Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 07:01 PM EDT

PDB ID	:	6W16
Title	:	Crystal structure of a human metapneumovirus monomeric fusion protein complexed with 458 Fab
Authors	:	Huang, J.; Mousa, J.J.
Deposited on	:	2020-03-03
Resolution	:	3.10 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:

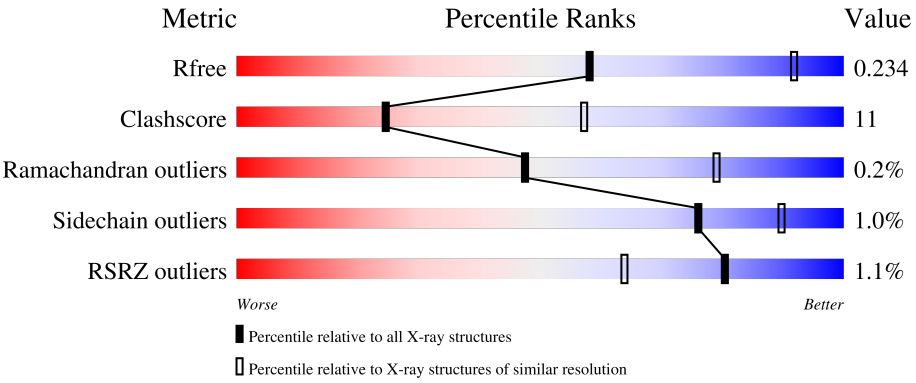
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	F	539	55% 16% 29%
2	H	219	2% 71% 28%
3	L	214	77% 23%
4	A	5	20% 80%

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
4	BMA	A	3	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6265 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 Fusion glycoprotein F0,Envelope glycoprotein fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	385	Total	C	N	O	S	0	0	0
			2901	1817	495	568	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	106	LYS	-	linker	UNP Q6W8S4
F	107	LYS	-	linker	UNP Q6W8S4
F	108	ARG	-	linker	UNP Q6W8S4
F	109	LYS	-	linker	UNP Q6W8S4
F	110	ARG	-	linker	UNP Q6W8S4
F	111	ARG	-	linker	UNP Q6W8S4
F	490	SER	-	linker	UNP Q6W8S4
F	491	GLY	-	linker	UNP Q6W8S4
F	492	ARG	-	linker	UNP Q6W8S4
F	493	GLU	-	linker	UNP Q6W8S4
F	494	ASN	-	linker	UNP Q6W8S4
F	495	LEU	-	linker	UNP Q6W8S4
F	496	TYR	-	linker	UNP Q6W8S4
F	497	PHE	-	linker	UNP Q6W8S4
F	498	GLN	-	linker	UNP Q6W8S4
F	499	GLY	-	linker	UNP Q6W8S4
F	500	GLY	-	linker	UNP Q6W8S4
F	501	GLY	-	linker	UNP Q6W8S4
F	502	GLY	-	linker	UNP Q6W8S4
F	503	GLY	-	linker	UNP Q6W8S4
F	504	SER	-	linker	UNP Q6W8S4
F	533	GLY	-	expression tag	UNP M1E1E4
F	534	THR	-	expression tag	UNP M1E1E4
F	535	GLU	-	expression tag	UNP M1E1E4
F	536	GLY	-	expression tag	UNP M1E1E4
F	537	ARG	-	expression tag	UNP M1E1E4
F	538	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	539	HIS	-	expression tag	UNP M1E1E4
F	540	HIS	-	expression tag	UNP M1E1E4
F	541	HIS	-	expression tag	UNP M1E1E4
F	542	HIS	-	expression tag	UNP M1E1E4
F	543	HIS	-	expression tag	UNP M1E1E4

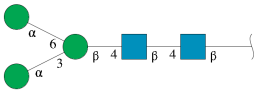
- Molecule 2 is a protein called 458 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1632	1026	279	319	8			

- Molecule 3 is a protein called 458 Fab light chain.

