Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 04:20 pm GMT

PDB ID	:	4D6W
Title	:	Crystal Structure of the low pH conformation of Chandipura Virus glycoprotein G ectodomain
Authors	:	Baquero, E.; Albertini, A.; Raux, H.; Bressanelli, S.; Gaudin, Y.
Deposited on	:	2014-11-18
Resolution	:	3.60 Å(reported)

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

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

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

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

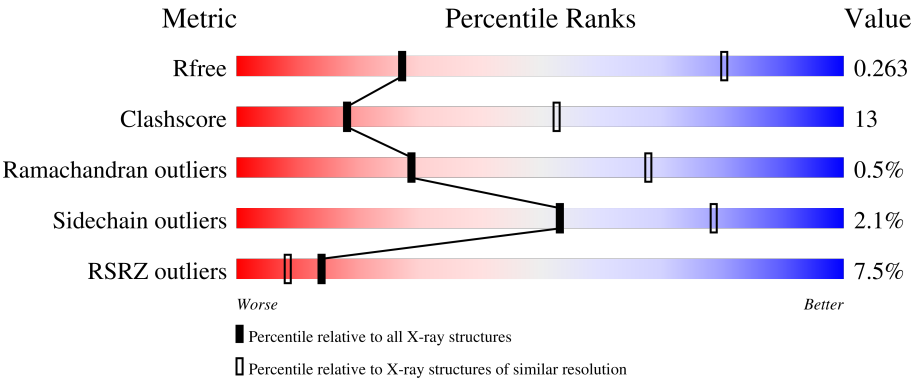
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	419	12% 70% 26%
1	B	419	5% 67% 31%
1	C	419	5% 69% 26%
2	D	2	100%
3	E	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9745 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 GLYCOPROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3197	2040	539	601	17			
1	B	416	Total	C	N	O	S	0	0	0
			3274	2091	551	614	18			
1	C	406	Total	C	N	O	S	0	0	0
			3190	2034	538	600	18			

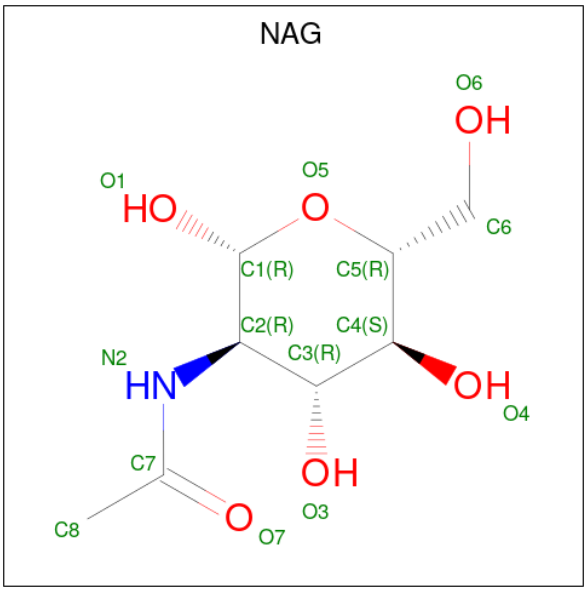
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			24	14	1	9			

- 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	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

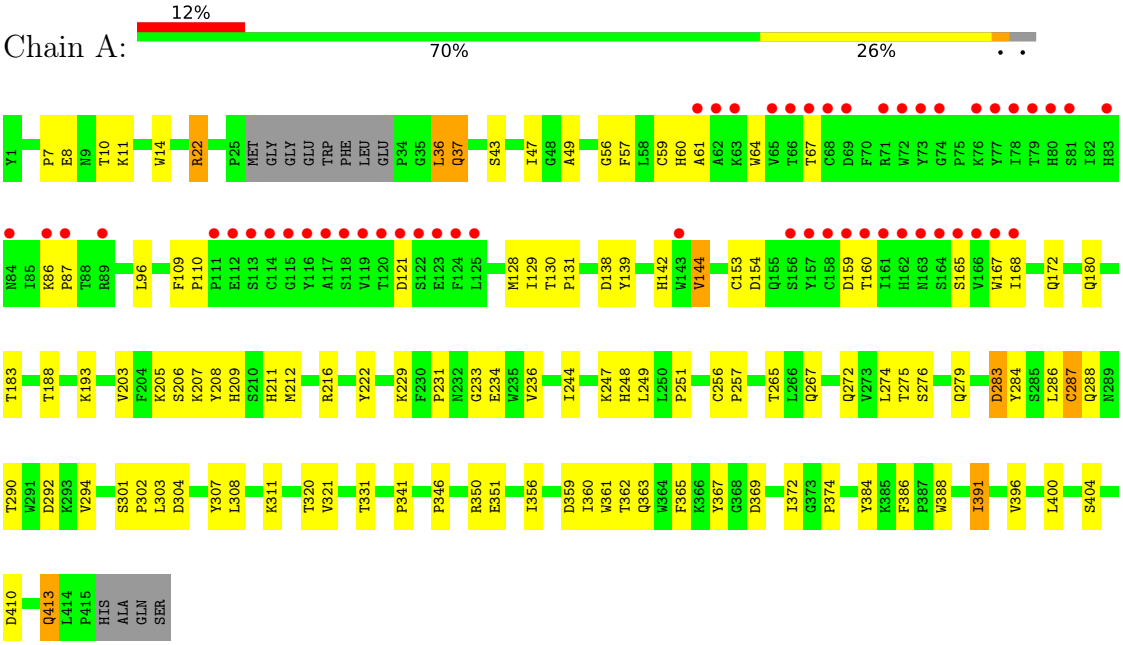
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0

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.

