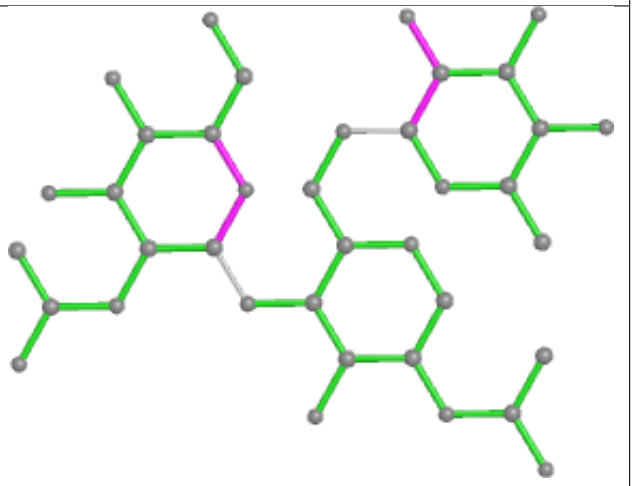
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	3	FUC	1	0
4	I	1	NAG	1	0
5	H	2	NAG	1	0
5	H	1	NAG	1	0
5	J	4	FUC	1	0

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

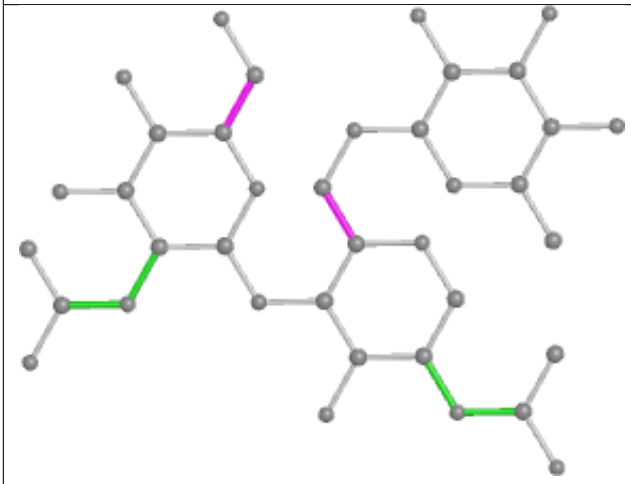
Oligosaccharide Chain G



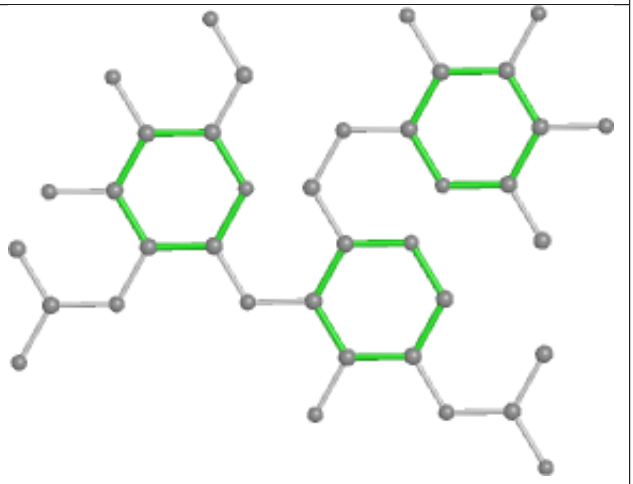
Bond lengths



Bond angles

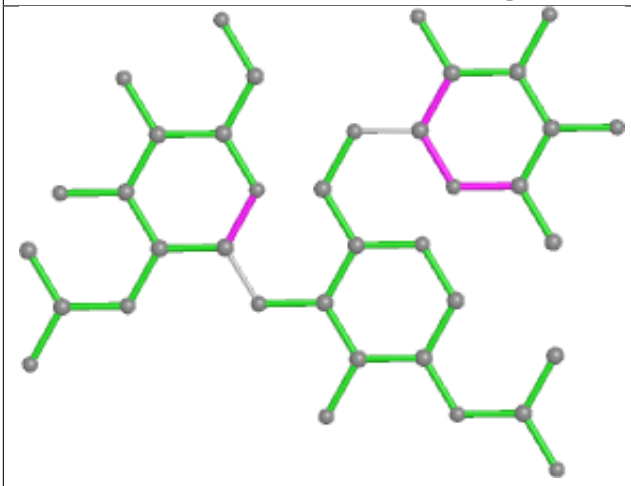


Torsions

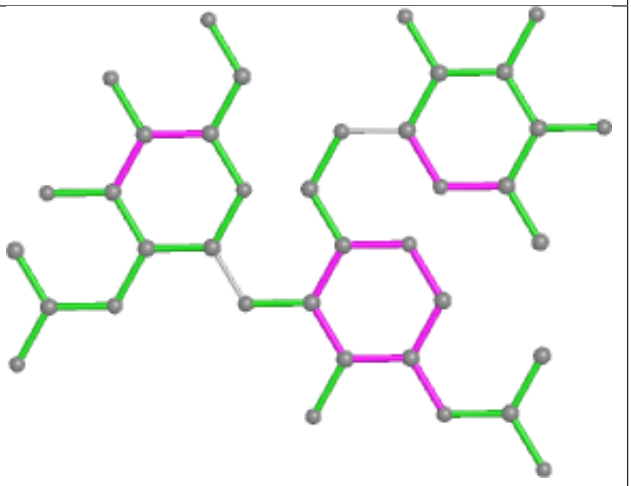


Rings

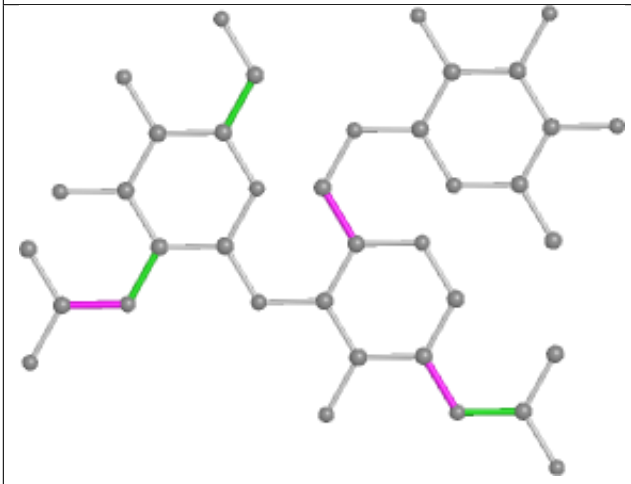
Oligosaccharide Chain I