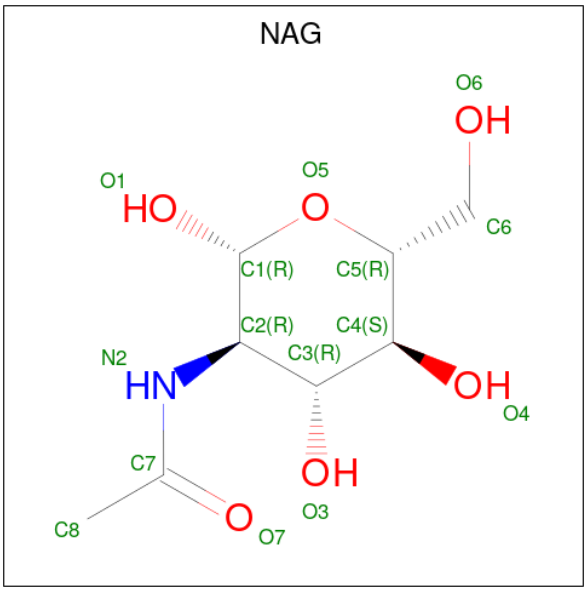
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1657	1033	284	334	6			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	A	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



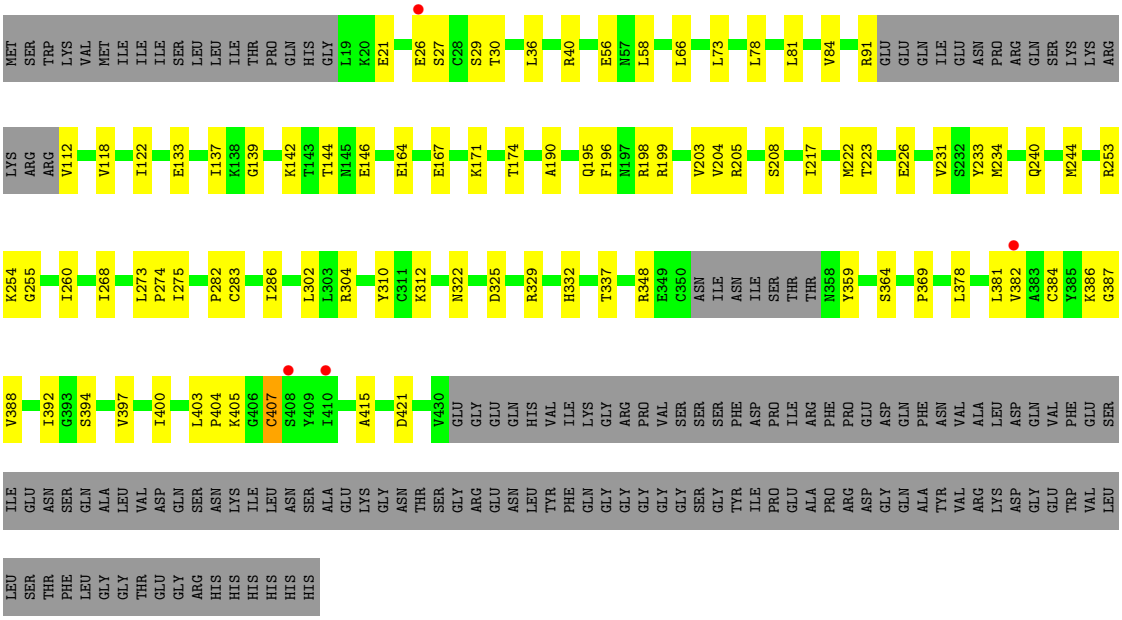
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	F	1	14	8	1	5	0	0

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.

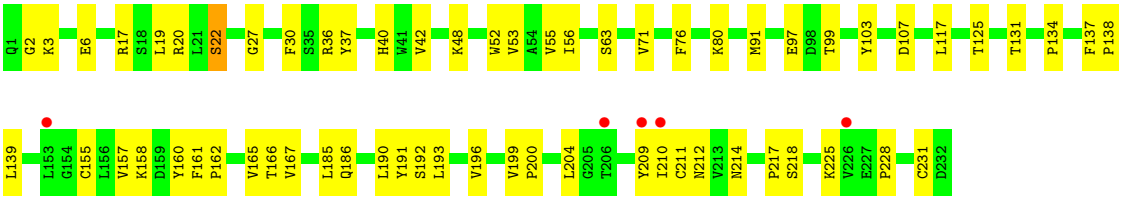
• Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein fusion

Chain F:



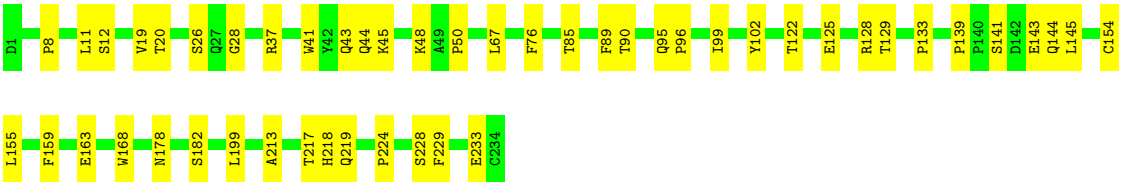
• Molecule 2: 458 Fab heavy chain

Chain H:



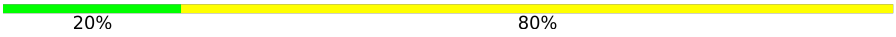
• Molecule 3: 458 Fab light chain

Chain L:



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	128.49Å 128.49Å 188.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.05 – 3.10 47.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.05-3.10) 100.0 (47.90-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.190 , 0.234 0.190 , 0.234	Depositor DCC
R_{free} test set	3242 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å^2)	106.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: MAN, 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	F	0.54	0/2940	0.71	0/3988
2	H	0.51	0/1670	0.69	1/2270 (0.0%)
3	L	0.51	0/1691	0.69	0/2292
All	All	0.53	0/6301	0.70	1/8550 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	211	CYS	CA-CB-SG	5.09	123.16	114.00

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	F	2901	0	2897	67	0
2	H	1632	0	1593	39	0
3	L	1657	0	1608	35	0
4	A	61	0	52	0	0
5	F	14	0	13	0	0
All	All	6265	0	6163	136	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 11.