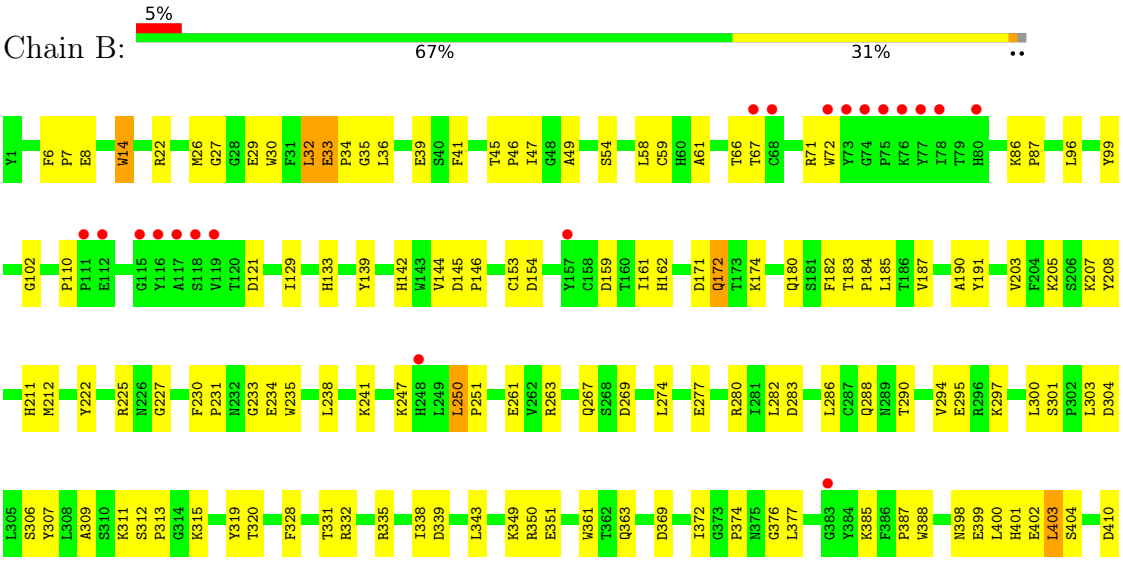
• Molecule 1: GLYCOPROTEIN G

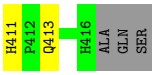
Chain A:



• Molecule 1: GLYCOPROTEIN G

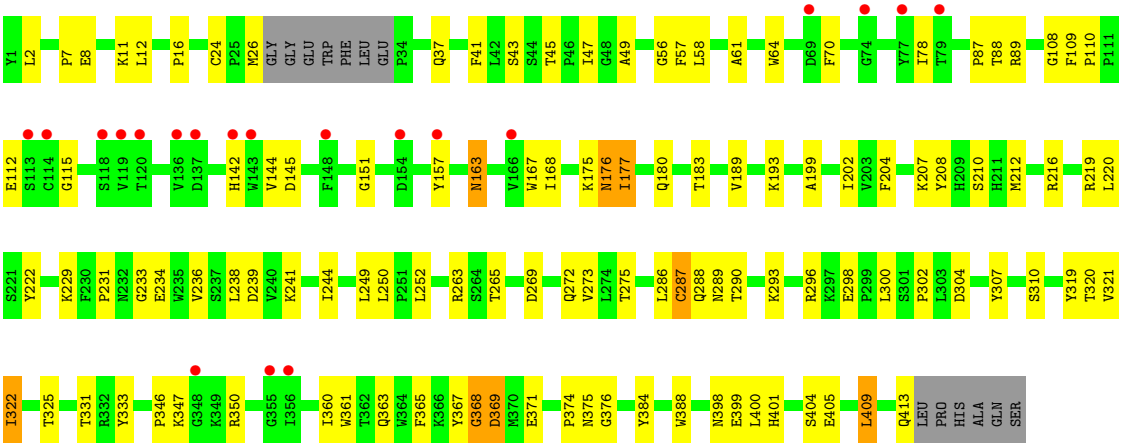
Chain B:





• Molecule 1: GLYCOPROTEIN G

Chain C:

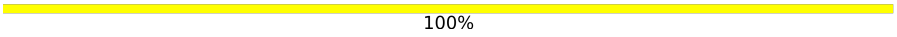


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	365.59Å 83.50Å 60.82Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	49.13 – 3.60 49.13 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.13-3.60) 99.3 (49.13-3.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.260 0.196 , 0.263	Depositor DCC
R_{free} test set	1057 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	86.0	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 87.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.040 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9745	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 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	0.63	1/3290 (0.0%)	0.77	0/4474
1	B	0.63	1/3372 (0.0%)	0.78	2/4587 (0.0%)
1	C	0.57	0/3282	0.74	2/4461 (0.0%)
All	All	0.61	2/9944 (0.0%)	0.76	4/13522 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	TRP	CB-CG	-6.98	1.37	1.50
1	A	287	CYS	CB-SG	-5.37	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	LEU	CA-CB-CG	7.70	133.01	115.30
1	B	282	LEU	CB-CG-CD2	-7.19	98.78	111.00
1	C	409	LEU	CA-CB-CG	6.28	129.75	115.30
1	C	409	LEU	CB-CG-CD2	-5.80	101.14	111.00

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	A	3197	0	3110	88	0
1	B	3274	0	3173	98	0
1	C	3190	0	3101	81	0
2	D	28	0	25	2	0
3	E	24	0	22	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	9745	0	9457	257	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 13.

