Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 07:22 AM EDT

PDB ID	:	5EJB
Title	:	Crystal structure of prefusion Hendra virus F protein
Authors	:	Wong, J.W.; Jardetzky, T.S.; Paterson, R.G.; Lamb, R.A.
Deposited on	:	2015-11-01
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 (i) 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 (1)) were used in the production of this report:

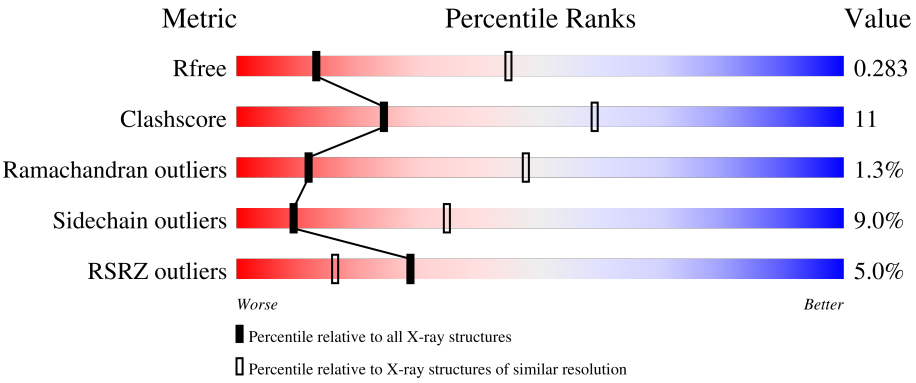
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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	501	3% 62% 23% • 12%
1	B	501	4% 63% 23% • 11%
1	C	501	7% 66% 21% • 9%
1	D	501	5% 64% 23% • 8%
1	E	501	5% 64% 21% • 13%

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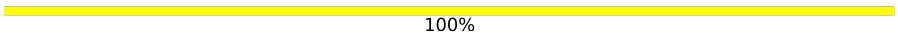
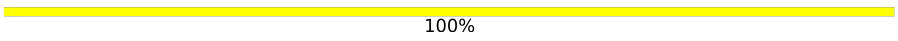
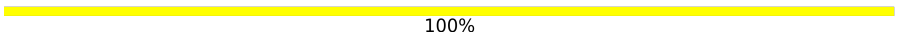
Mol	Chain	Length	Quality of chain
1	F	501	
2	G	2	
2	H	2	
2	I	2	

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	NAG	A	602	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20415 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.

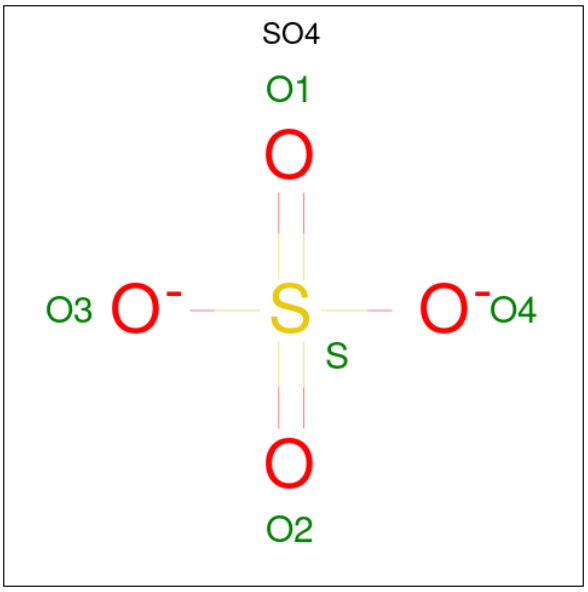
- Molecule 1 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	447	Total	C	N	O	S	0	0	0
			3376	2135	553	670	18			
1	C	454	Total	C	N	O	S	0	0	0
			3390	2142	558	672	18			
1	D	460	Total	C	N	O	S	0	0	0
			3441	2174	566	683	18			
1	F	436	Total	C	N	O	S	0	0	0
			3298	2086	540	654	18			
1	E	436	Total	C	N	O	S	0	0	0
			3298	2086	540	654	18			
1	A	440	Total	C	N	O	S	0	0	0
			3330	2107	545	660	18			

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

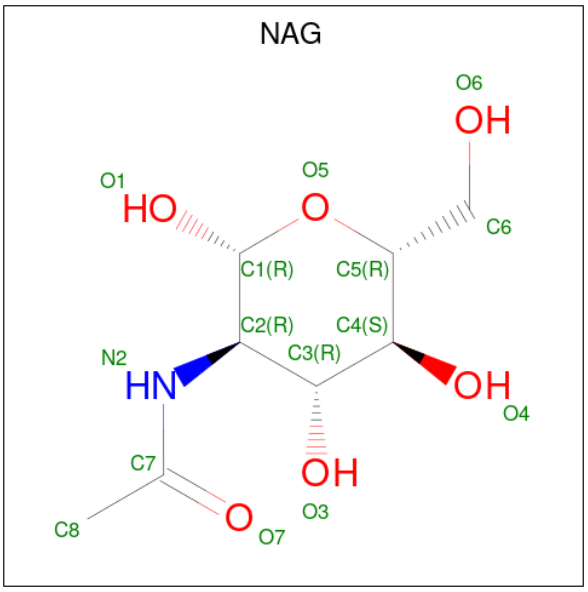
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



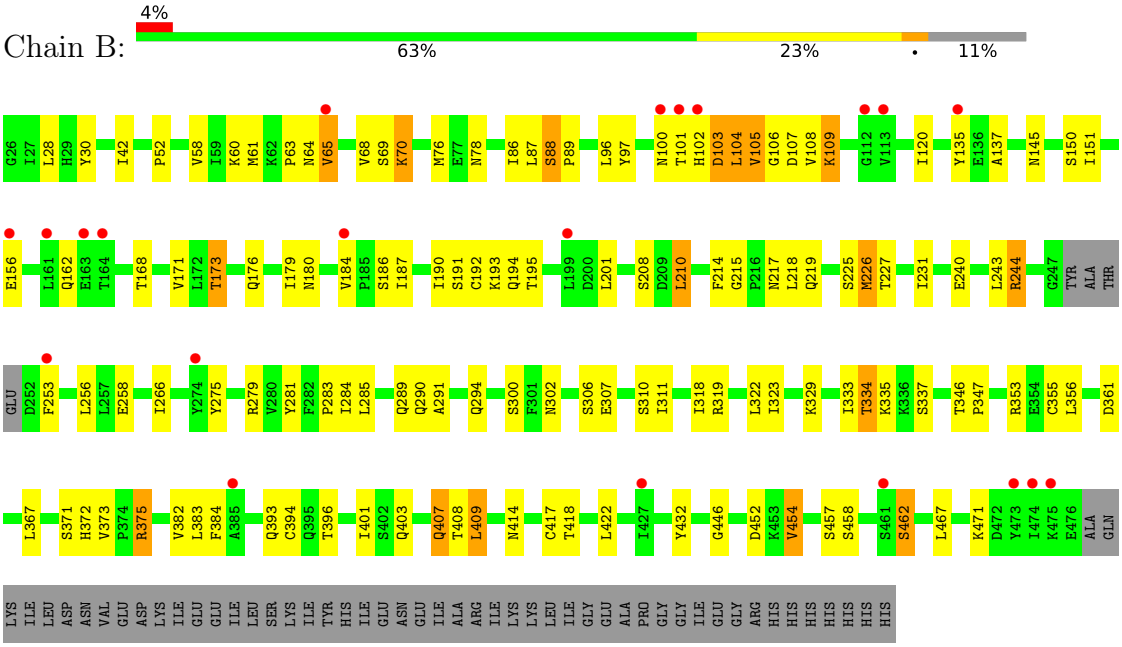
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 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.

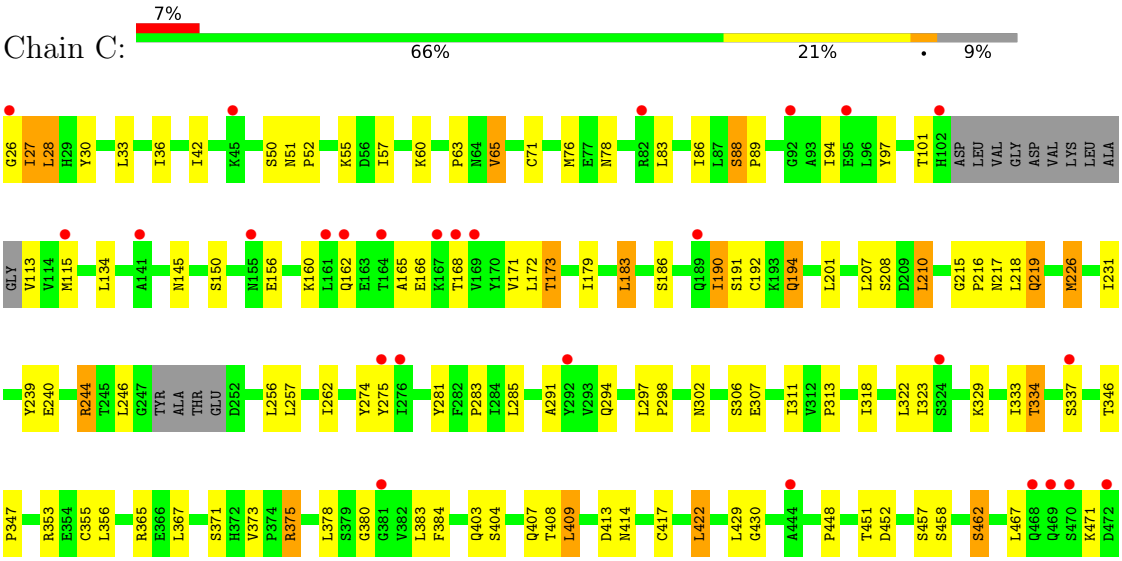
• Molecule 1: Fusion glycoprotein F0

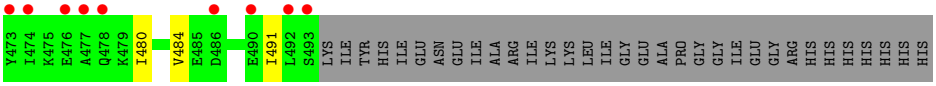
Chain B:



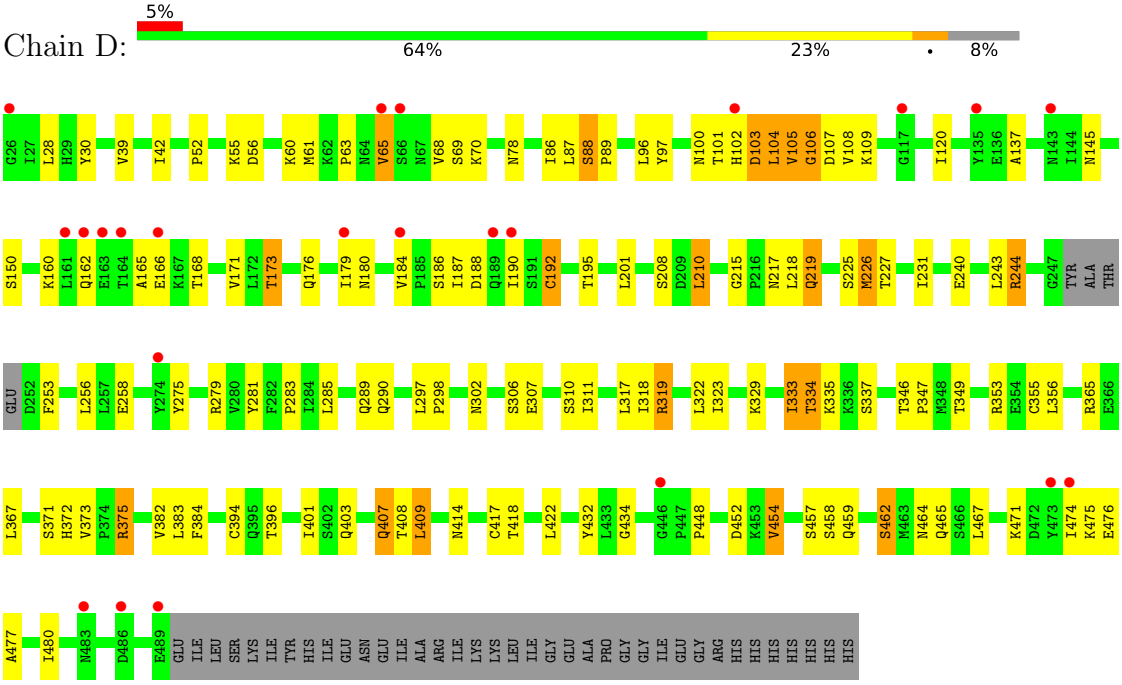
• Molecule 1: Fusion glycoprotein F0

Chain C:

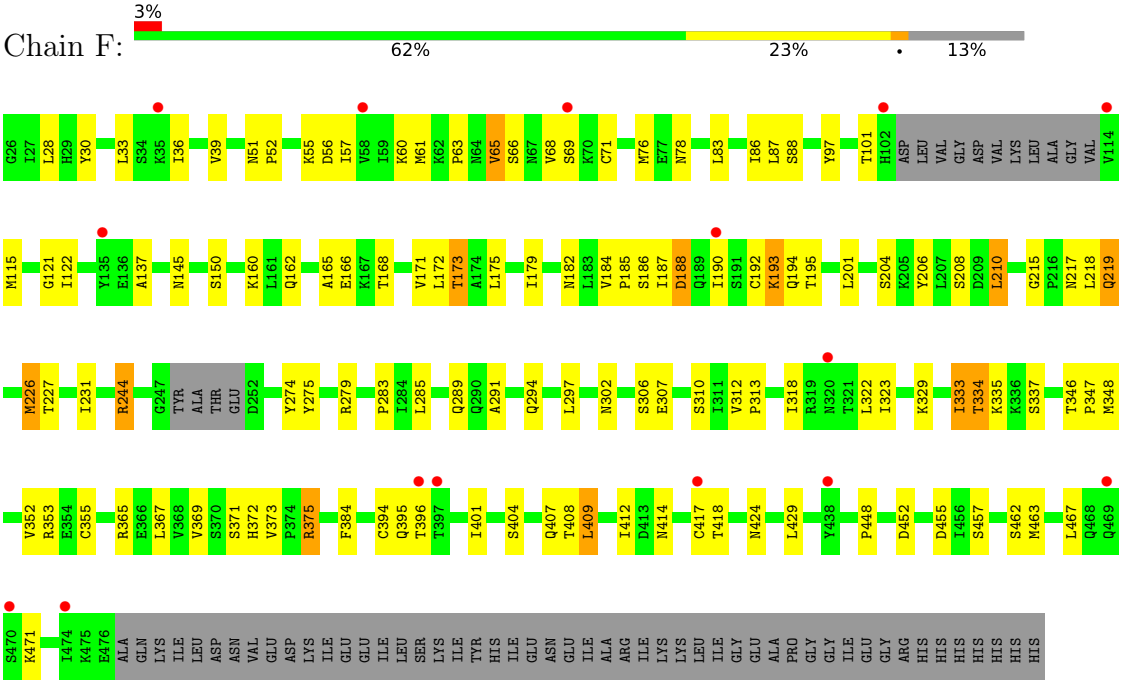




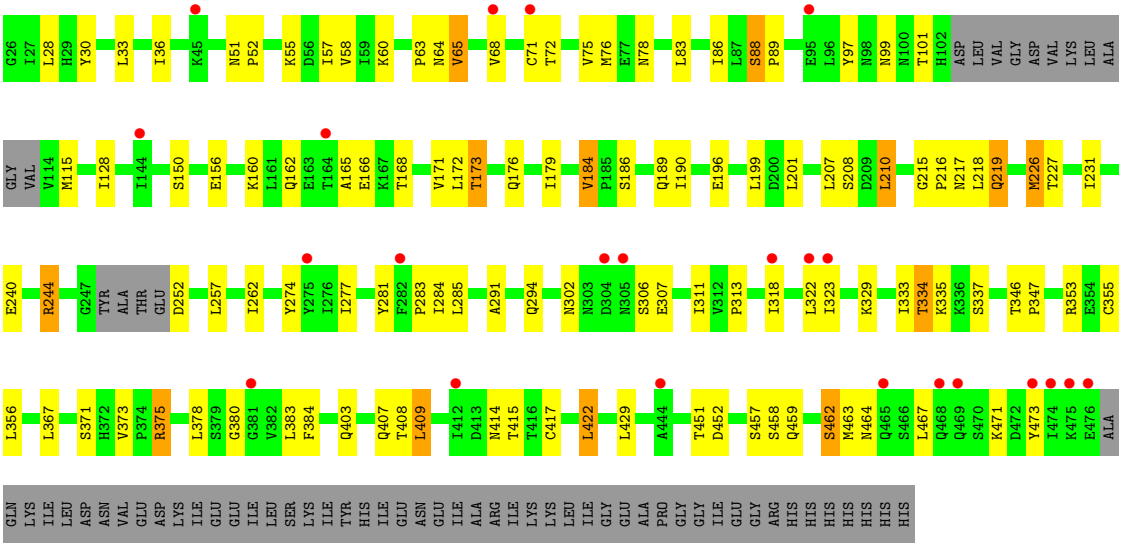
• Molecule 1: Fusion glycoprotein F0



• Molecule 1: Fusion glycoprotein F0

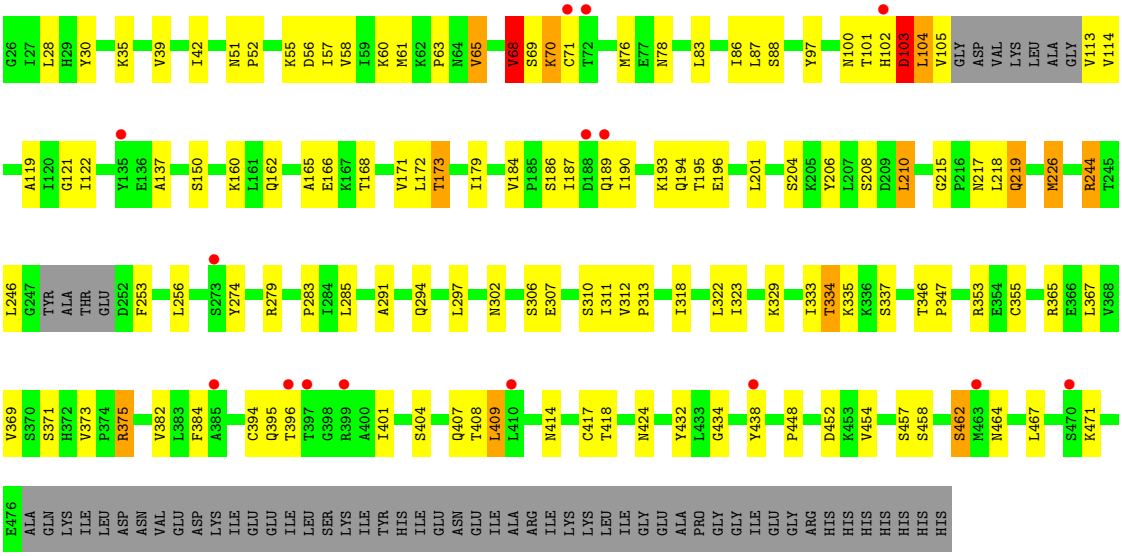


• Molecule 1: Fusion glycoprotein F0



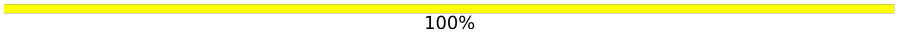
• Molecule 1: Fusion glycoprotein F0

Chain A:



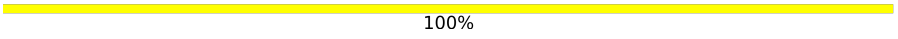
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



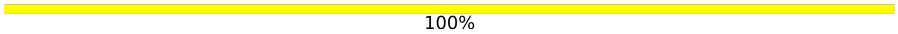
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.61Å 163.50Å 147.94Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	49.62 – 3.20 49.62 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.62-3.20) 99.7 (49.62-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.253 , 0.283 0.253 , 0.283	Depositor DCC
R_{free} test set	4233 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20415	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.87% 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: NAG, SO4

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	0.54	0/3375	0.73	1/4593 (0.0%)
1	B	0.59	0/3422	0.75	0/4657
1	C	0.53	0/3435	0.71	0/4677
1	D	0.59	0/3487	0.75	1/4748 (0.0%)
1	E	0.52	0/3343	0.71	0/4548
1	F	0.54	0/3343	0.72	0/4548
All	All	0.55	0/20405	0.73	2/27771 (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
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	319	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	253	PHE	N-CA-CB	-5.20	101.25	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Peptide
1	B	102	HIS	Peptide
1	D	102	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3324	87	0
1	B	3376	0	3377	86	1
1	C	3390	0	3336	75	0
1	D	3441	0	3403	88	0
1	E	3298	0	3288	75	0
1	F	3298	0	3290	84	1
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	28	0	26	0	0
4	C	14	0	13	0	0
4	D	42	0	39	2	0
4	E	56	0	52	1	0
4	F	28	0	26	2	0
All	All	20415	0	20249	449	1