All (136) 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:L:20:THR:HG22	3:L:90:THR:HG22	1.45	0.96
2:H:99:THR:HG23	2:H:125:THR:HA	1.67	0.76
1:F:369:PRO:HG2	1:F:386:LYS:HD3	1.67	0.75
1:F:81:LEU:HD22	1:F:204:VAL:HG22	1.72	0.70
1:F:382:VAL:O	1:F:407:CYS:HA	1.90	0.70
3:L:213:ALA:HB2	3:L:228:SER:HB3	1.73	0.70
3:L:233:GLU:OE1	3:L:233:GLU:N	2.19	0.68
2:H:158:LYS:HA	2:H:192:SER:HB2	1.74	0.67
1:F:387:GLY:HA2	1:F:405:LYS:HZ1	1.59	0.67
1:F:392:ILE:HG22	1:F:400:ILE:HG23	1.77	0.66
1:F:234:MET:HE1	1:F:275:ILE:HA	1.77	0.66
3:L:163:GLU:N	3:L:163:GLU:OE1	2.29	0.65
3:L:139:PRO:HB3	3:L:229:PHE:CE2	2.31	0.65
1:F:234:MET:HE3	1:F:275:ILE:HG12	1.80	0.64
3:L:217:THR:HG22	3:L:224:PRO:HB3	1.78	0.64
2:H:166:THR:HG23	2:H:214:ASN:HB3	1.80	0.63
2:H:199:VAL:HG11	2:H:209:TYR:CZ	2.34	0.63
3:L:12:SER:HB3	3:L:125:GLU:OE1	1.98	0.62
1:F:231:VAL:HG13	1:F:244:MET:HE2	1.80	0.62
2:H:165:VAL:CG1	2:H:193:LEU:HD21	2.30	0.61
2:H:42:VAL:O	2:H:103:TYR:HB2	2.01	0.59
1:F:112:VAL:HG13	1:F:112:VAL:O	2.02	0.58
1:F:112:VAL:HG11	1:F:253:ARG:O	2.02	0.58
2:H:2:GLY:HA3	2:H:27:GLY:HA3	1.84	0.58
3:L:20:THR:HG22	3:L:90:THR:CG2	2.26	0.58
1:F:387:GLY:H	1:F:405:LYS:HZ3	1.52	0.58
1:F:286:ILE:HD12	1:F:310:TYR:CE1	2.40	0.57
2:H:97:GLU:OE1	2:H:97:GLU:N	2.27	0.57
2:H:131:THR:HG22	2:H:218:SER:HB3	1.86	0.57
2:H:210:ILE:HG12	2:H:225:LYS:HG3	1.86	0.57
3:L:43:GLN:HB2	3:L:102:TYR:CE2	2.40	0.56
1:F:21:GLU:HB2	1:F:378:LEU:HD12	1.87	0.56
1:F:58:LEU:HD21	1:F:174:THR:HG23	1.87	0.56
1:F:407:CYS:SG	1:F:407:CYS:O	2.64	0.55
2:H:19:LEU:HD12	2:H:20:ARG:H	1.71	0.55
2:H:3:LYS:HA	2:H:117:LEU:HD11	1.87	0.55
1:F:66:LEU:HD23	1:F:190:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:GLU:O	1:F:137:ILE:HG13	2.08	0.54
2:H:165:VAL:HG11	2:H:193:LEU:HD21	1.89	0.54
1:F:30:THR:HG23	1:F:381:LEU:HD11	1.89	0.53
1:F:392:ILE:HG23	1:F:415:ALA:HB2	1.90	0.53
2:H:160:TYR:OH	2:H:193:LEU:HD23	2.08	0.53
2:H:186:GLN:NE2	2:H:190:LEU:O	2.41	0.53
1:F:27:SER:HB2	1:F:304:ARG:HD2	1.90	0.53
1:F:387:GLY:CA	1:F:405:LYS:HZ1	2.21	0.53
1:F:387:GLY:HA2	1:F:405:LYS:NZ	2.24	0.52
1:F:84:VAL:HG21	1:F:208:SER:HA	1.91	0.52
3:L:233:GLU:H	3:L:233:GLU:CD	2.12	0.52
2:H:199:VAL:HB	2:H:200:PRO:HD2	1.91	0.51
3:L:8:PRO:HG3	3:L:11:LEU:HD13	1.93	0.51
3:L:213:ALA:CB	3:L:228:SER:HB3	2.39	0.51
1:F:118:VAL:O	1:F:122:ILE:HG13	2.10	0.51
2:H:185:LEU:HD13	2:H:191:TYR:CE1	2.46	0.50
3:L:143:GLU:H	3:L:143:GLU:CD	2.10	0.50
1:F:231:VAL:HA	1:F:234:MET:SD	2.52	0.50
1:F:302:LEU:HD12	1:F:364:SER:O	2.12	0.50
2:H:37:TYR:O	2:H:80:LYS:NZ	2.45	0.50
3:L:11:LEU:CD2	3:L:19:VAL:HG13	2.40	0.50
3:L:41:TRP:CD2	3:L:89:PHE:HB2	2.48	0.49
1:F:348:ARG:NH1	1:F:359:TYR:HE2	2.10	0.49
1:F:384:CYS:HB3	1:F:405:LYS:HA	1.94	0.49
1:F:404:PRO:HG2	1:F:404:PRO:O	2.14	0.48
1:F:146:GLU:OE2	1:F:233:TYR:CE2	2.66	0.48
2:H:76:PHE:CE2	2:H:91:MET:HG2	2.49	0.48
2:H:161:PHE:CE1	2:H:162:PRO:HB3	2.49	0.48
2:H:134:PRO:HB2	2:H:157:VAL:HG13	1.96	0.47
3:L:128:ARG:HG2	3:L:129:THR:N	2.29	0.47
1:F:254:LYS:HB2	1:F:274:PRO:HG3	1.96	0.47
1:F:36:LEU:O	1:F:332:HIS:HA	2.15	0.47
1:F:205:ARG:NH1	2:H:63:SER:OG	2.48	0.47
1:F:195:GLN:HE22	1:F:198:ARG:HH11	1.62	0.47