All (257) 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:C:293:LYS:NZ	1:C:304:ASP:OD2	1.77	1.18
1:A:22:ARG:NH1	1:A:288:GLN:OE1	1.88	1.06
1:C:8:GLU:O	1:C:350:ARG:NH1	2.06	0.88
1:B:32:LEU:HD13	1:B:34:PRO:HD2	1.59	0.81
1:B:180:GLN:NE2	1:B:222:TYR:OH	2.14	0.81
1:A:180:GLN:NE2	1:A:222:TYR:OH	2.15	0.80
1:C:180:GLN:NE2	1:C:222:TYR:OH	2.14	0.80
1:A:7:PRO:HB3	1:A:331:THR:HG21	1.64	0.78
1:C:272:GLN:HE22	1:C:404:SER:HA	1.49	0.77
1:B:49:ALA:HA	1:B:180:GLN:HB3	1.68	0.76
1:A:22:ARG:NH2	1:A:292:ASP:OD1	2.20	0.74
1:A:212:MET:HG3	1:A:231:PRO:HD2	1.68	0.74
1:C:163:ASN:OD1	1:C:163:ASN:N	2.14	0.73
1:A:37:GLN:HG3	1:A:193:LYS:HG3	1.70	0.73
1:A:11:LYS:HG2	1:A:363:GLN:HB2	1.70	0.73
1:C:350:ARG:HH21	1:C:360:ILE:HA	1.53	0.72
1:B:7:PRO:HB3	1:B:331:THR:HG21	1.70	0.72
1:C:310:SER:HB3	1:C:333:TYR:CE2	2.26	0.71
1:A:144:VAL:HG11	1:A:413:GLN:HB2	1.71	0.70
1:B:22:ARG:HD3	1:B:288:GLN:OE1	1.91	0.70
1:A:37:GLN:HG2	1:A:193:LYS:HE2	1.73	0.69
1:C:210:SER:HB2	1:C:273:VAL:HG13	1.73	0.69
1:A:244:ILE:HG13	1:A:249:LEU:HD22	1.75	0.69
1:A:47:ILE:HD11	1:A:183:THR:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TRP:CE2	1:A:374:PRO:HD3	2.29	0.68
1:A:320:THR:OG1	1:A:321:VAL:N	2.27	0.67
1:C:212:MET:HG3	1:C:231:PRO:HD2	1.78	0.66
1:C:47:ILE:HD11	1:C:183:THR:HB	1.77	0.66
1:A:274:LEU:HB3	1:C:275:THR:HG21	1.78	0.66
1:C:11:LYS:HB3	1:C:363:GLN:HB2	1.78	0.65
1:B:250:LEU:HB3	1:B:251:PRO:HD3	1.78	0.65
1:B:139:TYR:OH	1:B:410:ASP:HB3	1.98	0.64
1:C:369:ASP:N	1:C:369:ASP:OD1	2.30	0.64
1:A:350:ARG:NH2	1:A:359:ASP:O	2.30	0.64
1:C:7:PRO:HB3	1:C:331:THR:HG21	1.79	0.64
1:C:263:ARG:HA	1:C:409:LEU:HA	1.79	0.63
1:B:402:GLU:HG2	1:C:207:LYS:HD3	1.81	0.63
1:B:142:HIS:HB3	1:B:154:ASP:HB3	1.80	0.63
1:C:24:CYS:SG	1:C:288:GLN:NE2	2.71	0.63
1:C:244:ILE:HG13	1:C:249:LEU:HD22	1.81	0.63
1:A:287:CYS:HB2	1:A:308:LEU:HD23	1.79	0.63
1:B:335:ARG:NH2	1:B:398:ASN:OD1	2.32	0.62
1:B:399:GLU:O	1:B:403:LEU:HB2	1.98	0.62
1:B:8:GLU:O	1:B:350:ARG:NH1	2.32	0.62
1:C:239:ASP:OD2	1:C:241:LYS:HB2	1.99	0.62
1:B:96:LEU:HD23	1:B:172:GLN:HE22	1.64	0.61
1:A:14:TRP:CD1	1:A:365:PHE:HZ	2.19	0.61
1:A:286:LEU:HB3	1:A:307:TYR:HD1	1.66	0.61
1:A:160:THR:OG1	1:A:165:SER:O	2.18	0.61
1:A:142:HIS:HB3	1:A:154:ASP:HB3	1.82	0.61
1:C:142:HIS:HA	1:C:177:ILE:HD11	1.83	0.60
1:B:47:ILE:HD11	1:B:183:THR:HB	1.84	0.60
1:B:212:MET:HE2	1:B:230:PHE:HB3	1.83	0.60
1:B:46:PRO:HA	1:B:182:PHE:HD1	1.66	0.60
1:C:89:ARG:HG3	1:C:157:TYR:CE1	2.37	0.60
1:C:64:TRP:CZ3	1:C:108:GLY:HA2	2.37	0.59
1:B:67:THR:HA	1:B:121:ASP:HB3	1.85	0.59
1:A:209:HIS:NE2	1:A:234:GLU:OE1	2.35	0.59
1:B:339:ASP:OD1	1:B:349:LYS:NZ	2.35	0.59
1:A:11:LYS:NZ	1:A:362:THR:HG23	2.18	0.58
1:B:144:VAL:HG11	1:B:413:GLN:HB2	1.85	0.58
1:B:171:ASP:OD2	1:B:174:LYS:NZ	2.29	0.58
1:A:302:PRO:HD3	1:A:367:TYR:OH	2.03	0.58
1:C:7:PRO:HD3	1:C:333:TYR:HE1	1.69	0.58
1:A:144:VAL:CG1	1:A:413:GLN:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HG3	1:B:22:ARG:HH11	1.70	0.57
1:B:283:ASP:OD2	1:B:311:LYS:HD2	2.05	0.57
1:A:57:PHE:HD1	1:A:131:PRO:HA	1.69	0.56
1:A:286:LEU:HD22	1:A:307:TYR:CE1	2.41	0.56
1:A:290:THR:O	1:A:294:VAL:HG23	2.05	0.56
1:A:272:GLN:HE22	1:A:404:SER:HB3	1.71	0.56
1:A:60:HIS:HB3	1:A:128:MET:HB3	1.86	0.56
1:B:61:ALA:HB2	1:B:87:PRO:HB3	1.87	0.56
1:C:346:PRO:HD3	1:C:384:TYR:CE1	2.41	0.56
1:B:212:MET:CE	1:B:230:PHE:HB3	2.35	0.55
1:B:203:VAL:HG21	1:B:211:HIS:CE1	2.41	0.55
1:C:142:HIS:CA	1:C:177:ILE:HD11	2.36	0.55
1:A:286:LEU:HB3	1:A:307:TYR:CD1	2.42	0.55
1:B:59:CYS:HA	1:B:129:ILE:HD13	1.88	0.55
1:C:287:CYS:HB2	1:C:307:TYR:O	2.07	0.55
1:B:208:TYR:OH	1:B:267:GLN:HG2	2.07	0.55
1:C:234:GLU:OE2	1:C:269:ASP:OD2	2.24	0.55
1:A:388:TRP:CZ2	1:B:26:MET:HB3	2.42	0.54
1:C:56:GLY:HA3	1:C:167:TRP:CZ2	2.42	0.54
1:A:203:VAL:HG21	1:A:211:HIS:CE1	2.43	0.54
1:B:6:PHE:CG	1:B:7:PRO:HD2	2.42	0.54
1:B:304:ASP:O	1:B:307:TYR:HB2	2.08	0.54
1:B:372:ILE:HD11	1:B:376:GLY:HA2	1.90	0.54