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 (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:ILE:HG12	1:F:323:ILE:HG22	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:ILE:HG12	1:E:323:ILE:HG22	1.52	0.91
1:C:65:VAL:HG21	1:C:76:MET:CE	2.00	0.91
1:D:307:GLU:HG3	1:D:375:ARG:HH21	1.36	0.91
1:E:65:VAL:HG21	1:E:76:MET:CE	2.01	0.91
1:F:184:VAL:O	1:F:187:ILE:HG12	1.70	0.91
1:B:318:ILE:HG12	1:B:323:ILE:HG22	1.53	0.91
1:C:318:ILE:HG12	1:C:323:ILE:HG22	1.50	0.91
1:B:307:GLU:HG3	1:B:375:ARG:HH21	1.35	0.90
1:D:318:ILE:HG12	1:D:323:ILE:HG22	1.54	0.90
1:A:318:ILE:HG12	1:A:323:ILE:HG22	1.55	0.87
1:B:65:VAL:HG21	1:B:76:MET:CE	2.04	0.87
1:C:307:GLU:HG3	1:C:375:ARG:HH21	1.41	0.86
1:F:307:GLU:HG3	1:F:375:ARG:HH21	1.41	0.85
1:F:414:ASN:HA	1:F:417:CYS:O	1.78	0.83
1:D:105:VAL:CG1	1:F:395:GLN:HE22	1.91	0.83
1:A:307:GLU:HG3	1:A:375:ARG:HH21	1.43	0.82
1:E:307:GLU:HG3	1:E:375:ARG:HH21	1.44	0.80
1:F:65:VAL:HG21	1:F:76:MET:CE	2.13	0.79
1:B:307:GLU:HG3	1:B:375:ARG:NH2	2.00	0.77
1:D:459:GLN:HG2	4:F:602:NAG:H83	1.67	0.76
1:A:414:ASN:HA	1:A:417:CYS:O	1.84	0.75
1:E:334:THR:HG22	1:E:337:SER:H	1.51	0.75
1:B:414:ASN:HA	1:B:417:CYS:O	1.87	0.74
1:C:334:THR:HG22	1:C:337:SER:H	1.51	0.73
1:D:307:GLU:HG3	1:D:375:ARG:NH2	2.03	0.73
1:A:334:THR:HG22	1:A:337:SER:H	1.54	0.73
1:B:28:LEU:HD22	1:B:356:LEU:HB3	1.70	0.72
1:D:28:LEU:HB2	1:D:30:TYR:CE1	2.24	0.72
1:D:372:HIS:HB2	3:D:606:SO4:O4	1.89	0.71
1:B:103:ASP:O	1:B:105:VAL:N	2.23	0.71
1:A:105:VAL:HG23	1:A:113:VAL:N	2.06	0.71
1:A:65:VAL:HG22	1:A:179:ILE:HD13	1.72	0.71
1:C:323:ILE:HD11	1:C:353:ARG:HG3	1.73	0.71
1:B:103:ASP:C	1:B:105:VAL:H	1.95	0.70
1:F:218:LEU:O	1:F:218:LEU:HG	1.92	0.70
1:B:396:THR:HG21	1:B:418:THR:OG1	1.91	0.70
1:F:334:THR:HG22	1:F:337:SER:H	1.57	0.70
1:E:65:VAL:HG21	1:E:76:MET:HE3	1.73	0.69
4:D:605:NAG:H83	1:E:459:GLN:HE21	1.56	0.69
1:B:60:LYS:HB3	1:B:173:THR:HB	1.73	0.69
1:B:104:LEU:HG	1:B:135:TYR:OH	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:HG11	1:F:395:GLN:HE22	1.58	0.69
1:D:323:ILE:HD11	1:D:353:ARG:HG3	1.75	0.69
1:A:190:ILE:HG23	1:A:194:GLN:HB3	1.74	0.69
1:B:323:ILE:HD11	1:B:353:ARG:HG3	1.75	0.68
1:D:186:SER:HB2	1:D:190:ILE:HD12	1.75	0.68
1:D:100:ASN:HD22	1:D:120:ILE:HD13	1.59	0.68
1:F:68:VAL:HG12	1:F:68:VAL:O	1.93	0.68
1:B:289:GLN:HB3	1:F:424:ASN:OD1	1.92	0.68
1:C:65:VAL:HG21	1:C:76:MET:HE3	1.74	0.68
1:B:184:VAL:HA	1:B:187:ILE:HD12	1.76	0.67
1:A:218:LEU:O	1:A:218:LEU:HG	1.93	0.67
1:A:323:ILE:HD11	1:A:353:ARG:HG3	1.75	0.67
1:E:323:ILE:HD11	1:E:353:ARG:HG3	1.76	0.67
1:D:61:MET:HE1	1:D:87:LEU:HD21	1.76	0.67
1:F:186:SER:HB2	1:F:190:ILE:HD12	1.77	0.67
1:D:334:THR:HG22	1:D:337:SER:H	1.61	0.66
1:F:323:ILE:HD11	1:F:353:ARG:HG3	1.75	0.66
1:D:60:LYS:HB3	1:D:173:THR:HB	1.78	0.66
1:E:60:LYS:HB3	1:E:173:THR:HB	1.78	0.65
1:B:28:LEU:HB2	1:B:30:TYR:CE1	2.31	0.65
1:D:289:GLN:OE1	1:A:424:ASN:ND2	2.30	0.65
1:C:307:GLU:HG3	1:C:375:ARG:NH2	2.11	0.65
1:A:346:THR:CG2	1:A:347:PRO:HD2	2.26	0.64
1:D:289:GLN:HB3	1:A:424:ASN:OD1	1.98	0.64
1:A:103:ASP:O	1:A:104:LEU:HB2	1.97	0.63
1:B:63:PRO:HB2	1:B:179:ILE:HD12	1.81	0.63
1:D:68:VAL:HG22	1:D:184:VAL:HG22	1.80	0.63
1:B:334:THR:HG22	1:B:337:SER:H	1.62	0.63
1:F:346:THR:CG2	1:F:347:PRO:HD2	2.29	0.63
1:A:103:ASP:CB	1:A:114:VAL:H	2.11	0.63
1:B:218:LEU:HG	1:B:218:LEU:O	1.99	0.63
1:A:307:GLU:HG3	1:A:375:ARG:NH2	2.14	0.63
1:F:182:ASN:O	1:F:186:SER:OG	2.15	0.63
1:A:103:ASP:HB3	1:A:114:VAL:H	1.64	0.63
1:D:218:LEU:O	1:D:218:LEU:HG	1.97	0.62
1:A:190:ILE:HG22	1:A:195:THR:HG23	1.81	0.62
1:F:372:HIS:HB2	3:F:603:SO4:O2	1.99	0.62
1:B:104:LEU:HD22	1:B:109:LYS:HA	1.82	0.62
1:B:289:GLN:OE1	1:F:424:ASN:ND2	2.32	0.62
1:B:105:VAL:CG1	1:A:395:GLN:HE22	2.13	0.61
1:D:396:THR:HG21	1:D:418:THR:OG1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:THR:HG22	1:A:347:PRO:HD2	1.80	0.61
1:B:97:TYR:O	1:B:101:THR:HG23	2.00	0.61
1:D:106:GLY:O	1:D:108:VAL:N	2.31	0.61
1:F:307:GLU:HG3	1:F:375:ARG:NH2	2.13	0.61
1:C:60:LYS:HB3	1:C:173:THR:HB	1.82	0.61
1:D:474:ILE:HD13	1:E:473:TYR:HD2	1.64	0.61
1:E:97:TYR:O	1:E:101:THR:HG23	2.00	0.61
1:B:226:MET:HE2	1:B:231:ILE:HG12	1.82	0.61
1:B:65:VAL:HG21	1:B:76:MET:HE3	1.80	0.61
1:B:103:ASP:C	1:B:105:VAL:N	2.51	0.61
1:F:60:LYS:HB3	1:F:173:THR:HB	1.83	0.61
1:E:307:GLU:HG3	1:E:375:ARG:NH2	2.13	0.61
1:F:65:VAL:HG21	1:F:76:MET:HE1	1.81	0.60
1:E:72:THR:O	1:E:75:VAL:HG22	2.01	0.60
4:D:605:NAG:C8	1:E:459:GLN:HE21	2.15	0.60
1:C:83:LEU:HD23	1:C:274:TYR:CD1	2.36	0.60
1:C:218:LEU:O	1:C:218:LEU:HG	2.01	0.60
1:D:414:ASN:HA	1:D:417:CYS:O	2.02	0.59
1:E:179:ILE:O	1:E:184:VAL:HG23	2.02	0.59
1:B:68:VAL:O	1:B:70:LYS:N	2.35	0.59
1:F:463:MET:HE1	1:E:463:MET:HB3	1.84	0.59
1:D:78:ASN:HB3	1:F:244:ARG:HH21	1.67	0.59
1:D:226:MET:HE2	1:D:231:ILE:HG12	1.85	0.59
1:F:57:ILE:HD11	1:F:172:LEU:HD13	1.85	0.59
1:E:218:LEU:HG	1:E:218:LEU:O	2.02	0.59
1:E:68:VAL:HG12	1:E:68:VAL:O	2.03	0.58
1:E:63:PRO:HB2	1:E:179:ILE:HD12	1.84	0.58
1:A:103:ASP:OD1	1:A:103:ASP:N	2.36	0.58
1:B:192:CYS:C	1:B:194:GLN:H	2.06	0.58
1:C:26:GLY:O	1:C:28:LEU:N	2.36	0.58
1:D:63:PRO:HB2	1:D:179:ILE:HD12	1.85	0.58
1:D:68:VAL:O	1:D:70:LYS:N	2.33	0.58
1:E:28:LEU:HB2	1:E:30:TYR:CE1	2.38	0.57
1:B:78:ASN:HB3	1:A:244:ARG:HH21	1.69	0.57
1:C:63:PRO:HB2	1:C:179:ILE:HD12	1.85	0.57
1:E:83:LEU:HD23	1:E:274:TYR:CD1	2.40	0.57
1:C:97:TYR:O	1:C:101:THR:HG23	2.05	0.57
1:F:346:THR:HG22	1:F:347:PRO:HD2	1.86	0.57
1:B:100:ASN:HD22	1:B:120:ILE:HD13	1.70	0.57
1:B:372:HIS:HB2	3:B:603:SO4:O2	2.05	0.57
1:A:65:VAL:HG21	1:A:76:MET:CE	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:HE22	1:A:168:THR:HG22	1.70	0.56
1:B:61:MET:HE3	1:B:87:LEU:HD21	1.86	0.56
1:D:333:ILE:HD12	1:E:219:GLN:OE1	2.05	0.56
1:A:105:VAL:CG2	1:A:113:VAL:N	2.69	0.56
1:A:60:LYS:HB3	1:A:173:THR:HB	1.88	0.56
1:A:63:PRO:HB2	1:A:179:ILE:HD12	1.89	0.55
1:D:346:THR:CG2	1:D:347:PRO:HD2	2.37	0.55
1:E:162:GLN:HE22	1:E:168:THR:HG22	1.72	0.55
1:E:226:MET:HE2	1:E:231:ILE:HG12	1.89	0.55
1:E:257:LEU:HD13	1:E:262:ILE:HD12	1.88	0.55
1:E:467:LEU:O	1:E:471:LYS:HB2	2.07	0.54
1:A:39:VAL:CG2	1:A:297:LEU:HB2	2.37	0.54
1:D:459:GLN:HG2	4:F:602:NAG:C8	2.35	0.54
1:F:39:VAL:CG2	1:F:297:LEU:HB2	2.37	0.54
1:A:30:TYR:OH	1:A:294:GLN:HG2	2.08	0.54
1:D:137:ALA:HB2	1:D:279:ARG:HD2	1.90	0.54
1:D:215:GLY:C	1:D:217:ASN:H	2.09	0.54
1:D:384:PHE:HB3	1:D:409:LEU:HD21	1.89	0.53
1:B:64:ASN:HB2	1:B:176:GLN:OE1	2.08	0.53
1:D:349:THR:HG22	1:F:455:ASP:OD2	2.08	0.53
1:D:467:LEU:O	1:D:471:LYS:HB2	2.09	0.53
1:F:190:ILE:HG22	1:F:195:THR:HG23	1.90	0.53
1:F:463:MET:HE1	1:E:463:MET:CB	2.38	0.53
1:C:333:ILE:HD12	1:A:219:GLN:OE1	2.08	0.53
1:B:106:GLY:O	1:B:108:VAL:N	2.33	0.53
1:D:61:MET:CE	1:D:87:LEU:HD21	2.39	0.53
1:A:186:SER:O	1:A:190:ILE:HD12	2.08	0.53
1:F:51:ASN:N	1:F:52:PRO:HD3	2.23	0.53
1:B:162:GLN:HE22	1:B:168:THR:HG22	1.74	0.52
1:B:401:ILE:HD11	1:B:417:CYS:SG	2.49	0.52
1:B:65:VAL:HG12	1:B:65:VAL:O	2.09	0.52
1:B:467:LEU:O	1:B:471:LYS:HB2	2.10	0.52
1:C:215:GLY:C	1:C:217:ASN:H	2.11	0.52
1:D:162:GLN:HE22	1:D:168:THR:HG22	1.75	0.52
1:A:467:LEU:O	1:A:471:LYS:HB2	2.10	0.52
1:C:257:LEU:HD13	1:C:262:ILE:HD12	1.92	0.52
1:D:145:ASN:ND2	1:D:275:TYR:OH	2.42	0.52
1:D:104:LEU:HD22	1:D:109:LYS:HA	1.90	0.52
1:D:475:LYS:C	1:D:477:ALA:H	2.13	0.52
1:F:56:ASP:OD1	1:F:279:ARG:HA	2.10	0.52
1:E:458:SER:O	1:E:462:SER:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:THR:HG21	1:A:418:THR:OG1	2.10	0.52
1:F:467:LEU:O	1:F:471:LYS:HB2	2.09	0.52
1:C:210:LEU:C	1:C:210:LEU:HD12	2.30	0.52
1:D:290:GLN:HE22	1:A:424:ASN:HA	1.74	0.52
1:E:384:PHE:HB3	1:E:409:LEU:HD21	1.92	0.51
1:B:467:LEU:CD1	1:C:467:LEU:HB2	2.41	0.51
1:B:52:PRO:HA	1:B:283:PRO:HA	1.91	0.51
1:F:122:ILE:HA	1:E:378:LEU:O	2.11	0.51
1:B:186:SER:O	1:B:190:ILE:HG12	2.10	0.51
1:D:65:VAL:HG22	1:D:68:VAL:HB	1.92	0.51
1:D:97:TYR:O	1:D:101:THR:HG23	2.11	0.51
1:A:97:TYR:O	1:A:101:THR:HG23	2.10	0.51
1:A:184:VAL:O	1:A:187:ILE:HG13	2.11	0.51
1:D:103:ASP:C	1:D:105:VAL:H	2.13	0.51
1:B:384:PHE:HB3	1:B:409:LEU:HD21	1.92	0.51
1:E:215:GLY:C	1:E:217:ASN:H	2.12	0.51
1:A:52:PRO:HA	1:A:283:PRO:HA	1.93	0.51
1:B:156:GLU:OE1	1:C:194:GLN:HG2	2.11	0.51
1:D:187:ILE:HD12	1:D:195:THR:HG21	1.93	0.51
1:E:281:TYR:O	1:E:283:PRO:HD3	2.11	0.51
1:B:28:LEU:CD2	1:B:356:LEU:HB3	2.39	0.51
1:E:75:VAL:HG21	1:E:199:LEU:HD23	1.93	0.51
1:B:210:LEU:HD12	1:B:210:LEU:C	2.32	0.50
1:D:190:ILE:HD11	1:F:185:PRO:HG3	1.92	0.50
1:D:382:VAL:HG21	1:D:432:TYR:CA	2.42	0.50
1:C:467:LEU:O	1:C:471:LYS:HB2	2.11	0.50
1:D:103:ASP:O	1:D:105:VAL:N	2.44	0.50
1:F:63:PRO:HB2	1:F:179:ILE:HD12	1.92	0.50
1:A:190:ILE:HG23	1:A:194:GLN:CB	2.40	0.50
1:E:383:LEU:HD21	1:E:422:LEU:CD2	2.42	0.50
1:C:162:GLN:HE22	1:C:168:THR:HG22	1.76	0.50
1:B:346:THR:CG2	1:B:347:PRO:HD2	2.41	0.50
1:C:186:SER:OG	1:C:190:ILE:HD11	2.12	0.50
1:F:83:LEU:HD23	1:F:274:TYR:CD1	2.47	0.50
1:A:365:ARG:O	1:A:448:PRO:HA	2.11	0.50
1:A:51:ASN:N	1:A:52:PRO:HD3	2.27	0.50
1:D:401:ILE:HD11	1:D:417:CYS:SG	2.52	0.49
1:F:162:GLN:HE22	1:F:168:THR:HG22	1.77	0.49
1:C:156:GLU:OE1	1:A:194:GLN:HG2	2.12	0.49
1:C:186:SER:O	1:C:190:ILE:HG13	2.12	0.49
1:F:78:ASN:HB3	1:E:244:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:O	1:A:122:ILE:HA	2.12	0.49
1:F:137:ALA:HB2	1:F:279:ARG:HD2	1.95	0.49
1:A:57:ILE:HD11	1:A:172:LEU:HD13	1.93	0.49
1:C:281:TYR:O	1:C:283:PRO:HD3	2.11	0.49
1:F:215:GLY:C	1:F:217:ASN:H	2.14	0.49
1:C:57:ILE:HD11	1:C:172:LEU:HD13	1.95	0.49
1:F:52:PRO:HA	1:F:283:PRO:HA	1.95	0.49
1:A:401:ILE:HD11	1:A:417:CYS:SG	2.53	0.49
1:E:28:LEU:CD2	1:E:356:LEU:HB3	2.43	0.49
1:A:215:GLY:C	1:A:217:ASN:H	2.15	0.49
1:C:240:GLU:HB3	1:A:204:SER:HB2	1.94	0.48
1:F:65:VAL:HG21	1:F:76:MET:HE3	1.95	0.48
1:B:382:VAL:HG21	1:B:432:TYR:CA	2.43	0.48
1:E:65:VAL:HG21	1:E:76:MET:HE1	1.90	0.48
1:A:61:MET:CE	1:A:87:LEU:HD21	2.43	0.48
1:C:346:THR:CG2	1:C:347:PRO:HD2	2.43	0.48
1:B:383:LEU:HD21	1:B:422:LEU:HD22	1.96	0.48