2:H:56:ILE:HD13	2:H:80:LYS:HB2	1.96	0.47
2:H:196:VAL:HG11	3:L:155:LEU:HD22	1.97	0.46
1:F:260:ILE:HB	1:F:268:ILE:O	2.16	0.46
1:F:282:PRO:HD2	1:F:312:LYS:O	2.16	0.46
2:H:17:ARG:HD2	2:H:17:ARG:HA	1.68	0.46
3:L:154:CYS:HB2	3:L:168:TRP:CH2	2.50	0.46
1:F:139:GLY:HA2	1:F:142:LYS:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:SER:HB3	1:F:304:ARG:HD3	1.99	0.45
1:F:40:ARG:O	1:F:337:THR:OG1	2.23	0.45
3:L:218:HIS:CD2	3:L:219:GLN:H	2.33	0.45
2:H:137:PHE:CG	3:L:144:GLN:HB2	2.51	0.45
1:F:234:MET:CE	1:F:275:ILE:HG12	2.46	0.45
3:L:219:GLN:HG2	3:L:219:GLN:O	2.17	0.45
1:F:26:GLU:H	1:F:26:GLU:CD	2.20	0.45
2:H:190:LEU:HD23	2:H:190:LEU:HA	1.62	0.45
3:L:67:LEU:HD11	3:L:76:PHE:O	2.17	0.45
2:H:6:GLU:HA	2:H:22:SER:O	2.17	0.44
2:H:40:HIS:NE2	2:H:107:ASP:HB2	2.31	0.44
3:L:95:GLN:HB3	3:L:96:PRO:HD2	1.98	0.44
1:F:392:ILE:HB	1:F:400:ILE:O	2.18	0.44
1:F:403:LEU:HD22	1:F:404:PRO:HD2	1.98	0.44
2:H:71:VAL:HB	2:H:76:PHE:CG	2.53	0.44
3:L:44:GLN:HB2	3:L:50:PRO:HA	1.99	0.44
3:L:133:PRO:HB3	3:L:159:PHE:HB3	2.00	0.44
1:F:388:VAL:HG22	1:F:421:ASP:HB2	2.00	0.44
3:L:45:LYS:O	3:L:48:LYS:HB2	2.18	0.44
3:L:178:ASN:ND2	3:L:199:LEU:HD11	2.33	0.44
3:L:178:ASN:OD1	3:L:178:ASN:N	2.45	0.44
3:L:141:SER:O	3:L:145:LEU:HD12	2.18	0.44
1:F:73:LEU:HD22	2:H:36:ARG:HB3	2.00	0.44
1:F:146:GLU:OE2	1:F:233:TYR:HE2	2.01	0.44
1:F:78:LEU:HA	1:F:78:LEU:HD23	1.73	0.43
1:F:81:LEU:HD12	1:F:81:LEU:HA	1.76	0.43
3:L:8:PRO:O	3:L:122:THR:HG22	2.17	0.43
2:H:138:PRO:O	2:H:139:LEU:HD23	2.19	0.43
2:H:167:VAL:HA	2:H:212:ASN:O	2.18	0.43
1:F:195:GLN:NE2	1:F:198:ARG:HH11	2.17	0.43
1:F:223:THR:HG23	1:F:226:GLU:OE1	2.19	0.43
2:H:134:PRO:HB3	2:H:160:TYR:HB3	2.01	0.43
1:F:195:GLN:OE1	1:F:198:ARG:NH1	2.52	0.43
1:F:322:ASN:O	1:F:325:ASP:HB2	2.19	0.42
3:L:28:GLY:HA2	3:L:85:THR:HG22	2.01	0.42
1:F:56:GLU:HG2	3:L:37:ARG:HD3	2.01	0.42
1:F:283:CYS:HA	1:F:310:TYR:O	2.18	0.42
1:F:273:LEU:HD23	1:F:273:LEU:HA	1.76	0.42
1:F:392:ILE:HG23	1:F:415:ALA:CB	2.50	0.42
2:H:162:PRO:HD2	2:H:217:PRO:CB	2.49	0.42
3:L:133:PRO:HD3	3:L:218:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:GLN:O	1:F:244:MET:HG3	2.20	0.42
1:F:199:ARG:O	1:F:203:VAL:HG23	2.20	0.41
3:L:128:ARG:HG2	3:L:129:THR:H	1.84	0.41
1:F:244:MET:HE3	1:F:244:MET:HB3	1.87	0.41
1:F:394:SER:HB3	1:F:397:VAL:O	2.20	0.41
2:H:30:PHE:CZ	2:H:80:LYS:HE3	2.54	0.41
1:F:58:LEU:HD23	1:F:58:LEU:HA	1.87	0.41
1:F:222:MET:SD	1:F:273:LEU:HD11	2.60	0.41
1:F:164:GLU:OE1	1:F:164:GLU:N	2.50	0.41
2:H:52:TRP:HZ2	2:H:55:VAL:HG12	1.85	0.41
1:F:167:GLU:O	1:F:171:LYS:HG2	2.21	0.41
1:F:91:ARG:HA	1:F:91:ARG:HD2	1.87	0.41
2:H:53:VAL:HG13	2:H:71:VAL:HG21	2.03	0.40
1:F:144:THR:HG23	1:F:146:GLU:H	1.86	0.40
2:H:204:LEU:HD22	2:H:228:PRO:HB2	2.03	0.40
1:F:217:ILE:HD11	1:F:255:GLY:HA3	2.04	0.40
3:L:99:ILE:HD12	3:L:99:ILE:HG23	1.87	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	F	379/539 (70%)	350 (92%)	28 (7%)	1 (0%)	41 73
2	H	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	29 64
3	L	212/214 (99%)	194 (92%)	18 (8%)	0	100 100
All	All	808/972 (83%)	750 (93%)	56 (7%)	2 (0%)	47 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	48	LYS
1	F	407	CYS