1:B:54:SER:OG	1:B:133:HIS:NE2	2.41	0.54
1:B:388:TRP:CZ2	1:C:26:MET:HB3	2.43	0.54
1:B:306:SER:HB3	1:B:387:PRO:HG2	1.88	0.53
1:C:144:VAL:HG11	1:C:413:GLN:HB2	1.91	0.53
1:A:303:LEU:HG	1:A:307:TYR:HE2	1.74	0.53
1:B:261:GLU:OE1	1:B:411:HIS:HD2	1.91	0.53
1:B:361:TRP:NE1	1:B:363:GLN:O	2.40	0.53
1:C:78:ILE:HG13	1:C:112:GLU:OE1	2.09	0.53
1:A:283:ASP:OD2	1:A:311:LYS:NZ	2.34	0.53
1:C:189:VAL:HG13	1:C:202:ILE:HG23	1.91	0.53
1:A:303:LEU:HG	1:A:307:TYR:CE2	2.44	0.52
1:C:319:TYR:O	1:C:375:ASN:N	2.32	0.52
1:A:57:PHE:CD2	1:A:96:LEU:HD11	2.45	0.52
1:B:36:LEU:HD21	1:B:190:ALA:HB1	1.91	0.52
1:C:263:ARG:NH1	1:C:405:GLU:O	2.43	0.52
1:A:67:THR:HG23	1:A:121:ASP:HB3	1.90	0.52
1:C:41:PHE:HE1	1:C:43:SER:HB2	1.74	0.52
1:C:216:ARG:HB2	1:C:231:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:HB	1:A:205:LYS:HB2	1.92	0.51
1:A:208:TYR:OH	1:A:267:GLN:HG3	2.10	0.51
1:B:399:GLU:OE2	1:C:207:LYS:O	2.28	0.51
1:C:49:ALA:HA	1:C:180:GLN:HB3	1.93	0.51
1:B:234:GLU:OE2	1:B:269:ASP:OD2	2.29	0.51
1:A:284:TYR:HE2	1:C:388:TRP:HB3	1.76	0.50
1:B:30:TRP:HE3	1:B:33:GLU:HG3	1.77	0.50
1:B:227:GLY:HA3	1:B:235:TRP:CZ2	2.46	0.50
1:A:207:LYS:O	1:C:399:GLU:OE2	2.28	0.50
1:C:361:TRP:CE2	1:C:374:PRO:HD3	2.47	0.50
1:A:139:TYR:HE1	1:A:222:TYR:CE2	2.30	0.50
1:A:206:SER:OG	1:A:209:HIS:ND1	2.45	0.49
1:B:45:THR:OG1	1:B:46:PRO:HD2	2.12	0.49
1:A:367:TYR:HB2	1:A:372:ILE:HG22	1.93	0.49
1:B:54:SER:HG	1:B:133:HIS:CE1	2.29	0.49
1:C:175:LYS:O	1:C:176:ASN:HB2	2.13	0.49
1:A:248:HIS:CD2	1:A:251:PRO:HG2	2.48	0.49
1:A:276:SER:HA	1:A:279:GLN:HG2	1.94	0.49
1:A:142:HIS:HB2	1:A:153:CYS:O	2.13	0.48
1:B:309:ALA:O	1:B:311:LYS:NZ	2.32	0.48
1:B:39:GLU:OE2	1:B:191:TYR:OH	2.32	0.48
1:B:145:ASP:OD1	1:B:146:PRO:HD2	2.14	0.48
1:C:367:TYR:O	1:C:368:GLY:C	2.52	0.48
1:A:61:ALA:HB2	1:A:87:PRO:HB3	1.96	0.47
1:C:322:ILE:HG22	1:C:365:PHE:CG	2.49	0.47
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.59	0.47
1:A:168:ILE:HG21	1:A:172:GLN:HE21	1.78	0.47
1:A:361:TRP:NE1	1:A:363:GLN:O	2.46	0.47
1:C:61:ALA:HB2	1:C:87:PRO:HB3	1.97	0.47
1:C:287:CYS:O	1:C:290:THR:HB	2.15	0.47
1:C:320:THR:OG1	1:C:321:VAL:N	2.48	0.47
1:B:203:VAL:HG11	1:B:211:HIS:ND1	2.29	0.47
1:B:401:HIS:O	1:B:404:SER:N	2.46	0.47
1:A:396:VAL:O	1:A:400:LEU:HB2	2.14	0.47
1:C:229:LYS:HE2	1:C:233:GLY:HA2	1.96	0.46
1:A:86:LYS:NZ	1:A:159:ASP:OD1	2.36	0.46
1:C:272:GLN:NE2	1:C:404:SER:HA	2.25	0.46
1:C:263:ARG:HB3	1:C:409:LEU:HB3	1.97	0.46
1:B:22:ARG:NH2	1:B:295:GLU:OE2	2.45	0.46
1:C:89:ARG:HD2	1:C:157:TYR:CE2	2.50	0.46
1:C:293:LYS:HZ3	1:C:304:ASP:CG	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:PRO:HB3	1:C:376:GLY:O	2.15	0.46
1:A:229:LYS:HE2	1:A:233:GLY:HA2	1.97	0.46
1:A:36:LEU:HD13	1:A:36:LEU:HA	1.76	0.46
1:C:41:PHE:CE1	1:C:43:SER:HB2	2.51	0.46
1:A:11:LYS:HZ3	1:A:362:THR:HG23	1.81	0.46
1:A:57:PHE:HD2	1:A:96:LEU:HD11	1.81	0.46
1:C:41:PHE:CZ	1:C:238:LEU:HD13	2.51	0.46
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.79	0.45
1:C:37:GLN:HB2	1:C:193:LYS:HE2	1.98	0.45
1:C:212:MET:CG	1:C:231:PRO:HD2	2.45	0.45
1:C:109:PHE:HA	1:C:110:PRO:HD3	1.78	0.45
1:B:41:PHE:CE1	1:B:187:VAL:HB	2.50	0.45
1:C:400:LEU:HD23	1:C:400:LEU:HA	1.78	0.45
1:A:56:GLY:HA3	1:A:167:TRP:CZ2	2.52	0.45
1:A:10:THR:HB	1:A:362:THR:HG22	1.98	0.45
1:B:71:ARG:HB3	1:B:72:TRP:CE3	2.52	0.45
1:B:96:LEU:CD2	1:B:172:GLN:HE22	2.29	0.45
1:C:347:LYS:HE2	1:C:347:LYS:HB3	1.68	0.45
1:B:183:THR:OG1	1:B:184:PRO:HD2	2.17	0.45
1:A:138:ASP:OD2	1:A:410:ASP:OD2	2.35	0.44
1:A:275:THR:OG1	1:B:274:LEU:HD13	2.17	0.44
1:A:139:TYR:HE1	1:A:222:TYR:HE2	1.63	0.44
1:B:172:GLN:H	1:B:172:GLN:HG2	1.31	0.44
1:B:274:LEU:HA	1:B:274:LEU:HD23	1.80	0.44
1:A:43:SER:OG	1:A:236:VAL:HB	2.17	0.44
1:B:261:GLU:OE1	1:B:411:HIS:CD2	2.70	0.44
1:C:310:SER:HB3	1:C:333:TYR:CD2	2.53	0.44
1:A:130:THR:OG1	1:B:102:GLY:HA2	2.18	0.44
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.80	0.44