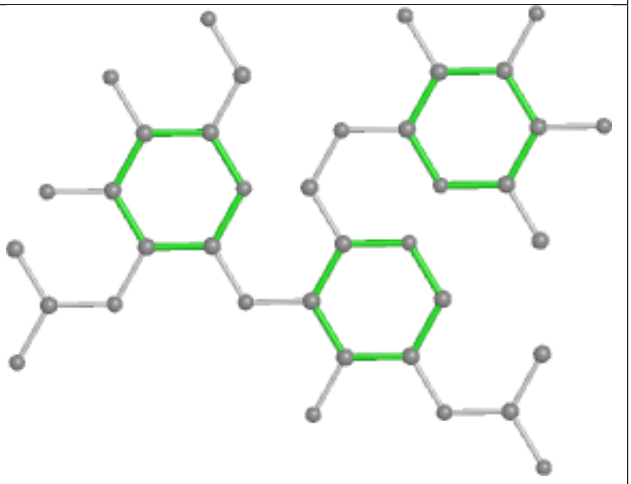
Bond lengths



Bond angles

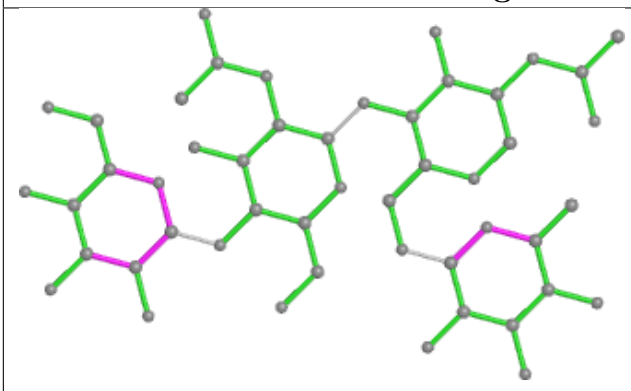


Torsions

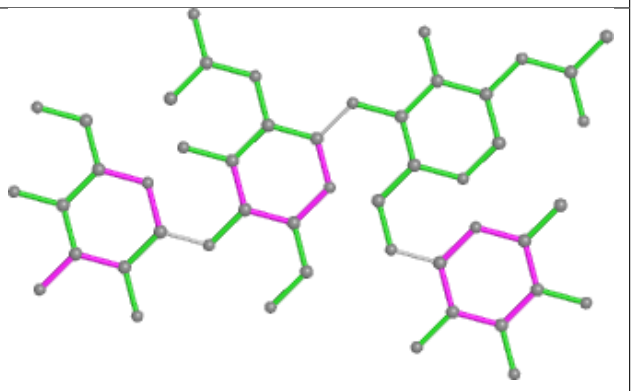


Rings

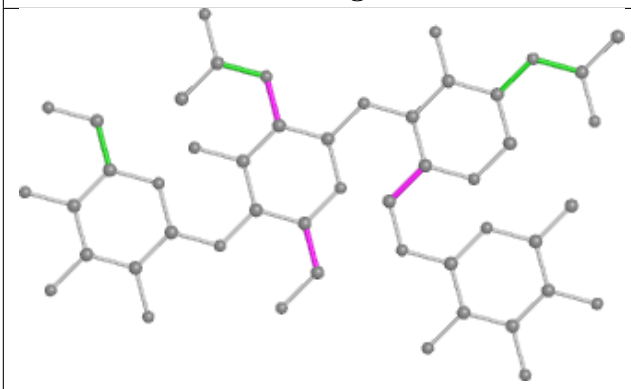
Oligosaccharide Chain H



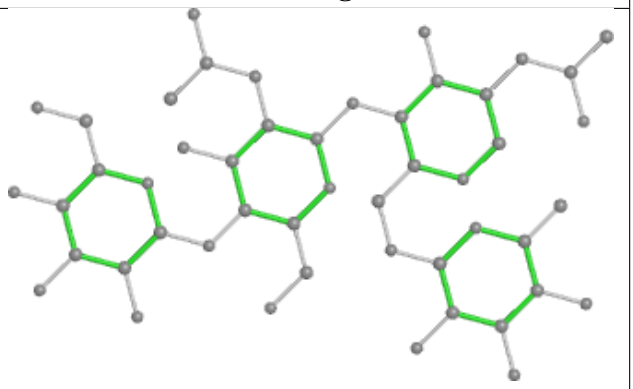
Bond lengths



Bond angles

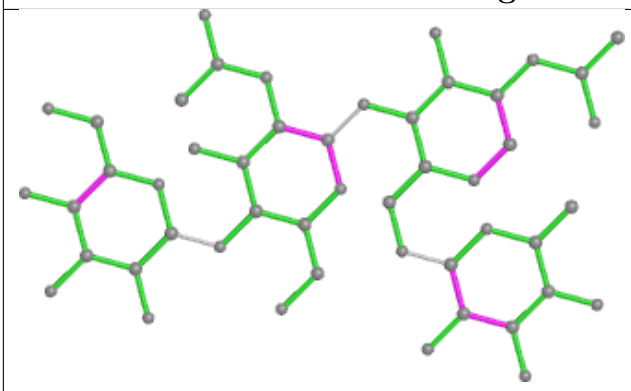


Torsions

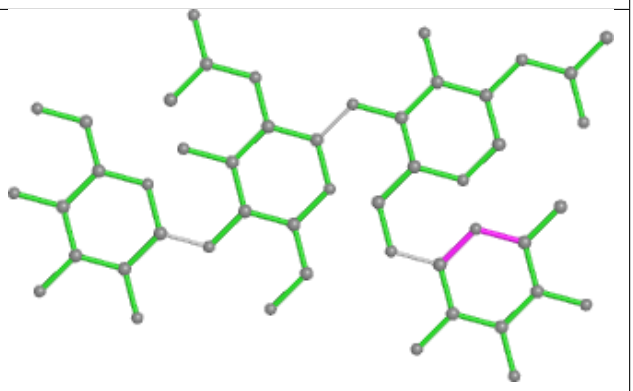


Rings

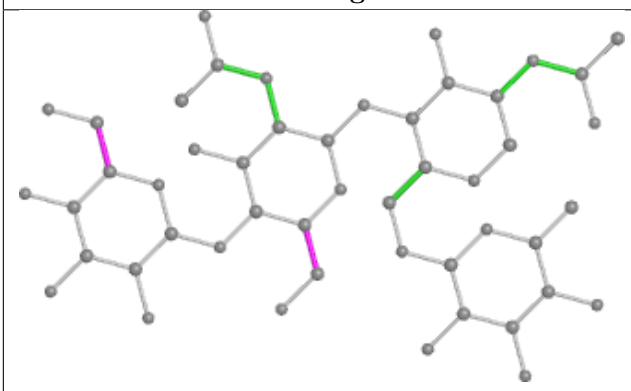
Oligosaccharide Chain J



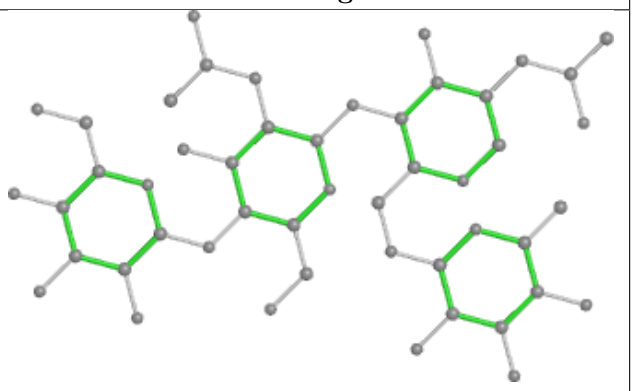