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	F	319/456 (70%)	317 (99%)	2 (1%)	86 94
2	H	180/182 (99%)	177 (98%)	3 (2%)	60 83
3	L	188/188 (100%)	186 (99%)	2 (1%)	73 89
All	All	687/826 (83%)	680 (99%)	7 (1%)	76 90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	196	PHE
1	F	329	ARG
2	H	22	SER
2	H	155	CYS
2	H	231	CYS
3	L	26	SER
3	L	182	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

5 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	A	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	0.84	0
4	NAG	A	2	4	14,14,15	0.55	0	17,19,21	0.79	0
4	BMA	A	3	4	11,11,12	2.50	6 (54%)	15,15,17	1.85	4 (26%)
4	MAN	A	4	4	11,11,12	0.71	0	15,15,17	1.92	5 (33%)
4	MAN	A	5	4	11,11,12	1.91	3 (27%)	15,15,17	1.20	2 (13%)

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	A	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	MAN	A	4	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5	4	-	1/2/19/22	1/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	C2-C3	4.63	1.59	1.52
4	A	5	MAN	C1-C2	3.70	1.60	1.52
4	A	5	MAN	C2-C3	3.36	1.57	1.52
4	A	3	BMA	C4-C3	3.30	1.60	1.52
4	A	3	BMA	O3-C3	3.26	1.50	1.43
4	A	3	BMA	C4-C5	2.85	1.59	1.53
4	A	3	BMA	C1-C2	2.73	1.58	1.52
4	A	1	NAG	O5-C1	2.68	1.48	1.43
4	A	5	MAN	O5-C5	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	BMA	C6-C5	2.00	1.58	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	4	MAN	C1-O5-C5	4.70	118.56	112.19
4	A	3	BMA	C1-C2-C3	3.49	113.96	109.67
4	A	3	BMA	C1-O5-C5	3.44	116.85	112.19
4	A	3	BMA	C3-C4-C5	3.15	115.85	110.24
4	A	4	MAN	C6-C5-C4	-3.05	105.86	113.00
4	A	5	MAN	C1-O5-C5	3.03	116.29	112.19
4	A	3	BMA	C2-C3-C4	2.88	115.88	110.89
4	A	4	MAN	O3-C3-C4	-2.47	104.64	110.35
4	A	4	MAN	C2-C3-C4	-2.47	106.63	110.89
4	A	4	MAN	O2-C2-C3	-2.44	105.24	110.14
4	A	5	MAN	O2-C2-C1	2.37	114.01	109.15

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

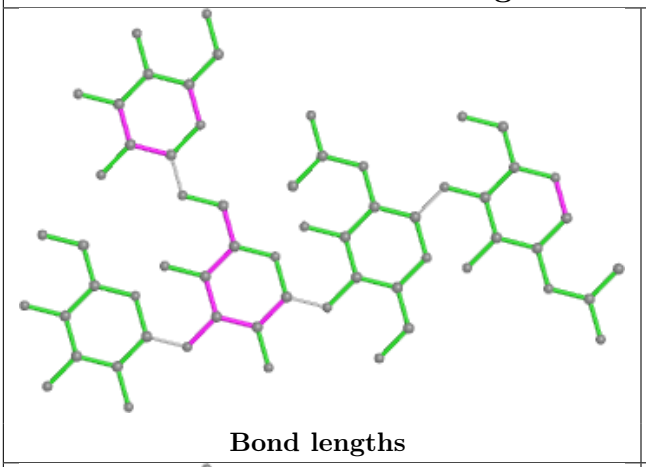
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5	MAN	C1-C2-C3-C4-C5-O5