1:B:303:LEU:HD12	1:B:303:LEU:HA	1.72	0.44
1:B:377:LEU:HD12	1:B:385:LYS:O	2.17	0.44
1:B:315:LYS:HA	1:B:332:ARG:HA	2.00	0.44
1:C:398:ASN:O	1:C:401:HIS:HB3	2.17	0.44
1:A:279:GLN:O	1:A:283:ASP:HB2	2.17	0.44
1:B:86:LYS:HE3	1:B:159:ASP:OD1	2.18	0.44
1:C:207:LYS:NZ	1:C:208:TYR:CZ	2.86	0.44
1:A:350:ARG:HE	1:A:350:ARG:HB2	1.70	0.43
1:B:142:HIS:HB2	1:B:153:CYS:O	2.17	0.43
1:C:45:THR:HB	1:C:236:VAL:HG12	2.00	0.43
1:B:46:PRO:HA	1:B:182:PHE:CD1	2.51	0.43
1:B:212:MET:HE3	1:B:231:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:TYR:CE2	1:C:388:TRP:HB3	2.52	0.43
1:A:369:ASP:OD1	1:A:369:ASP:N	2.52	0.43
1:A:346:PRO:O	1:A:360:ILE:HG12	2.19	0.43
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.72	0.43
1:B:290:THR:O	1:B:294:VAL:HG23	2.18	0.43
1:B:361:TRP:CZ2	1:B:363:GLN:HB3	2.54	0.43
1:C:175:LYS:HB3	1:C:175:LYS:HE2	1.78	0.43
1:A:346:PRO:HD3	1:A:384:TYR:CZ	2.53	0.43
1:B:277:GLU:HA	1:B:280:ARG:HD3	2.00	0.43
1:C:57:PHE:N	1:C:168:ILE:O	2.46	0.43
1:A:301:SER:H	1:A:304:ASP:HB2	1.84	0.42
1:B:27:GLY:HA3	1:B:280:ARG:HG2	2.01	0.42
1:C:12:LEU:HD13	1:C:331:THR:HB	2.01	0.42
1:B:301:SER:OG	1:B:304:ASP:OD2	2.36	0.42
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.62	0.42
1:C:16:PRO:HB3	1:C:325:THR:HG21	2.00	0.42
1:B:369:ASP:OD1	1:B:369:ASP:N	2.51	0.42
2:D:1:NAG:H5	2:D:1:NAG:HN2	1.85	0.42
1:C:70:PHE:HB3	1:C:115:GLY:O	2.19	0.42
1:A:14:TRP:CD1	1:A:365:PHE:CZ	3.04	0.42
1:B:233:GLY:O	1:B:263:ARG:N	2.34	0.42
1:A:130:THR:HG21	1:B:99:TYR:O	2.20	0.42
1:B:71:ARG:HB3	1:B:72:TRP:HE3	1.84	0.42
1:B:222:TYR:HB3	1:B:235:TRP:CZ2	2.55	0.41
1:A:8:GLU:O	1:A:350:ARG:NH1	2.54	0.41
1:B:306:SER:O	1:B:311:LYS:HE3	2.19	0.41
1:A:256:CYS:HA	1:A:257:PRO:HD3	1.90	0.41
1:B:207:LYS:NZ	1:B:208:TYR:CE2	2.88	0.41
1:C:89:ARG:HG3	1:C:157:TYR:CZ	2.55	0.41
1:C:286:LEU:O	1:C:289:ASN:HB3	2.20	0.41
1:A:49:ALA:HA	1:A:180:GLN:HA	2.03	0.41
1:A:275:THR:HG21	1:B:274:LEU:HB3	2.02	0.41
1:C:220:LEU:CD2	1:C:222:TYR:HB2	2.50	0.41
1:B:227:GLY:HA2	1:B:238:LEU:H	1.85	0.41
1:A:11:LYS:HA	1:A:363:GLN:OE1	2.20	0.41
1:A:109:PHE:HA	1:A:110:PRO:HD3	1.85	0.41
1:B:14:TRP:CE3	1:B:320:THR:HG22	2.56	0.41
1:C:296:ARG:NE	1:C:298:GLU:OE2	2.53	0.41
1:B:312:SER:HA	1:B:313:PRO:HD3	1.83	0.41
1:A:386:PHE:N	1:A:386:PHE:CD1	2.88	0.41
1:B:121:ASP:OD1	1:B:121:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HG13	1:B:162:HIS:N	2.36	0.41
1:A:216:ARG:HB2	1:A:231:PRO:HG3	2.03	0.41
1:A:276:SER:O	1:A:279:GLN:HG2	2.21	0.41
1:B:319:TYR:CE1	1:B:328:PHE:HB3	2.55	0.41
1:B:338:ILE:HB	1:B:343:LEU:HD21	2.02	0.41
1:C:189:VAL:HG22	1:C:204:PHE:CE1	2.56	0.41
1:C:219:ARG:HD3	1:C:250:LEU:HD11	2.02	0.41
1:A:287:CYS:HB3	1:A:307:TYR:O	2.20	0.41
1:B:182:PHE:HE2	1:B:225:ARG:HD3	1.86	0.41
1:B:241:LYS:HA	1:B:241:LYS:HD3	1.72	0.41
1:B:301:SER:O	1:B:304:ASP:HB2	2.21	0.41
2:D:1:NAG:H4	2:D:2:NAG:H2	1.90	0.41
1:A:64:TRP:CD1	1:A:64:TRP:N	2.89	0.40
1:A:247:LYS:HE2	1:A:247:LYS:HB3	1.82	0.40
1:A:341:PRO:HA	1:A:391:ILE:HD11	2.03	0.40
1:C:2:LEU:HD23	1:C:2:LEU:HA	1.83	0.40
1:C:145:ASP:O	1:C:151:GLY:HA2	2.21	0.40
1:C:199:ALA:HB2	1:C:252:LEU:O	2.20	0.40
1:C:302:PRO:HD3	1:C:367:TYR:OH	2.21	0.40
1:A:11:LYS:HZ2	1:A:362:THR:HG23	1.86	0.40
1:B:66:THR:OG1	1:B:110:PRO:HD2	2.20	0.40
1:B:361:TRP:CE2	1:B:374:PRO:HD3	2.56	0.40
1:B:29:GLU:OE2	1:B:205:LYS:HD2	2.21	0.40
1:B:247:LYS:HE2	1:B:247:LYS:HB3	1.83	0.40
1:A:59:CYS:HA	1:A:129:ILE:HD13	2.03	0.40
1:A:244:ILE:CG1	1:A:249:LEU:HD22	2.47	0.40
1:B:6:PHE:CD1	1:B:7:PRO:HD2	2.56	0.40
1:B:171:ASP:HB3	1:B:174:LYS:HZ3	1.86	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	403/419 (96%)	393 (98%)	10 (2%)	0	100	100
1	B	414/419 (99%)	397 (96%)	14 (3%)	3 (1%)	22	61
1	C	402/419 (96%)	387 (96%)	12 (3%)	3 (1%)	22	61
All	All	1219/1257 (97%)	1177 (97%)	36 (3%)	6 (0%)	29	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	176	ASN
1	C	177	ILE
1	C	368	GLY
1	B	351	GLU
1	B	33	GLU
1	B	35	GLY