1:B:61:MET:CE	1:B:87:LEU:HD21	2.44	0.48
1:A:83:LEU:HD23	1:A:274:TYR:CD1	2.49	0.48
1:D:210:LEU:HD12	1:D:210:LEU:C	2.35	0.48
1:D:349:THR:HG22	1:F:455:ASP:CG	2.34	0.48
1:E:64:ASN:HB2	1:E:176:GLN:OE1	2.14	0.47
1:C:380:GLY:N	1:A:121:GLY:O	2.47	0.47
1:D:103:ASP:C	1:D:105:VAL:N	2.68	0.47
1:B:333:ILE:HD12	1:C:219:GLN:OE1	2.15	0.47
1:C:190:ILE:HG22	1:C:191:SER:H	1.78	0.47
1:D:454:VAL:HG11	1:E:313:PRO:HD3	1.95	0.47
1:F:65:VAL:HG22	1:F:179:ILE:HD13	1.97	0.47
1:B:137:ALA:HB2	1:B:279:ARG:HD2	1.96	0.47
1:D:103:ASP:OD1	1:D:103:ASP:N	2.44	0.47
1:F:57:ILE:HD11	1:F:172:LEU:CD1	2.44	0.47
1:A:193:LYS:HA	1:A:196:GLU:HG2	1.97	0.47
1:B:454:VAL:HG11	1:C:313:PRO:HD3	1.97	0.47
1:B:104:LEU:CG	1:B:135:TYR:OH	2.62	0.46
1:C:226:MET:HE2	1:C:231:ILE:HG12	1.97	0.46
1:F:66:SER:HA	1:F:69:SER:HB3	1.97	0.46
1:F:175:LEU:HD21	1:F:206:TYR:HB2	1.97	0.46
1:C:33:LEU:O	1:C:36:ILE:HG22	2.16	0.46
1:D:68:VAL:HG22	1:D:184:VAL:CG2	2.42	0.46
1:F:101:THR:CG2	1:F:115:MET:SD	3.04	0.46
1:C:384:PHE:HB3	1:C:409:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:NH2	1:F:369:VAL:O	2.44	0.46
1:E:71:CYS:O	1:E:196:GLU:HB3	2.15	0.46
1:E:210:LEU:C	1:E:210:LEU:HD12	2.35	0.46
1:A:189:GLN:O	1:A:190:ILE:HG13	2.14	0.46
1:F:30:TYR:OH	1:F:294:GLN:HG2	2.16	0.46
1:E:186:SER:O	1:E:190:ILE:HG13	2.15	0.46
1:B:103:ASP:OD1	1:B:103:ASP:N	2.49	0.46
1:C:239:TYR:HE1	1:C:257:LEU:HD21	1.80	0.46
1:D:52:PRO:HA	1:D:283:PRO:HA	1.98	0.46
1:D:346:THR:HG22	1:D:347:PRO:HD2	1.98	0.46
1:F:365:ARG:O	1:F:448:PRO:HA	2.15	0.46
1:A:137:ALA:HB2	1:A:279:ARG:HD2	1.98	0.46
1:A:61:MET:HE3	1:A:87:LEU:HD21	1.98	0.46
1:D:334:THR:O	1:D:335:LYS:C	2.54	0.46
1:D:458:SER:O	1:D:462:SER:HB2	2.16	0.46
1:D:225:SER:O	1:D:226:MET:C	2.54	0.45
1:D:290:GLN:O	1:D:319:ARG:HA	2.17	0.45
1:E:51:ASN:N	1:E:52:PRO:HD3	2.31	0.45
1:E:346:THR:CG2	1:E:347:PRO:HD2	2.46	0.45
1:B:383:LEU:HD21	1:B:422:LEU:CD2	2.46	0.45
1:F:187:ILE:HG13	1:F:188:ASP:H	1.81	0.45
1:A:65:VAL:HG22	1:A:179:ILE:CD1	2.43	0.45
1:A:334:THR:O	1:A:335:LYS:C	2.55	0.45
1:B:290:GLN:O	1:B:319:ARG:HA	2.16	0.45
1:F:334:THR:O	1:F:335:LYS:C	2.54	0.45
1:A:65:VAL:HG12	1:A:65:VAL:O	2.17	0.45
1:C:383:LEU:HD21	1:C:422:LEU:CD2	2.46	0.45
1:F:194:GLN:HG2	1:E:156:GLU:OE1	2.16	0.45
1:E:291:ALA:HA	1:E:318:ILE:O	2.16	0.45
1:A:311:ILE:HD13	1:A:311:ILE:HA	1.71	0.45
1:B:319:ARG:NH2	1:A:369:VAL:O	2.47	0.45
1:B:215:GLY:C	1:B:217:ASN:H	2.20	0.45
1:B:291:ALA:HA	1:B:318:ILE:O	2.17	0.45
1:D:215:GLY:C	1:D:217:ASN:N	2.70	0.45
1:E:226:MET:HE2	1:E:226:MET:HB3	1.94	0.45
1:A:432:TYR:CZ	1:A:434:GLY:HA3	2.51	0.45
1:D:28:LEU:HD22	1:D:356:LEU:HB3	1.98	0.45
1:C:65:VAL:HG21	1:C:76:MET:HE2	1.92	0.45
1:C:467:LEU:CD1	1:A:467:LEU:HB2	2.46	0.45
1:D:240:GLU:HG3	1:E:207:LEU:HB3	1.97	0.45
1:E:415:THR:HG22	4:E:603:NAG:H82	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:N	1:B:89:PRO:HD2	2.32	0.45
1:C:30:TYR:OH	1:C:294:GLN:HG2	2.17	0.45
1:F:396:THR:HG21	1:F:418:THR:OG1	2.17	0.45
1:B:151:ILE:HG21	1:B:275:TYR:CD2	2.52	0.44
1:B:334:THR:O	1:B:335:LYS:C	2.55	0.44
1:F:63:PRO:CB	1:F:179:ILE:HD12	2.48	0.44
1:F:204:SER:HB2	1:E:240:GLU:HB3	2.00	0.44
1:C:26:GLY:O	1:C:27:ILE:C	2.55	0.44
1:D:171:VAL:HG12	1:D:173:THR:HG22	2.00	0.44
1:F:33:LEU:O	1:F:36:ILE:HG22	2.17	0.44
1:E:57:ILE:HD11	1:E:172:LEU:HD13	1.98	0.44
1:B:58:VAL:HG12	1:B:171:VAL:HG13	1.98	0.44
1:A:162:GLN:NE2	1:A:168:THR:HG22	2.32	0.44
1:F:384:PHE:HB3	1:F:409:LEU:HD21	2.00	0.44
1:B:244:ARG:HH21	1:C:78:ASN:HB3	1.82	0.44
1:C:28:LEU:CD2	1:C:356:LEU:HB3	2.47	0.44
1:C:302:ASN:O	1:C:408:THR:HA	2.18	0.44
1:F:145:ASN:ND2	1:F:275:TYR:OH	2.51	0.44
1:A:404:SER:HB3	1:A:407:GLN:OE1	2.18	0.44
1:B:105:VAL:HG11	1:A:395:GLN:HE22	1.83	0.44
1:B:279:ARG:HD3	1:B:281:TYR:OH	2.18	0.44
1:D:382:VAL:HG21	1:D:432:TYR:HA	1.99	0.44
1:F:210:LEU:C	1:F:210:LEU:HD12	2.38	0.44
1:B:30:TYR:OH	1:B:294:GLN:HG2	2.18	0.44
1:B:240:GLU:HG3	1:C:207:LEU:HB3	2.00	0.44
1:A:56:ASP:OD1	1:A:279:ARG:HG3	2.18	0.44
1:C:413:ASP:HB2	1:C:430:GLY:O	2.18	0.43
1:A:165:ALA:O	1:A:166:GLU:CB	2.66	0.43
1:B:176:GLN:NE2	1:B:180:ASN:OD1	2.51	0.43
1:B:382:VAL:HG21	1:B:432:TYR:HA	2.00	0.43
1:D:88:SER:N	1:D:89:PRO:HD2	2.33	0.43
1:E:58:VAL:HG22	1:E:277:ILE:HG12	2.01	0.43
1:B:284:ILE:HD12	1:B:284:ILE:HA	1.93	0.43
1:C:51:ASN:N	1:C:52:PRO:HD3	2.33	0.43
1:C:414:ASN:HB3	1:C:429:LEU:O	2.18	0.43
1:A:39:VAL:HG22	1:A:297:LEU:HB2	2.00	0.43
1:A:382:VAL:HG21	1:A:432:TYR:HA	2.01	0.43
1:E:414:ASN:HB3	1:E:429:LEU:O	2.18	0.43
1:F:101:THR:HG22	1:F:115:MET:SD	2.59	0.43
1:C:291:ALA:HA	1:C:318:ILE:O	2.19	0.43
1:D:244:ARG:HH21	1:E:78:ASN:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:OD1	1:A:279:ARG:HA	2.18	0.43
1:B:458:SER:O	1:B:462:SER:HB2	2.19	0.43
1:D:243:LEU:HB3	1:D:253:PHE:HZ	1.83	0.43
1:E:284:ILE:HD12	1:E:284:ILE:HA	1.95	0.43
1:B:145:ASN:ND2	1:B:275:TYR:OH	2.51	0.43
1:C:244:ARG:HH21	1:A:78:ASN:HB3	1.84	0.43
1:F:219:GLN:OE1	1:E:333:ILE:HD12	2.18	0.43
1:F:348:MET:SD	1:F:352:VAL:HG12	2.59	0.43
1:E:162:GLN:NE2	1:E:168:THR:HG22	2.32	0.43
1:A:291:ALA:HA	1:A:318:ILE:O	2.18	0.43
1:B:214:PHE:HE1	1:B:266:ILE:HD11	1.84	0.43
1:C:71:CYS:HB3	1:C:192:CYS:HB3	1.85	0.43
1:C:403:GLN:HG3	1:C:407:GLN:HG3	2.01	0.43
1:C:458:SER:O	1:C:462:SER:HB2	2.18	0.43
1:D:162:GLN:NE2	1:D:168:THR:HG22	2.34	0.43
1:F:165:ALA:O	1:F:166:GLU:CB	2.67	0.43
1:E:58:VAL:HG12	1:E:171:VAL:HG13	2.00	0.43
1:F:193:LYS:H	1:F:193:LYS:HG2	1.33	0.42
1:E:463:MET:O	1:E:464:ASN:C	2.57	0.42
1:F:160:LYS:HE2	1:F:168:THR:HG21	2.02	0.42
1:F:412:ILE:O	1:F:429:LEU:HD13	2.19	0.42
1:A:171:VAL:HG12	1:A:173:THR:HG22	2.01	0.42
1:B:225:SER:O	1:B:226:MET:C	2.55	0.42
1:C:297:LEU:HA	1:C:298:PRO:HD3	1.89	0.42
1:F:121:GLY:O	1:E:380:GLY:N	2.52	0.42
1:E:160:LYS:HE2	1:E:168:THR:HG21	2.02	0.42
1:B:302:ASN:O	1:B:408:THR:HA	2.20	0.42
1:D:464:ASN:O	1:D:465:GLN:C	2.57	0.42
1:F:97:TYR:O	1:F:101:THR:HG23	2.18	0.42
1:F:302:ASN:O	1:F:408:THR:HA	2.20	0.42
1:A:226:MET:HE2	1:A:226:MET:HB3	1.98	0.42
1:A:302:ASN:O	1:A:408:THR:HA	2.19	0.42
1:B:162:GLN:NE2	1:B:168:THR:HG22	2.34	0.42
1:B:403:GLN:HG3	1:B:407:GLN:HG3	2.01	0.42
1:C:365:ARG:O	1:C:448:PRO:HA	2.19	0.42
1:D:219:GLN:OE1	1:F:333:ILE:HD12	2.20	0.42
1:D:297:LEU:HA	1:D:298:PRO:HD3	1.93	0.42
1:E:101:THR:CG2	1:E:115:MET:SD	3.08	0.42
1:C:404:SER:HB3	1:C:407:GLN:OE1	2.19	0.42
1:D:279:ARG:HD3	1:D:281:TYR:OH	2.19	0.42
1:F:39:VAL:HG22	1:F:297:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:VAL:HG13	1:F:313:PRO:HD2	2.02	0.42
1:E:302:ASN:O	1:E:408:THR:HA	2.18	0.42
1:E:403:GLN:HG3	1:E:407:GLN:HG3	2.01	0.42
1:E:33:LEU:O	1:E:36:ILE:HG22	2.20	0.42
1:A:100:ASN:ND2	1:A:119:ALA:HB1	2.35	0.42
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.81	0.42
1:D:302:ASN:O	1:D:408:THR:HA	2.20	0.42
1:E:215:GLY:C	1:E:217:ASN:N	2.73	0.42
1:B:68:VAL:C	1:B:70:LYS:H	2.23	0.42
1:C:414:ASN:HA	1:C:417:CYS:O	2.20	0.42
1:E:88:SER:N	1:E:89:PRO:HD2	2.35	0.42
1:E:311:ILE:HD13	1:E:311:ILE:HA	1.77	0.42
1:A:382:VAL:HG21	1:A:432:TYR:CA	2.50	0.42
1:C:165:ALA:O	1:C:166:GLU:CB	2.68	0.42
1:D:226:MET:HE2	1:D:226:MET:HB3	1.89	0.42
1:D:403:GLN:HG3	1:D:407:GLN:HG3	2.02	0.42
1:D:432:TYR:CZ	1:D:434:GLY:HA3	2.55	0.42
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.85	0.42
1:B:311:ILE:HD13	1:B:311:ILE:HA	1.77	0.41
1:C:215:GLY:C	1:C:217:ASN:N	2.73	0.41
1:A:68:VAL:C	1:A:70:LYS:H	2.23	0.41
1:B:171:VAL:HG12	1:B:173:THR:HG22	2.01	0.41
1:B:243:LEU:HB3	1:B:253:PHE:HZ	1.84	0.41
1:D:56:ASP:OD1	1:D:279:ARG:HA	2.20	0.41
1:D:160:LYS:HE2	1:D:168:THR:HG21	2.03	0.41
1:D:165:ALA:O	1:D:166:GLU:CB	2.68	0.41
1:F:291:ALA:HA	1:F:318:ILE:O	2.20	0.41
1:F:463:MET:CE	1:E:463:MET:HB3	2.49	0.41
1:B:361:ASP:HA	1:B:446:GLY:HA2	2.03	0.41
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.41
1:A:160:LYS:HE2	1:A:168:THR:HG21	2.02	0.41
1:D:365:ARG:O	1:D:448:PRO:HA	2.20	0.41
1:F:226:MET:HE2	1:F:231:ILE:HG12	2.02	0.41
1:B:258:GLU:HG3	1:C:216:PRO:HD2	2.02	0.41
1:C:94:ILE:HG23	1:C:134:LEU:HD21	2.02	0.41
1:C:311:ILE:HG22	1:C:311:ILE:O	2.21	0.41
1:E:165:ALA:O	1:E:166:GLU:CB	2.68	0.41
1:C:162:GLN:NE2	1:C:168:THR:HG22	2.35	0.41
1:F:61:MET:CE	1:F:87:LEU:HD21	2.50	0.41
1:F:68:VAL:HG23	1:F:184:VAL:HG22	2.03	0.41
1:F:171:VAL:HG12	1:F:173:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:ILE:HD11	1:F:417:CYS:SG	2.60	0.41
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.83	0.41
1:C:50:SER:O	1:C:51:ASN:C	2.59	0.41
1:C:101:THR:CG2	1:C:115:MET:SD	3.08	0.41
1:D:39:VAL:CG2	1:D:297:LEU:HB2	2.50	0.41
1:D:176:GLN:NE2	1:D:180:ASN:OD1	2.52	0.41
1:F:87:LEU:HD23	1:F:87:LEU:HA	1.94	0.41
1:E:334:THR:O	1:E:335:LYS:C	2.59	0.41
1:A:58:VAL:HG12	1:A:171:VAL:HG13	2.03	0.41
1:A:215:GLY:C	1:A:217:ASN:N	2.74	0.41
1:A:312:VAL:HG13	1:A:313:PRO:HD2	2.02	0.41
1:C:257:LEU:HD12	1:C:257:LEU:HA	1.84	0.41
1:D:311:ILE:HD13	1:D:311:ILE:HA	1.76	0.41
1:F:215:GLY:C	1:F:217:ASN:N	2.74	0.41
1:E:101:THR:HG22	1:E:115:MET:SD	2.61	0.41
1:A:384:PHE:HB3	1:A:409:LEU:HD21	2.02	0.41
1:C:145:ASN:ND2	1:C:275:TYR:OH	2.54	0.40
1:D:258:GLU:HG3	1:E:216:PRO:HD2	2.03	0.40
1:A:100:ASN:CG	1:A:119:ALA:HB1	2.40	0.40
1:A:206:TYR:CZ	1:A:210:LEU:HD23	2.56	0.40
1:A:458:SER:O	1:A:462:SER:HB2	2.20	0.40
1:B:346:THR:HG22	1:B:347:PRO:HD2	2.03	0.40
1:C:160:LYS:HE2	1:C:168:THR:HG21	2.02	0.40
1:C:183:LEU:HD12	1:C:183:LEU:HA	1.81	0.40
1:C:226:MET:HE2	1:C:226:MET:HB3	1.94	0.40
1:D:383:LEU:HD21	1:D:422:LEU:CD2	2.51	0.40
1:F:404:SER:HB3	1:F:407:GLN:OE1	2.20	0.40
1:E:115:MET:HE2	1:E:128:ILE:HG23	2.03	0.40
1:E:414:ASN:HA	1:E:417:CYS:O	2.21	0.40
1:A:57:ILE:HD11	1:A:172:LEU:CD1	2.51	0.40
1:B:64:ASN:N	1:B:176:GLN:OE1	2.53	0.40
1:C:83:LEU:HD23	1:C:274:TYR:HD1	1.82	0.40
1:C:171:VAL:HG12	1:C:173:THR:HG22	2.03	0.40
1:E:30:TYR:OH	1:E:294:GLN:HG2	2.21	0.40
1:A:35:LYS:HG3	1:A:438:TYR:CZ	2.56	0.40
1:C:88:SER:N	1:C:89:PRO:HD2	2.37	0.40
1:F:56:ASP:OD1	1:F:279:ARG:HG3	2.22	0.40
1:A:65:VAL:HG11	1:A:76:MET:HE2	2.04	0.40