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	195/195 (100%)	-0.01	3 (1%) 73 61	28, 47, 79, 95	0
1	B	195/195 (100%)	0.07	6 (3%) 49 32	30, 51, 105, 137	0
2	C	218/239 (91%)	-0.02	0 100 100	40, 58, 79, 100	0
2	E	218/239 (91%)	0.40	15 (6%) 16 9	39, 74, 108, 137	0
3	D	219/240 (91%)	0.21	3 (1%) 75 63	47, 66, 86, 97	0
3	F	219/240 (91%)	0.10	3 (1%) 75 63	36, 71, 110, 116	0
All	All	1264/1348 (93%)	0.13	30 (2%) 59 44	28, 62, 101, 137	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	THR	4.0
3	F	187	LEU	3.6
2	E	138	SER	3.4
1	B	520	ALA	2.9
2	E	122	THR	2.9
2	E	216	LYS	2.9
2	E	136	SER	2.7
1	A	517	LEU	2.6
3	D	30	LEU	2.6
1	B	527	PRO	2.6
1	B	392	PHE	2.5
2	E	201	ILE	2.5
2	E	213	VAL	2.5
2	E	189	THR	2.5
2	E	129	PRO	2.4
3	D	129	GLU	2.4
1	B	524	VAL	2.3
2	E	217	ALA	2.3
1	A	516	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	4	LEU	2.2
2	E	137	THR	2.2
1	A	365	TYR	2.1
2	E	123	LYS	2.1
2	E	165	LEU	2.1
1	B	412	PRO	2.1
2	E	204	VAL	2.0
2	E	132	PRO	2.0
3	D	131	LEU	2.0
3	F	161	GLN	2.0
3	F	198	TYR	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)