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	355/364 (98%)	345 (97%)	10 (3%)	43	72
1	B	362/364 (100%)	357 (99%)	5 (1%)	67	85
1	C	354/364 (97%)	346 (98%)	8 (2%)	50	76
All	All	1071/1092 (98%)	1048 (98%)	23 (2%)	53	78

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	36	LEU
1	A	37	GLN
1	A	144	VAL
1	A	265	THR
1	A	283	ASP
1	A	351	GLU

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Mol	Chain	Res	Type
1	A	356	ILE
1	A	391	ILE
1	A	413	GLN
1	B	32	LEU
1	B	172	GLN
1	B	185	LEU
1	B	297	LYS
1	B	403	LEU
1	C	88	THR
1	C	163	ASN
1	C	265	THR
1	C	287	CYS
1	C	300	LEU
1	C	322	ILE
1	C	369	ASP
1	C	371	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	211	HIS
1	A	248	HIS
1	A	272	GLN
1	A	413	GLN
1	B	60	HIS
1	B	83	HIS
1	B	172	GLN
1	B	180	GLN
1	B	248	HIS
1	B	411	HIS
1	C	9	ASN
1	C	60	HIS
1	C	180	GLN
1	C	272	GLN

5.3.3 RNA

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)

4 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	D	1	1,2	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
2	NAG	D	2	2	14,14,15	0.91	1 (7%)	17,19,21	0.62	0
3	NAG	E	1	1,3	14,14,15	1.14	1 (7%)	17,19,21	1.18	1 (5%)
3	FUC	E	2	3	10,10,11	1.55	2 (20%)	14,14,16	1.94	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C1-C2	4.09	1.58	1.52
3	E	2	FUC	C2-C3	3.23	1.57	1.52
2	D	2	NAG	C1-C2	3.22	1.57	1.52
3	E	2	FUC	C1-C2	2.69	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	FUC	O5-C1-C2	4.25	117.33	110.77
3	E	1	NAG	C1-O5-C5	4.13	117.79	112.19
3	E	2	FUC	C1-C2-C3	3.97	114.54	109.67
3	E	2	FUC	C1-O5-C5	3.28	120.20	112.78
2	D	1	NAG	C1-O5-C5	2.40	115.44	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6

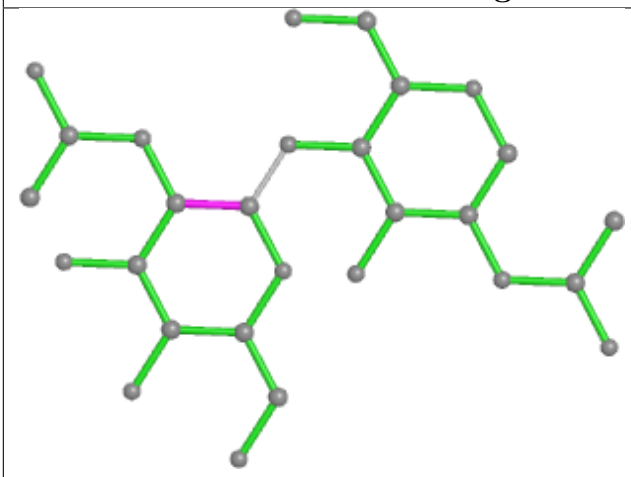
There are no ring outliers.