All (1) 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)
1:B:393:GLN:OE1	1:F:289:GLN:OE1[2_656]	2.12	0.08

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	434/501 (87%)	393 (91%)	34 (8%)	7 (2%)	9	43
1	B	443/501 (88%)	392 (88%)	43 (10%)	8 (2%)	8	41
1	C	448/501 (89%)	399 (89%)	42 (9%)	7 (2%)	9	43
1	D	456/501 (91%)	406 (89%)	41 (9%)	9 (2%)	7	38
1	E	430/501 (86%)	388 (90%)	40 (9%)	2 (0%)	29	67
1	F	430/501 (86%)	386 (90%)	42 (10%)	2 (0%)	29	67
All	All	2641/3006 (88%)	2364 (90%)	242 (9%)	35 (1%)	12	47

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	104	LEU
1	B	107	ASP
1	B	371	SER
1	C	27	ILE
1	C	371	SER
1	D	69	SER
1	D	104	LEU
1	D	107	ASP
1	D	371	SER
1	F	65	VAL
1	F	371	SER
1	E	371	SER
1	A	65	VAL
1	A	371	SER

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Mol	Chain	Res	Type
1	B	65	VAL
1	B	191	SER
1	C	65	VAL
1	D	192	CYS
1	E	65	VAL
1	A	70	LYS
1	B	193	LYS
1	C	480	ILE
1	A	69	SER
1	B	105	VAL
1	C	28	LEU
1	C	484	VAL
1	D	105	VAL
1	D	480	ILE
1	D	106	GLY
1	D	476	GLU
1	A	103	ASP
1	A	464	ASN
1	C	491	ILE
1	A	68	VAL

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	377/443 (85%)	341 (90%)	36 (10%)	8 32
1	B	382/443 (86%)	347 (91%)	35 (9%)	9 33
1	C	374/443 (84%)	342 (91%)	32 (9%)	10 38
1	D	382/443 (86%)	345 (90%)	37 (10%)	8 31
1	E	373/443 (84%)	342 (92%)	31 (8%)	11 40
1	F	373/443 (84%)	340 (91%)	33 (9%)	10 36
All	All	2261/2658 (85%)	2057 (91%)	204 (9%)	9 34

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	ILE
1	B	70	LYS
1	B	86	ILE
1	B	88	SER
1	B	96	LEU
1	B	103	ASP
1	B	109	LYS
1	B	150	SER
1	B	173	THR
1	B	195	THR
1	B	201	LEU
1	B	208	SER
1	B	210	LEU
1	B	219	GLN
1	B	226	MET
1	B	227	THR
1	B	244	ARG
1	B	285	LEU
1	B	300	SER
1	B	306	SER
1	B	310	SER
1	B	322	LEU
1	B	329	LYS
1	B	334	THR
1	B	355	CYS
1	B	367	LEU
1	B	373	VAL
1	B	375	ARG
1	B	394	CYS
1	B	407	GLN
1	B	409	LEU
1	B	452	ASP
1	B	454	VAL
1	B	457	SER
1	B	462	SER
1	C	42	ILE
1	C	55	LYS
1	C	86	ILE
1	C	88	SER
1	C	113	VAL
1	C	150	SER
1	C	173	THR
1	C	183	LEU

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Mol	Chain	Res	Type
1	C	190	ILE
1	C	194	GLN
1	C	201	LEU
1	C	208	SER
1	C	210	LEU
1	C	219	GLN
1	C	226	MET
1	C	244	ARG
1	C	246	LEU
1	C	285	LEU
1	C	306	SER
1	C	322	LEU
1	C	329	LYS
1	C	334	THR
1	C	355	CYS
1	C	367	LEU
1	C	373	VAL
1	C	375	ARG
1	C	409	LEU
1	C	422	LEU
1	C	451	THR
1	C	452	ASP
1	C	457	SER
1	C	462	SER
1	D	42	ILE
1	D	55	LYS
1	D	65	VAL
1	D	86	ILE
1	D	88	SER
1	D	96	LEU
1	D	103	ASP
1	D	150	SER
1	D	173	THR
1	D	188	ASP
1	D	192	CYS
1	D	201	LEU
1	D	208	SER
1	D	210	LEU
1	D	219	GLN
1	D	226	MET
1	D	227	THR
1	D	244	ARG