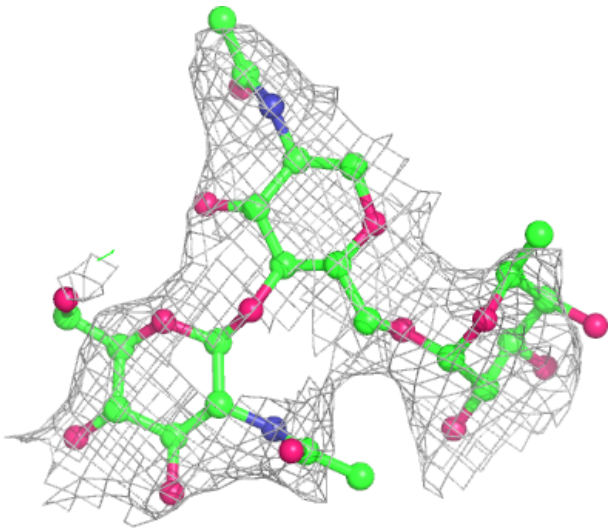
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

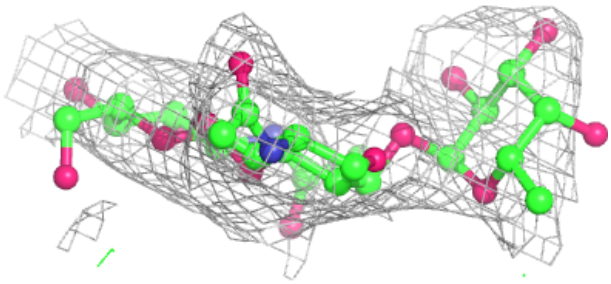
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	H	3	11/12	0.66	0.49	128,131,138,141	0
4	FUC	G	3	10/11	0.74	0.31	87,104,115,119	0
5	BMA	J	3	11/12	0.74	0.50	119,128,133,134	0
5	NAG	J	2	14/15	0.75	0.56	115,125,129,130	0
4	NAG	G	2	14/15	0.75	0.33	94,103,108,112	0
5	NAG	H	2	14/15	0.81	0.32	93,123,129,131	0
5	FUC	H	4	10/11	0.82	0.64	92,109,112,114	0
5	NAG	J	1	14/15	0.82	0.31	79,97,110,119	0
5	NAG	H	1	14/15	0.84	0.30	76,99,114,118	0
4	NAG	I	2	14/15	0.88	0.26	104,118,126,131	0
4	FUC	I	3	10/11	0.88	0.19	95,106,107,109	0
4	NAG	I	1	14/15	0.88	0.27	75,97,105,107	0
5	FUC	J	4	10/11	0.89	0.26	88,94,102,105	0
4	NAG	G	1	14/15	0.93	0.25	46,74,96,98	0

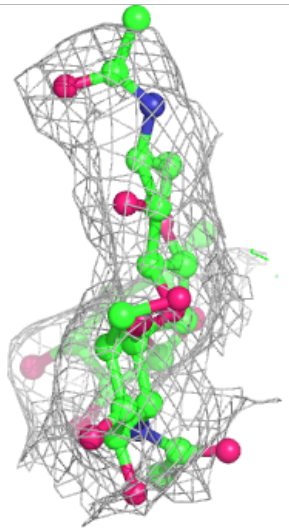
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