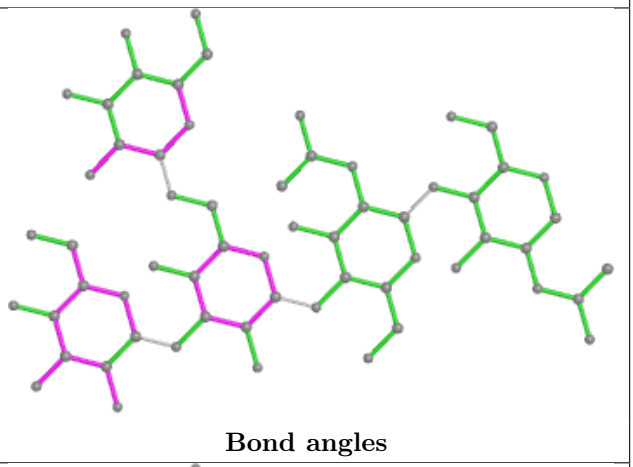
No monomer is involved in short contacts.

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

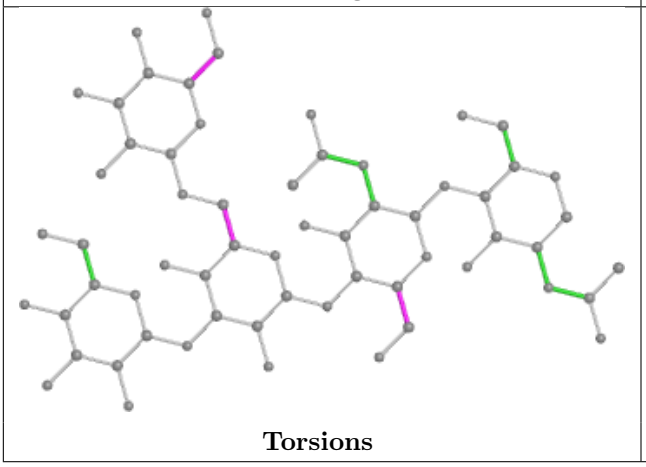
Oligosaccharide Chain A



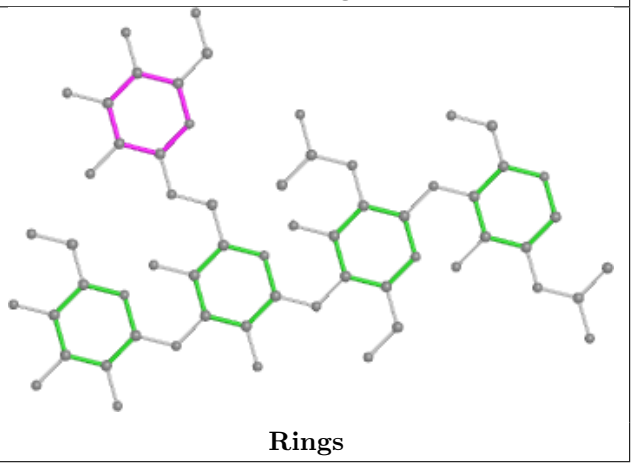
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	NAG	F	606	1	14,14,15	1.35	1 (7%)	17,19,21	1.08	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	606	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	606	NAG	O5-C1	4.84	1.51	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	606	NAG	C1-O5-C5	3.55	117.00	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	606	NAG	O5-C5-C6-O6
5	F	606	NAG	C4-C5-C6-O6

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^{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	F	385/539 (71%)	-0.06	4 (1%) 82 67	68, 98, 140, 188	0
2	H	219/219 (100%)	-0.02	5 (2%) 60 39	70, 99, 142, 165	0
3	L	214/214 (100%)	-0.11	0 100 100	74, 99, 117, 126	0
All	All	818/972 (84%)	-0.06	9 (1%) 80 64	68, 98, 137, 188	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	410	ILE	2.8
1	F	382	VAL	2.8
1	F	26	GLU	2.4
1	F	408	SER	2.4
2	H	209	TYR	2.2
2	H	210	ILE	2.1
2	H	206	THR	2.1
2	H	153	LEU	2.0
2	H	226	VAL	2.0