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Mol	Chain	Res	Type
1	D	285	LEU
1	D	306	SER
1	D	310	SER
1	D	317	LEU
1	D	322	LEU
1	D	329	LYS
1	D	333	ILE
1	D	334	THR
1	D	355	CYS
1	D	367	LEU
1	D	373	VAL
1	D	375	ARG
1	D	394	CYS
1	D	407	GLN
1	D	409	LEU
1	D	452	ASP
1	D	454	VAL
1	D	457	SER
1	D	462	SER
1	F	28	LEU
1	F	55	LYS
1	F	71	CYS
1	F	86	ILE
1	F	88	SER
1	F	150	SER
1	F	173	THR
1	F	188	ASP
1	F	192	CYS
1	F	193	LYS
1	F	201	LEU
1	F	208	SER
1	F	210	LEU
1	F	219	GLN
1	F	226	MET
1	F	227	THR
1	F	244	ARG
1	F	285	LEU
1	F	306	SER
1	F	310	SER
1	F	322	LEU
1	F	329	LYS
1	F	333	ILE

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Mol	Chain	Res	Type
1	F	334	THR
1	F	355	CYS
1	F	367	LEU
1	F	373	VAL
1	F	375	ARG
1	F	394	CYS
1	F	409	LEU
1	F	452	ASP
1	F	457	SER
1	F	462	SER
1	E	55	LYS
1	E	86	ILE
1	E	88	SER
1	E	99	ASN
1	E	150	SER
1	E	173	THR
1	E	184	VAL
1	E	189	GLN
1	E	201	LEU
1	E	208	SER
1	E	210	LEU
1	E	219	GLN
1	E	226	MET
1	E	227	THR
1	E	244	ARG
1	E	252	ASP
1	E	285	LEU
1	E	306	SER
1	E	322	LEU
1	E	329	LYS
1	E	334	THR
1	E	355	CYS
1	E	367	LEU
1	E	373	VAL
1	E	375	ARG
1	E	409	LEU
1	E	422	LEU
1	E	451	THR
1	E	452	ASP
1	E	457	SER
1	E	462	SER
1	A	28	LEU

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Mol	Chain	Res	Type
1	A	42	ILE
1	A	55	LYS
1	A	68	VAL
1	A	71	CYS
1	A	86	ILE
1	A	88	SER
1	A	102	HIS
1	A	103	ASP
1	A	104	LEU
1	A	150	SER
1	A	173	THR
1	A	201	LEU
1	A	208	SER
1	A	210	LEU
1	A	219	GLN
1	A	226	MET
1	A	244	ARG
1	A	246	LEU
1	A	285	LEU
1	A	306	SER
1	A	310	SER
1	A	322	LEU
1	A	329	LYS
1	A	333	ILE
1	A	334	THR
1	A	355	CYS
1	A	367	LEU
1	A	373	VAL
1	A	375	ARG
1	A	394	CYS
1	A	409	LEU
1	A	452	ASP
1	A	454	VAL
1	A	457	SER
1	A	462	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	100	ASN
1	B	145	ASN
1	B	162	GLN

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Mol	Chain	Res	Type
1	B	290	GLN
1	B	314	ASN
1	B	325	ASN
1	C	145	ASN
1	C	162	GLN
1	C	314	ASN
1	C	395	GLN
1	D	100	ASN
1	D	145	ASN
1	D	162	GLN
1	D	189	GLN
1	D	290	GLN
1	D	314	ASN
1	D	325	ASN
1	F	145	ASN
1	F	162	GLN
1	F	314	ASN
1	F	325	ASN
1	F	395	GLN
1	E	145	ASN
1	E	162	GLN
1	E	314	ASN
1	E	325	ASN
1	E	459	GLN
1	A	127	GLN
1	A	145	ASN
1	A	162	GLN
1	A	314	ASN
1	A	325	ASN
1	A	395	GLN

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)

6 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	$\#\|Z\| > 2$
2	NAG	G	1	2,1	14,14,15	0.61	0	17,19,21	1.57	3 (17%)
2	NAG	G	2	2	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.84	0	17,19,21	1.56	1 (5%)
2	NAG	H	2	2	14,14,15	0.69	0	17,19,21	1.47	3 (17%)
2	NAG	I	1	2,1	14,14,15	0.85	0	17,19,21	2.31	7 (41%)
2	NAG	I	2	2	14,14,15	0.57	0	17,19,21	1.79	4 (23%)

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
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NAG	C2-N2-C7	5.17	130.26	122.90
2	I	1	NAG	C1-O5-C5	4.54	118.35	112.19
2	I	1	NAG	C4-C3-C2	4.26	117.26	111.02
2	G	1	NAG	C1-O5-C5	4.05	117.68	112.19
2	I	2	NAG	C1-C2-N2	3.84	117.04	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	NAG	C3-C4-C5	3.69	116.82	110.24
2	H	2	NAG	C1-O5-C5	3.60	117.07	112.19
2	I	2	NAG	C1-O5-C5	3.58	117.04	112.19
2	I	1	NAG	C1-C2-N2	-3.54	104.44	110.49
2	G	1	NAG	C2-N2-C7	-3.39	118.08	122.90
2	H	2	NAG	C4-C3-C2	3.34	115.91	111.02
2	I	1	NAG	O7-C7-N2	3.02	127.51	121.95
2	G	2	NAG	C1-O5-C5	2.71	115.86	112.19
2	I	2	NAG	C3-C4-C5	2.60	114.87	110.24
2	H	2	NAG	C2-N2-C7	2.34	126.23	122.90
2	I	1	NAG	C8-C7-N2	-2.32	112.17	116.10
2	I	2	NAG	O5-C1-C2	-2.25	107.74	111.29
2	G	1	NAG	C4-C3-C2	2.24	114.29	111.02
2	I	1	NAG	O3-C3-C4	-2.20	105.27	110.35
2	G	2	NAG	O5-C5-C6	2.09	110.48	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

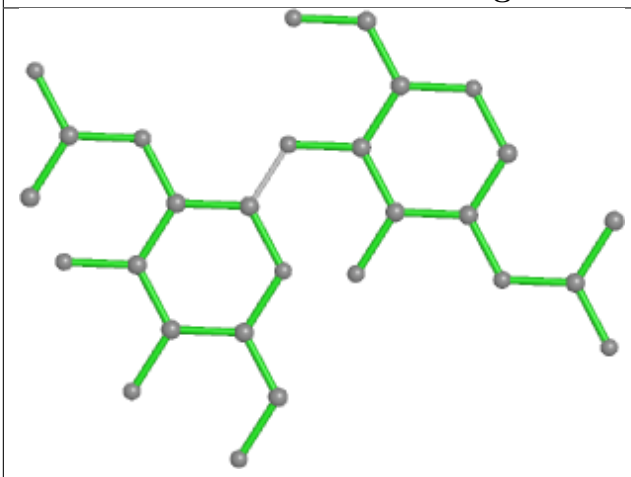
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7

There are no ring outliers.

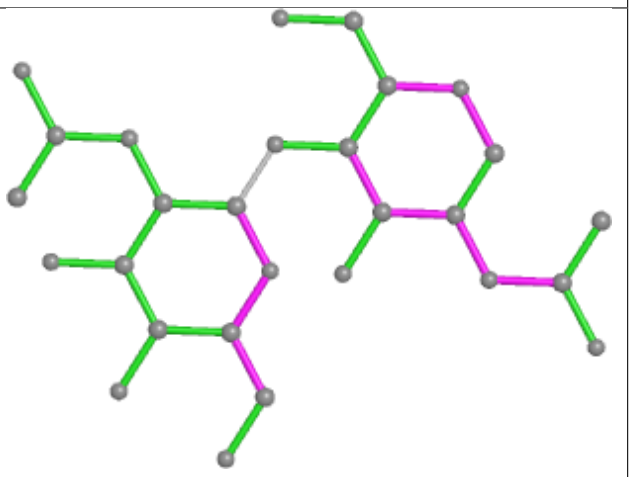
No monomer is involved in short contacts.