2 monomers are involved in 2 short contacts:

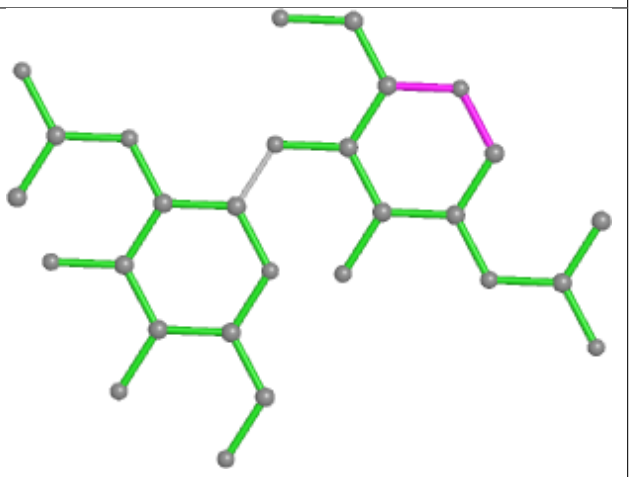
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
2	D	2	NAG	1	0

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

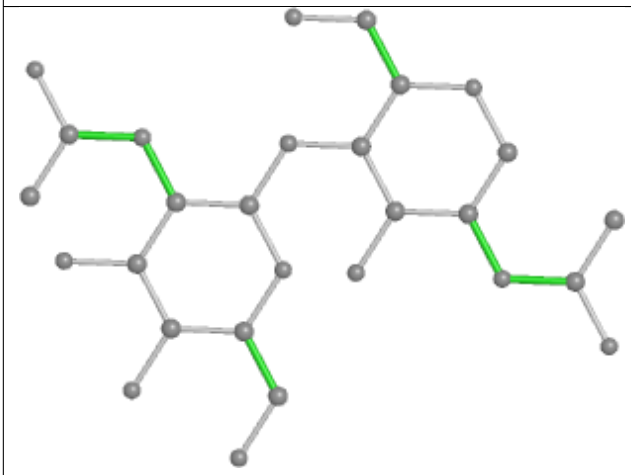
Oligosaccharide Chain D



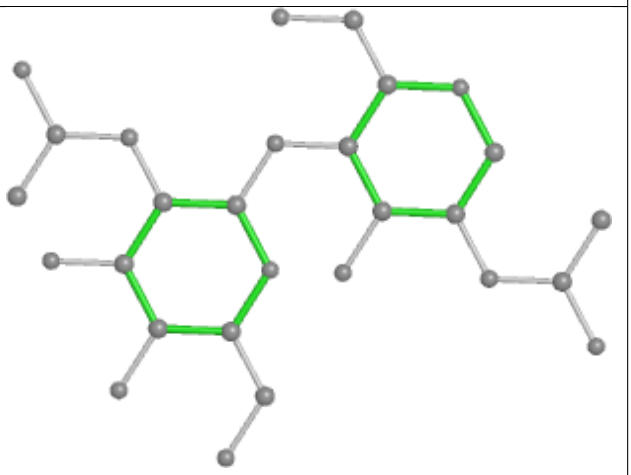
Bond lengths



Bond angles

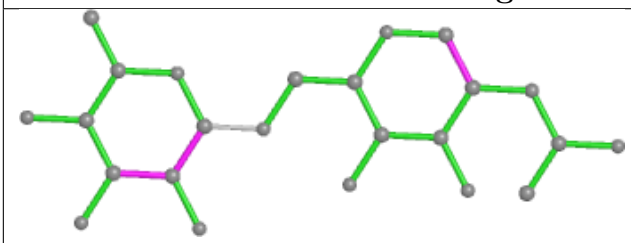


Torsions

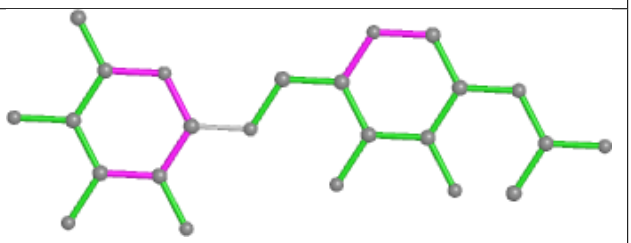


Rings

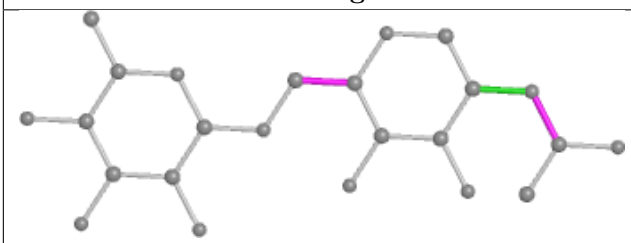
Oligosaccharide Chain E



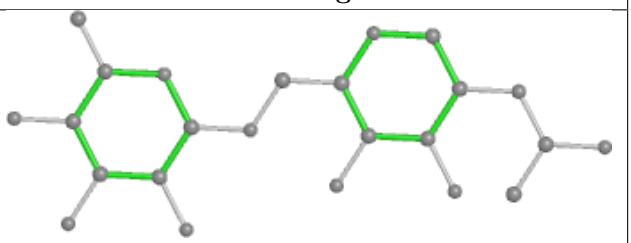
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

2 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	C	1004	1	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
4	NAG	B	1001	1	14,14,15	1.09	1 (7%)	17,19,21	0.80	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
4	NAG	C	1004	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1001	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)
4	B	1001	NAG	O5-C1	3.59	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1004	NAG	C1-O5-C5	3.05	116.32	112.19
4	B	1001	NAG	C1-O5-C5	2.95	116.19	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1004	NAG	O5-C5-C6-O6
4	C	1004	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1004	NAG	C1-C2-N2-C7
4	B	1001	NAG	C1-C2-N2-C7
4	C	1004	NAG	C3-C2-N2-C7
4	B	1001	NAG	C3-C2-N2-C7