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

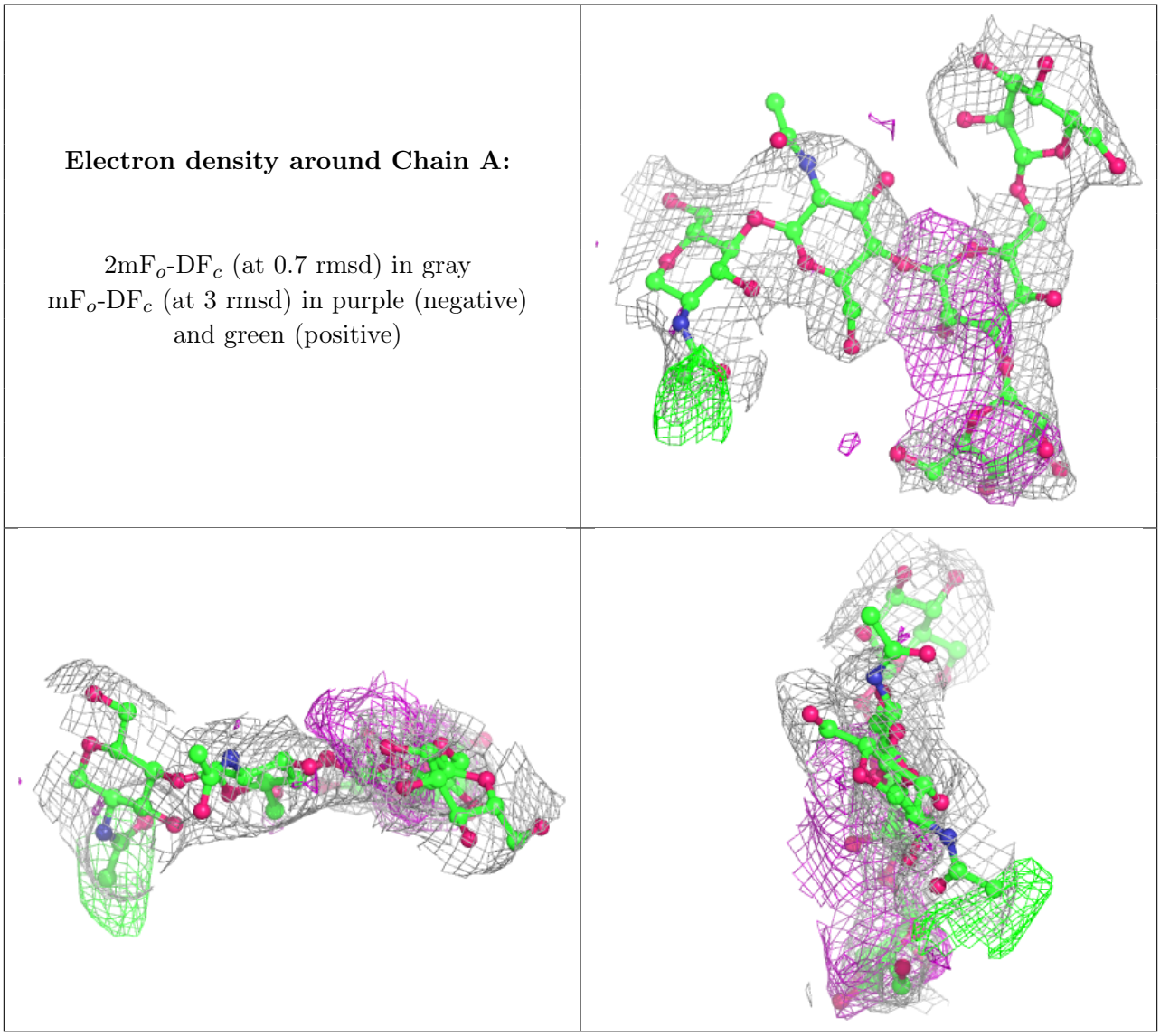
There are no non-standard protein/DNA/RNA residues in this entry.

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^{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
4	BMA	A	3	11/12	0.71	0.49	130,149,162,166	0
4	MAN	A	5	11/12	0.78	0.27	165,174,179,180	0
4	MAN	A	4	11/12	0.81	0.60	109,137,144,145	0
4	NAG	A	1	14/15	0.82	0.15	103,121,128,131	0
4	NAG	A	2	14/15	0.90	0.28	115,135,150,151	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

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	NAG	F	606	14/15	0.87	0.17	102,116,130,133	0

6.5 Other polymers (i)

There are no such residues in this entry.