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

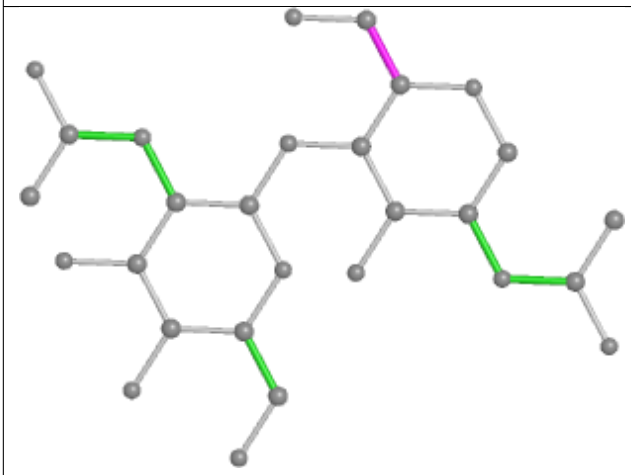
Oligosaccharide Chain G



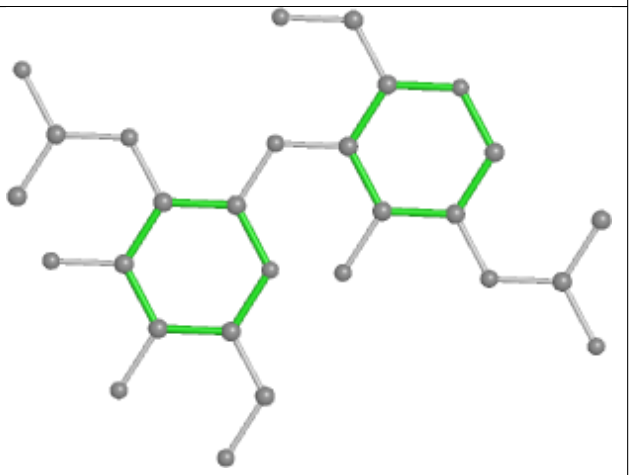
Bond lengths



Bond angles

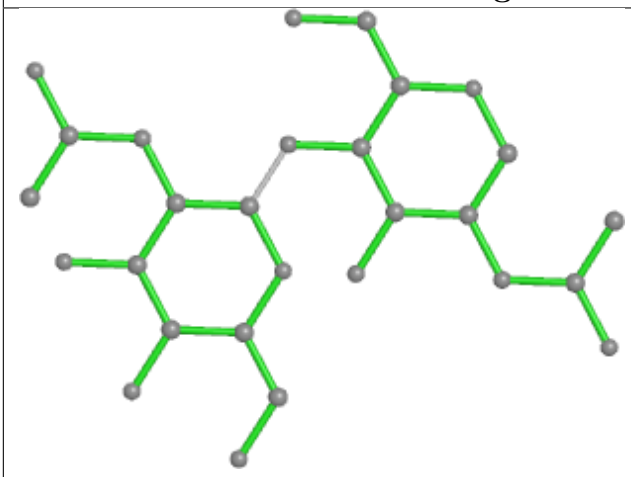


Torsions

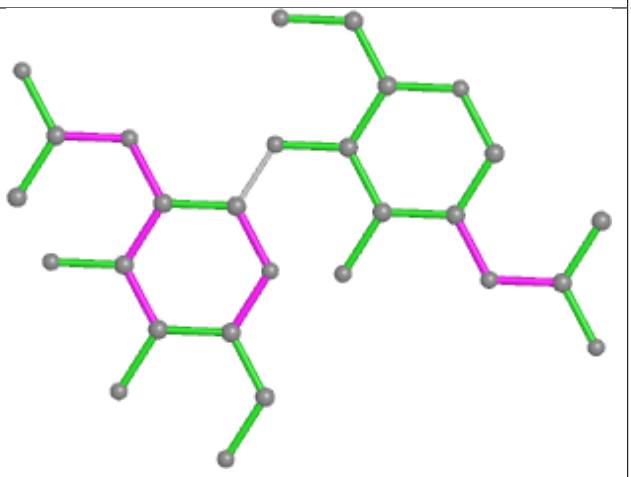


Rings

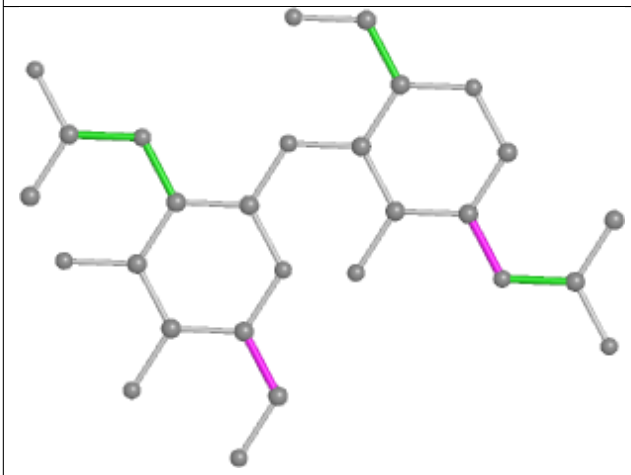
Oligosaccharide Chain H



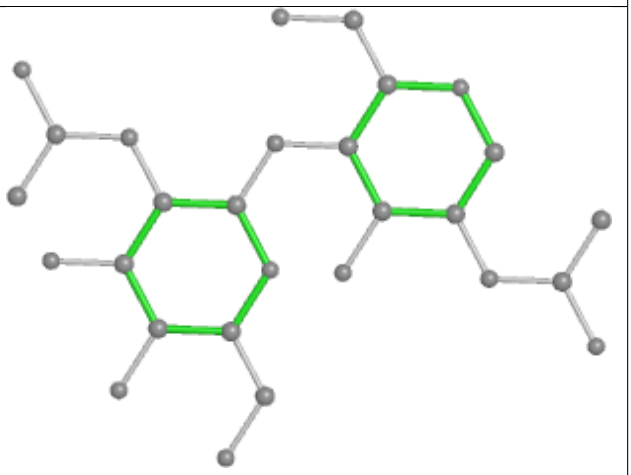
Bond lengths



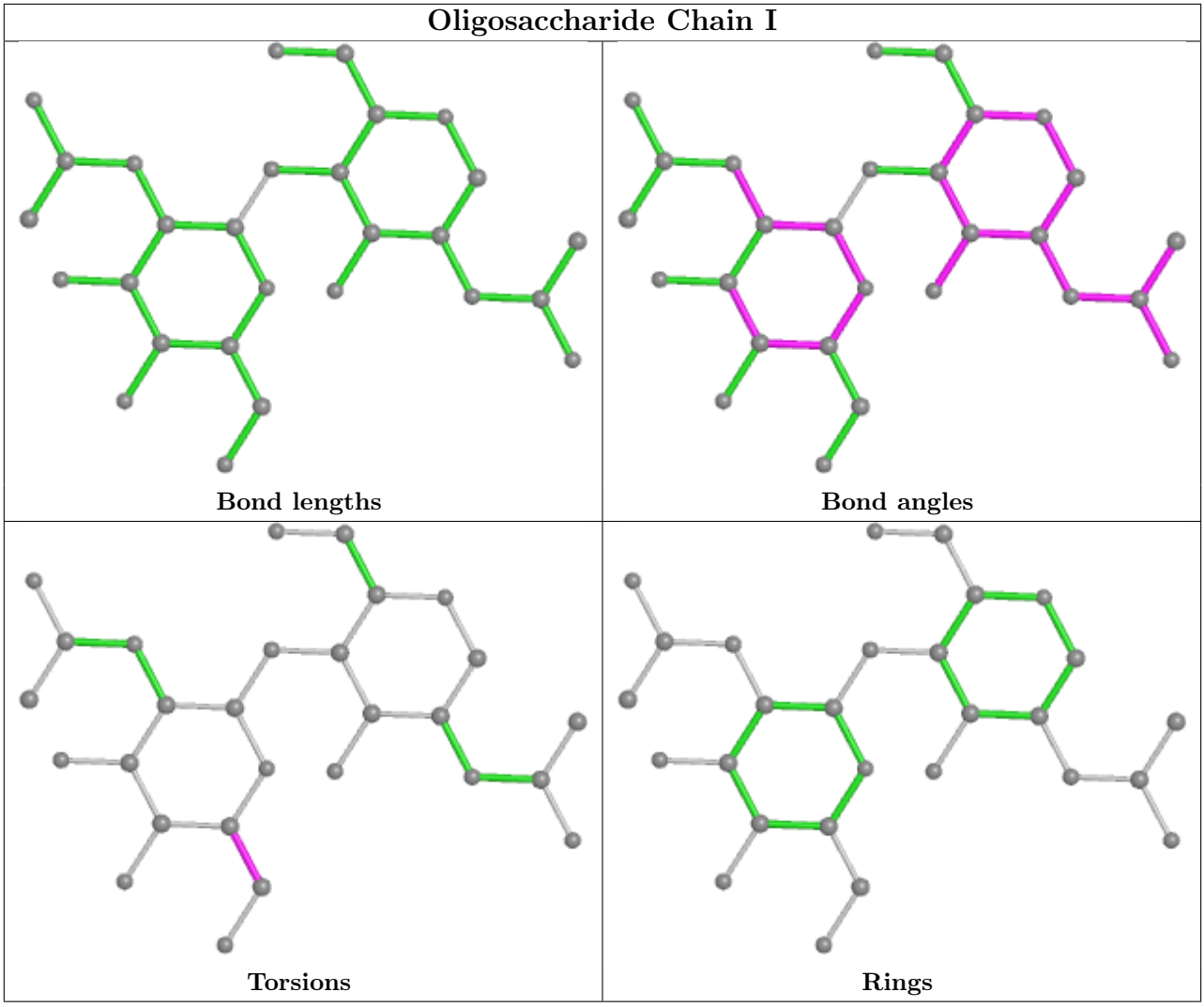
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	605	1	14,14,15	0.60	0	17,19,21	1.18	3 (17%)
4	NAG	D	601	1	14,14,15	0.78	0	17,19,21	1.56	3 (17%)
4	NAG	F	601	1	14,14,15	0.64	0	17,19,21	1.58	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	E	602	1	14,14,15	0.57	0	17,19,21	1.52	2 (11%)
3	SO4	F	603	-	4,4,4	0.51	0	6,6,6	0.88	0
4	NAG	D	602	1	14,14,15	0.44	0	17,19,21	1.58	2 (11%)
3	SO4	B	603	-	4,4,4	0.34	0	6,6,6	0.20	0
4	NAG	F	602	1	14,14,15	0.66	0	17,19,21	1.47	3 (17%)
3	SO4	A	603	-	4,4,4	0.61	0	6,6,6	0.75	0
3	SO4	E	605	-	4,4,4	0.40	0	6,6,6	1.21	0
4	NAG	C	603	1	14,14,15	0.83	1 (7%)	17,19,21	2.17	3 (17%)
4	NAG	E	601	1	14,14,15	0.64	0	17,19,21	1.96	5 (29%)
4	NAG	E	604	1	14,14,15	0.60	0	17,19,21	1.34	4 (23%)
4	NAG	A	601	1	14,14,15	0.68	0	17,19,21	1.72	3 (17%)
4	NAG	E	603	1	14,14,15	0.54	0	17,19,21	2.13	4 (23%)
3	SO4	C	604	-	4,4,4	0.86	0	6,6,6	1.74	1 (16%)
3	SO4	D	606	-	4,4,4	0.38	0	6,6,6	0.42	0
4	NAG	A	602	1	14,14,15	0.57	0	17,19,21	2.38	5 (29%)

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	605	1	-	1/6/23/26	0/1/1/1
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	F	601	1	-	1/6/23/26	0/1/1/1
4	NAG	E	602	1	-	2/6/23/26	0/1/1/1
4	NAG	F	602	1	-	2/6/23/26	0/1/1/1
4	NAG	E	601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	603	1	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	E	604	1	-	2/6/23/26	0/1/1/1
4	NAG	E	603	1	-	1/6/23/26	0/1/1/1
4	NAG	D	602	1	-	2/6/23/26	0/1/1/1
4	NAG	A	602	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	NAG	C1-C2	2.13	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	NAG	C1-O5-C5	6.84	121.46	112.19
4	C	603	NAG	C1-O5-C5	6.81	121.42	112.19
4	E	603	NAG	C1-O5-C5	5.88	120.16	112.19
4	A	601	NAG	C1-O5-C5	4.70	118.56	112.19
4	E	601	NAG	C2-N2-C7	4.35	129.09	122.90
4	D	602	NAG	C1-O5-C5	4.32	118.04	112.19
4	A	602	NAG	O5-C1-C2	-4.22	104.62	111.29
4	E	603	NAG	O5-C1-C2	-4.17	104.70	111.29
4	E	602	NAG	C4-C3-C2	-4.13	104.97	111.02
4	F	601	NAG	C1-O5-C5	4.02	117.64	112.19
4	E	601	NAG	C4-C3-C2	3.87	116.69	111.02
4	C	603	NAG	O5-C5-C6	3.57	112.79	107.20
4	D	601	NAG	C4-C3-C2	3.53	116.18	111.02
4	F	602	NAG	C4-C3-C2	3.43	116.04	111.02
4	E	602	NAG	C1-O5-C5	3.11	116.41	112.19
4	F	601	NAG	C1-C2-N2	3.09	115.76	110.49
4	A	602	NAG	O5-C5-C4	3.06	118.26	110.83
4	D	601	NAG	C3-C4-C5	3.01	115.62	110.24
4	E	601	NAG	C1-C2-N2	-2.95	105.45	110.49
3	C	604	SO4	O4-S-O2	-2.86	94.37	109.31
4	A	601	NAG	C1-C2-N2	2.84	115.34	110.49
4	D	605	NAG	C2-N2-C7	2.83	126.93	122.90
4	E	604	NAG	C4-C3-C2	2.78	115.09	111.02
4	E	601	NAG	C3-C4-C5	2.74	115.12	110.24
4	D	602	NAG	O5-C1-C2	-2.59	107.20	111.29
4	E	604	NAG	C1-O5-C5	2.58	115.69	112.19
4	E	603	NAG	C3-C4-C5	2.53	114.74	110.24
4	E	604	NAG	C2-N2-C7	2.50	126.47	122.90
4	A	602	NAG	C3-C4-C5	2.47	114.65	110.24
4	E	603	NAG	C1-C2-N2	2.34	114.48	110.49
4	C	603	NAG	C1-C2-N2	2.27	114.36	110.49
4	D	605	NAG	O5-C5-C6	2.23	110.70	107.20
4	E	604	NAG	O5-C1-C2	2.20	114.76	111.29
4	F	602	NAG	O7-C7-C8	-2.17	118.03	122.06
4	A	602	NAG	C1-C2-N2	2.15	114.15	110.49
4	F	602	NAG	C2-N2-C7	2.10	125.89	122.90
4	D	605	NAG	O7-C7-N2	2.07	125.76	121.95
4	D	601	NAG	C1-C2-N2	2.06	114.02	110.49
4	E	601	NAG	O5-C5-C6	2.05	110.42	107.20
4	A	601	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	602	NAG	O5-C5-C6-O6
4	E	602	NAG	C4-C5-C6-O6
4	E	602	NAG	O5-C5-C6-O6
4	F	602	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	D	602	NAG	C4-C5-C6-O6
4	E	604	NAG	O5-C5-C6-O6
4	E	604	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	F	602	NAG	O5-C5-C6-O6
4	A	602	NAG	O5-C5-C6-O6
4	D	605	NAG	O5-C5-C6-O6
4	E	603	NAG	O5-C5-C6-O6
4	C	603	NAG	O5-C5-C6-O6
4	F	601	NAG	C4-C5-C6-O6
4	E	601	NAG	C1-C2-N2-C7
4	E	601	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	605	NAG	2	0
3	F	603	SO4	1	0
3	B	603	SO4	1	0
4	F	602	NAG	2	0
4	E	603	NAG	1	0
3	D	606	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	440/501 (87%)	0.27	15 (3%)	45	29	43, 91, 149, 193	0
1	B	447/501 (89%)	0.30	21 (4%)	31	19	52, 81, 147, 170	0
1	C	454/501 (90%)	0.43	36 (7%)	12	6	51, 94, 151, 183	0
1	D	460/501 (91%)	0.34	23 (5%)	28	16	54, 84, 155, 194	0
1	E	436/501 (87%)	0.35	23 (5%)	26	14	55, 91, 154, 203	0
1	F	436/501 (87%)	0.23	15 (3%)	45	29	48, 90, 149, 184	0
All	All	2673/3006 (88%)	0.32	133 (4%)	28	16	43, 88, 151, 203	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	102	HIS	7.1
1	D	164	THR	7.0
1	A	102	HIS	6.7
1	B	164	THR	5.8
1	D	474	ILE	4.8
1	C	493	SER	4.7
1	D	102	HIS	4.6
1	B	163	GLU	4.2
1	C	469	GLN	4.2
1	C	476	GLU	4.1
1	C	474	ILE	4.1
1	E	474	ILE	4.1
1	B	253	PHE	4.0
1	E	164	THR	3.9
1	C	169	VAL	3.9
1	D	163	GLU	3.9
1	F	396	THR	3.9
1	F	190	ILE	3.9
1	C	381	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	475	LYS	3.6
1	D	65	VAL	3.6
1	C	478	GLN	3.6
1	B	474	ILE	3.5
1	C	164	THR	3.5
1	A	463	MET	3.4
1	B	102	HIS	3.4
1	A	397	THR	3.4
1	B	112	GLY	3.3
1	A	135	TYR	3.2
1	D	486	ASP	3.1
1	F	35	LYS	3.1
1	E	468	GLN	3.1
1	B	161	LEU	3.1
1	E	469	GLN	3.1
1	D	274	TYR	3.1
1	D	190	ILE	3.1
1	C	477	ALA	3.0
1	A	470	SER	3.0
1	D	189	GLN	3.0
1	C	324	SER	2.9
1	E	95	GLU	2.9
1	C	162	GLN	2.9
1	E	381	GLY	2.8
1	B	65	VAL	2.8
1	B	156	GLU	2.8
1	B	473	TYR	2.8
1	D	446	GLY	2.8
1	B	100	ASN	2.7
1	C	189	GLN	2.7
1	D	179	ILE	2.7
1	C	102	HIS	2.7
1	D	161	LEU	2.7
1	F	470	SER	2.7
1	C	490	GLU	2.7
1	B	385	ALA	2.7
1	C	470	SER	2.7
1	E	318	ILE	2.7
1	E	305	ASN	2.6
1	C	168	THR	2.6
1	F	397	THR	2.6
1	D	66	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	71	CYS	2.6
1	E	68	VAL	2.6
1	B	274	TYR	2.6
1	B	461	SER	2.6
1	C	26	GLY	2.6
1	E	444	ALA	2.6
1	A	396	THR	2.5
1	E	476	GLU	2.5
1	C	92	GLY	2.5
1	A	410	LEU	2.5
1	C	275	TYR	2.5
1	C	161	LEU	2.5
1	F	469	GLN	2.5
1	F	69	SER	2.5
1	E	475	LYS	2.4
1	C	468	GLN	2.4
1	D	166	GLU	2.4
1	E	304	ASP	2.4
1	B	113	VAL	2.4
1	F	114	VAL	2.4
1	A	273	SER	2.4
1	F	135	TYR	2.4
1	F	438	TYR	2.4
1	B	199	LEU	2.4
1	C	444	ALA	2.3
1	E	473	TYR	2.3
1	E	323	ILE	2.3
1	A	438	TYR	2.3
1	C	473	TYR	2.3
1	E	275	TYR	2.3
1	A	188	ASP	2.3
1	C	337	SER	2.3
1	D	162	GLN	2.3
1	B	101	THR	2.3
1	C	115	MET	2.3
1	A	71	CYS	2.2
1	A	189	GLN	2.2
1	A	399	ARG	2.2
1	D	483	ASN	2.2
1	F	58	VAL	2.2
1	B	427	ILE	2.2
1	C	82	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	2.2
1	C	45	LYS	2.2
1	D	135	TYR	2.2
1	E	412	ILE	2.2
1	C	492	LEU	2.2
1	F	320	ASN	2.2
1	E	45	LYS	2.2
1	C	276	ILE	2.2
1	B	184	VAL	2.2
1	C	292	TYR	2.2
1	C	167	LYS	2.2
1	C	155	ASN	2.1
1	D	473	TYR	2.1
1	D	184	VAL	2.1
1	C	141	ALA	2.1
1	A	385	ALA	2.1
1	A	72	THR	2.1
1	E	144	ILE	2.1
1	E	282	PHE	2.1
1	E	465	GLN	2.1
1	E	322	LEU	2.1
1	B	135	TYR	2.1
1	C	486	ASP	2.1
1	D	117	GLY	2.1
1	C	95	GLU	2.1
1	D	489	GLU	2.1
1	F	417	CYS	2.0
1	D	143	ASN	2.0
1	F	474	ILE	2.0
1	C	472	ASP	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)