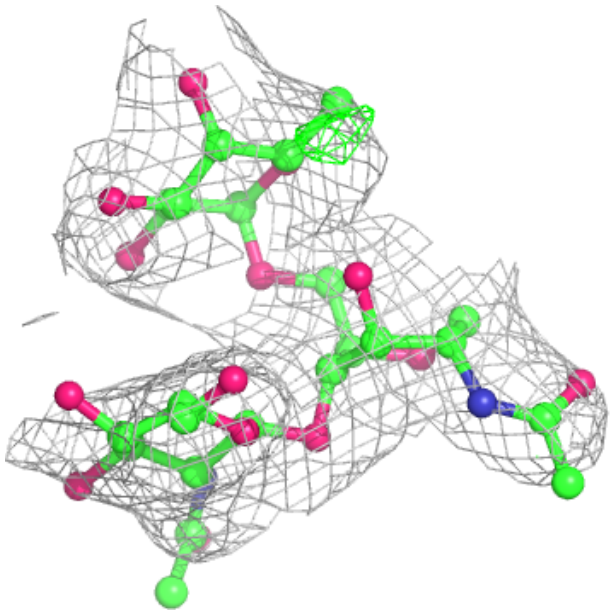


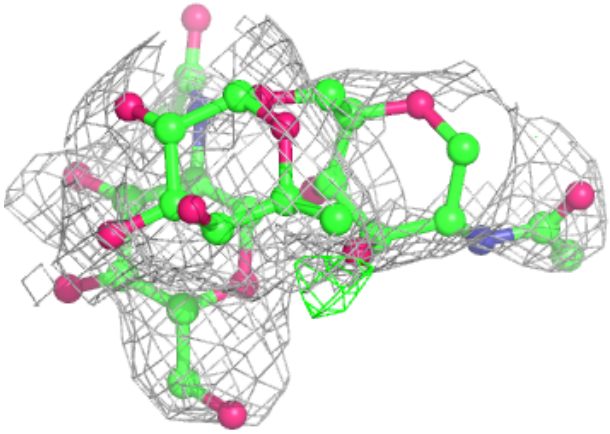


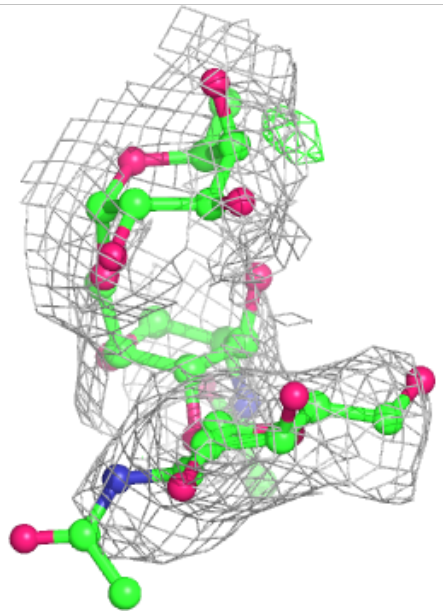


Electron density around Chain I:

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

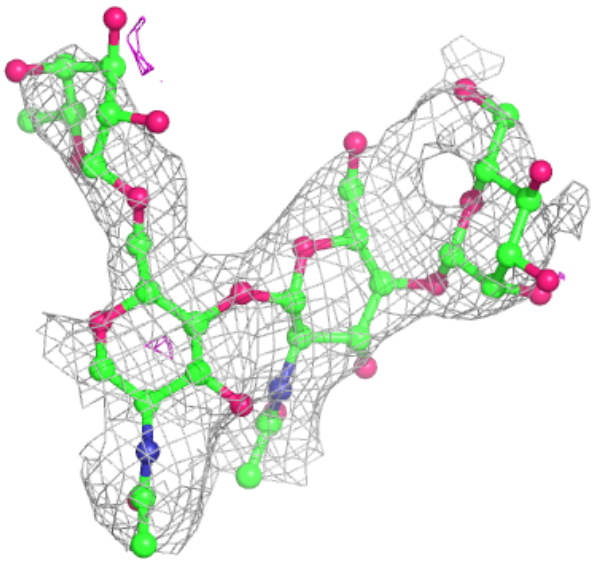


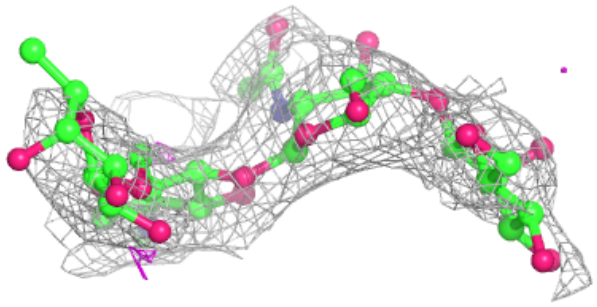


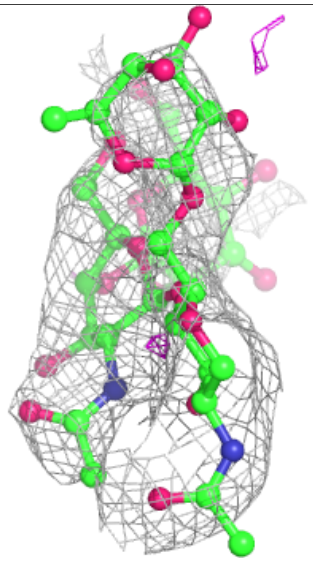


Electron density around Chain H:

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

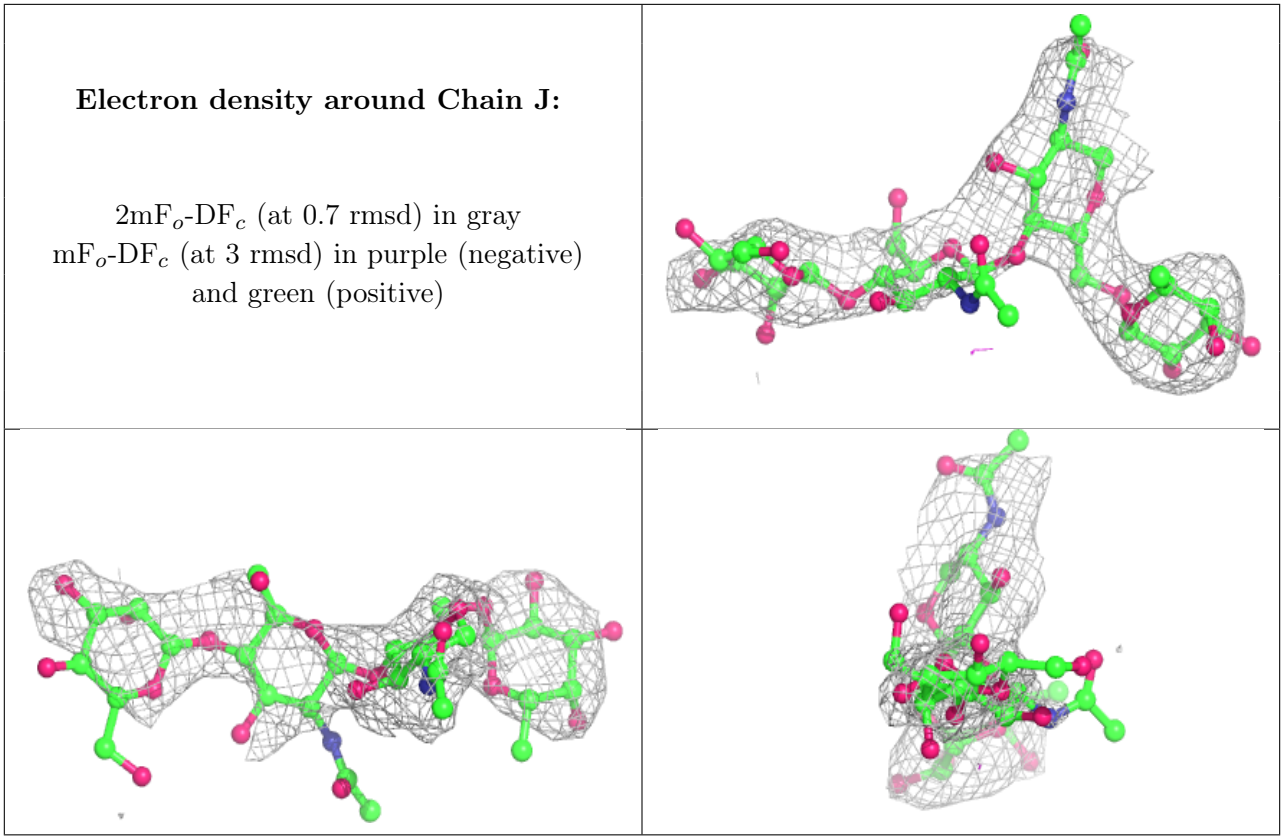






Electron density around Chain J:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.