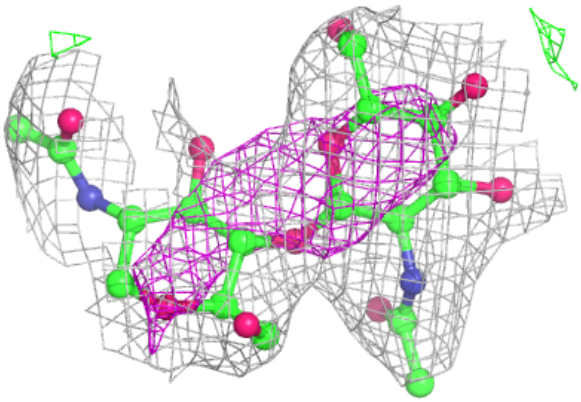
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

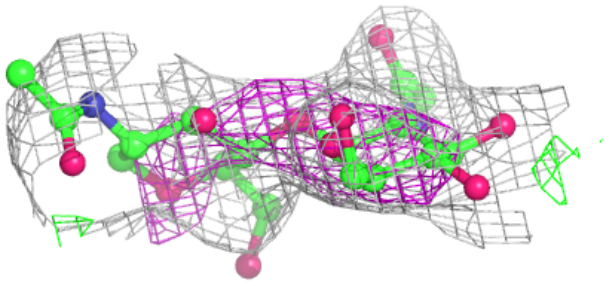
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.56	0.34	156,169,176,185	0
2	NAG	I	1	14/15	0.76	0.29	66,92,103,111	0
2	NAG	H	1	14/15	0.84	0.29	83,109,134,154	0
2	NAG	G	2	14/15	0.85	0.29	79,86,99,100	0
2	NAG	G	1	14/15	0.85	0.26	63,78,95,101	0
2	NAG	I	2	14/15	0.90	0.28	74,90,109,124	0

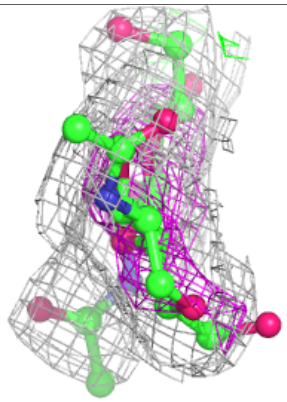
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

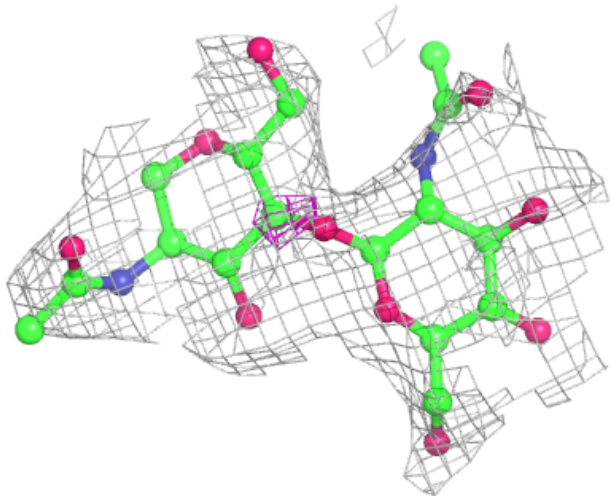


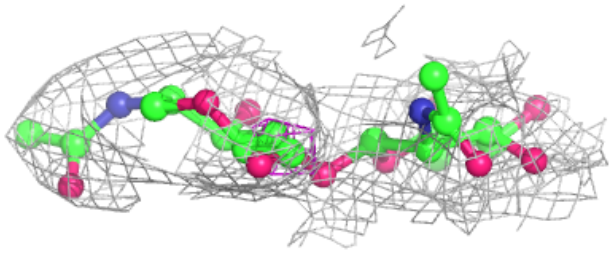


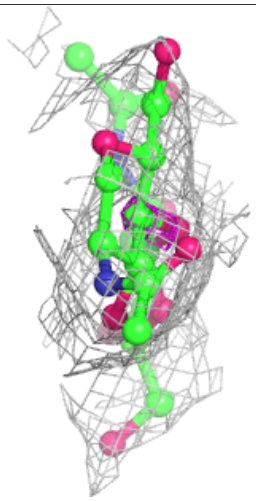


Electron density around Chain H:

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

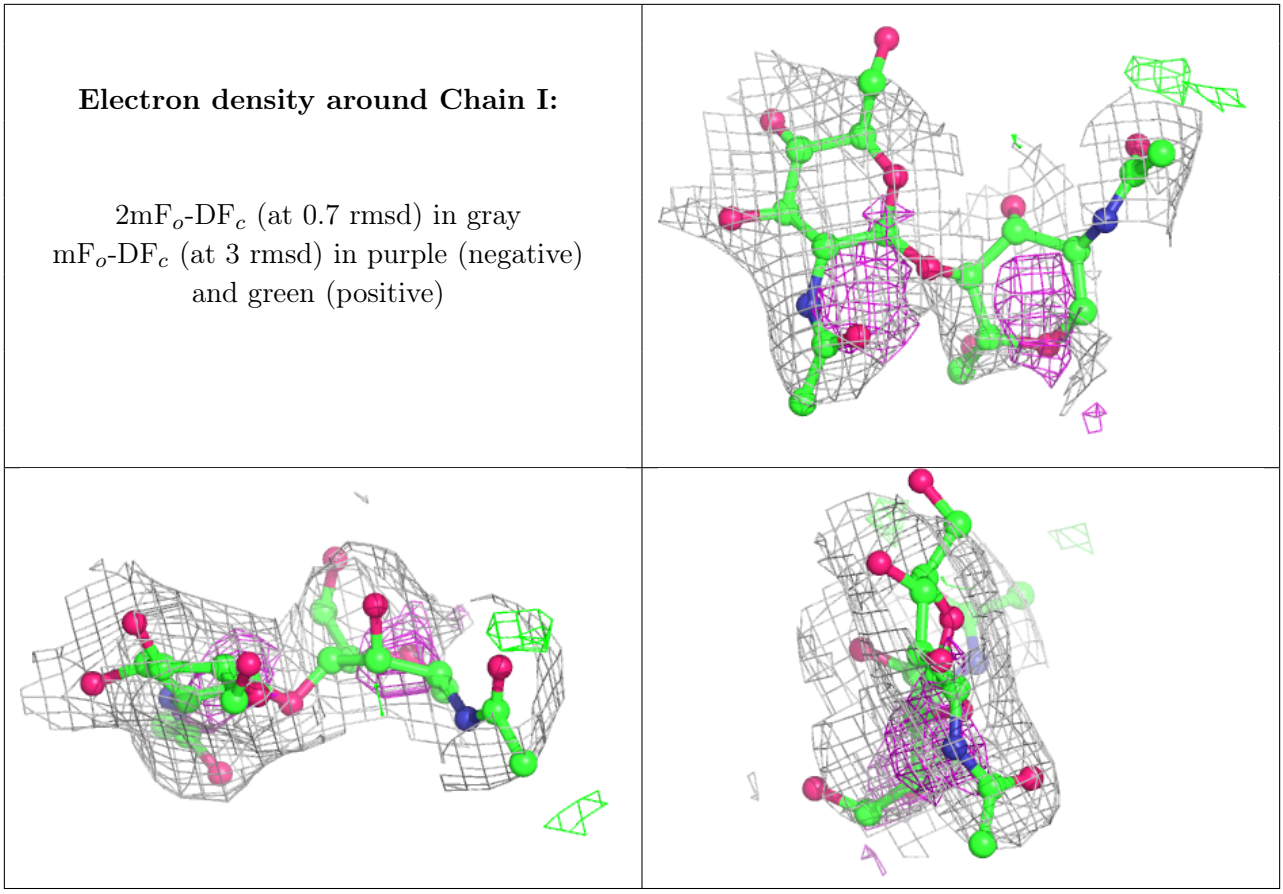






Electron density around Chain I:

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



6.4 Ligands

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	NAG	E	603	14/15	0.61	0.32	110,134,146,149	0
4	NAG	A	602	14/15	0.61	0.41	108,123,132,139	0
4	NAG	D	602	14/15	0.65	0.21	130,150,165,168	0
4	NAG	F	601	14/15	0.65	0.29	116,132,146,150	0
4	NAG	E	602	14/15	0.66	0.29	122,149,159,160	0
4	NAG	C	603	14/15	0.71	0.26	90,111,122,123	0
4	NAG	D	601	14/15	0.72	0.23	103,132,141,146	0
4	NAG	A	601	14/15	0.73	0.25	113,129,140,146	0
4	NAG	F	602	14/15	0.74	0.39	98,112,127,129	0
4	NAG	E	604	14/15	0.77	0.27	110,132,162,162	0
4	NAG	E	601	14/15	0.78	0.35	100,128,139,142	0
4	NAG	D	605	14/15	0.79	0.20	102,122,135,137	0
3	SO4	B	603	5/5	0.82	0.22	125,127,137,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	606	5/5	0.88	0.29	111,124,131,137	0
3	SO4	F	603	5/5	0.92	0.22	53,66,68,68	0
3	SO4	C	604	5/5	0.94	0.21	38,50,56,61	0
3	SO4	E	605	5/5	0.94	0.20	59,59,69,75	0
3	SO4	A	603	5/5	0.96	0.19	51,52,68,73	0

6.5 Other polymers (i)

There are no such residues in this entry.