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	A	407/419 (97%)	0.46	52 (12%) 3 2	54, 85, 220, 348	0
1	B	416/419 (99%)	0.02	20 (4%) 30 19	41, 85, 188, 284	0
1	C	406/419 (96%)	0.14	20 (4%) 29 18	42, 101, 204, 346	0
All	All	1229/1257 (97%)	0.21	92 (7%) 14 8	41, 91, 206, 348	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	THR	12.2
1	A	119	VAL	10.0
1	A	115	GLY	8.6
1	A	113	SER	6.5
1	A	114	CYS	6.4
1	B	75	PRO	6.4
1	A	61	ALA	6.1
1	A	65	VAL	5.7
1	A	121	ASP	5.4
1	A	117	ALA	5.3
1	A	77	TYR	5.3
1	B	76	LYS	5.2
1	A	161	ILE	4.9
1	A	67	THR	4.8
1	B	74	GLY	4.7
1	A	166	VAL	4.4
1	A	122	SER	4.4
1	A	81	SER	4.3
1	A	116	TYR	4.3
1	C	355	GLY	4.3
1	B	116	TYR	4.3
1	A	111	PRO	4.2
1	A	162	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	72	TRP	4.2
1	A	157	TYR	4.1
1	B	78	ILE	4.0
1	A	69	ASP	3.8
1	A	73	TYR	3.8
1	B	115	GLY	3.8
1	A	160	THR	3.7
1	A	83	HIS	3.7
1	C	120	THR	3.6
1	A	123	GLU	3.6
1	A	79	THR	3.6
1	A	158	CYS	3.5
1	A	167	TRP	3.4
1	A	80	HIS	3.4
1	A	112	GLU	3.3
1	C	142	HIS	3.3
1	A	164	SER	3.2
1	A	78	ILE	3.2
1	A	87	PRO	3.2
1	A	74	GLY	3.1
1	B	77	TYR	3.0
1	A	66	THR	3.0
1	B	118	SER	2.9
1	B	112	GLU	2.9
1	A	165	SER	2.9
1	A	168	ILE	2.8
1	C	143	TRP	2.8
1	A	68	CYS	2.8
1	A	156	SER	2.7
1	B	117	ALA	2.7
1	A	71	ARG	2.7
1	A	84	ASN	2.7
1	C	137	ASP	2.6
1	C	79	THR	2.6
1	A	76	LYS	2.6
1	B	67	THR	2.6
1	B	111	PRO	2.6
1	C	166	VAL	2.6
1	C	119	VAL	2.5
1	A	63	LYS	2.5
1	A	62	ALA	2.5
1	C	157	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	73	TYR	2.4
1	C	114	CYS	2.4
1	B	80	HIS	2.4
1	A	125	LEU	2.4
1	A	163	ASN	2.4
1	A	143	TRP	2.4
1	A	118	SER	2.4
1	B	119	VAL	2.4
1	B	383	GLY	2.3
1	C	77	TYR	2.3
1	A	159	ASP	2.3
1	A	124	PHE	2.3
1	A	86	LYS	2.3
1	B	72	TRP	2.2
1	A	89	ARG	2.2
1	C	113	SER	2.2
1	C	69	ASP	2.2
1	C	118	SER	2.2
1	C	154	ASP	2.2
1	C	348	GLY	2.1
1	B	68	CYS	2.1
1	B	157	TYR	2.1
1	C	74	GLY	2.1
1	B	248	HIS	2.0
1	C	136	VAL	2.0
1	C	356	ILE	2.0
1	C	148	PHE	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	D	2	14/15	0.69	0.29	94,151,158,165	0

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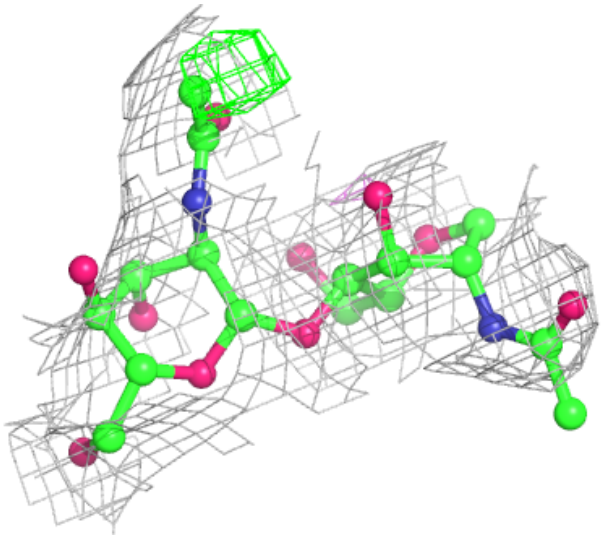
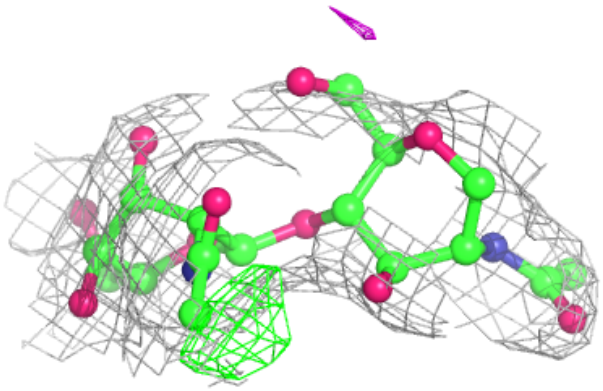
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	1	14/15	0.83	0.17	85,112,137,147	0
2	NAG	D	1	14/15	0.89	0.34	102,131,150,154	0
3	FUC	E	2	10/11	0.89	0.22	158,165,171,171	0

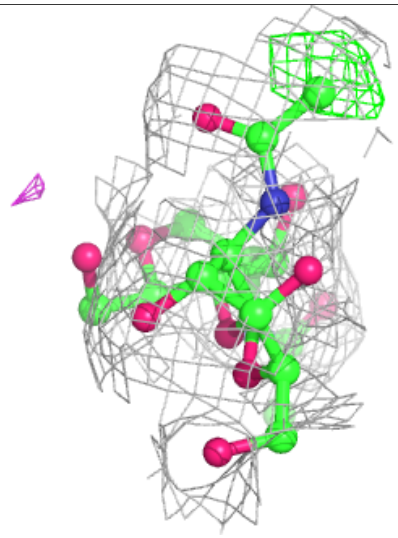
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

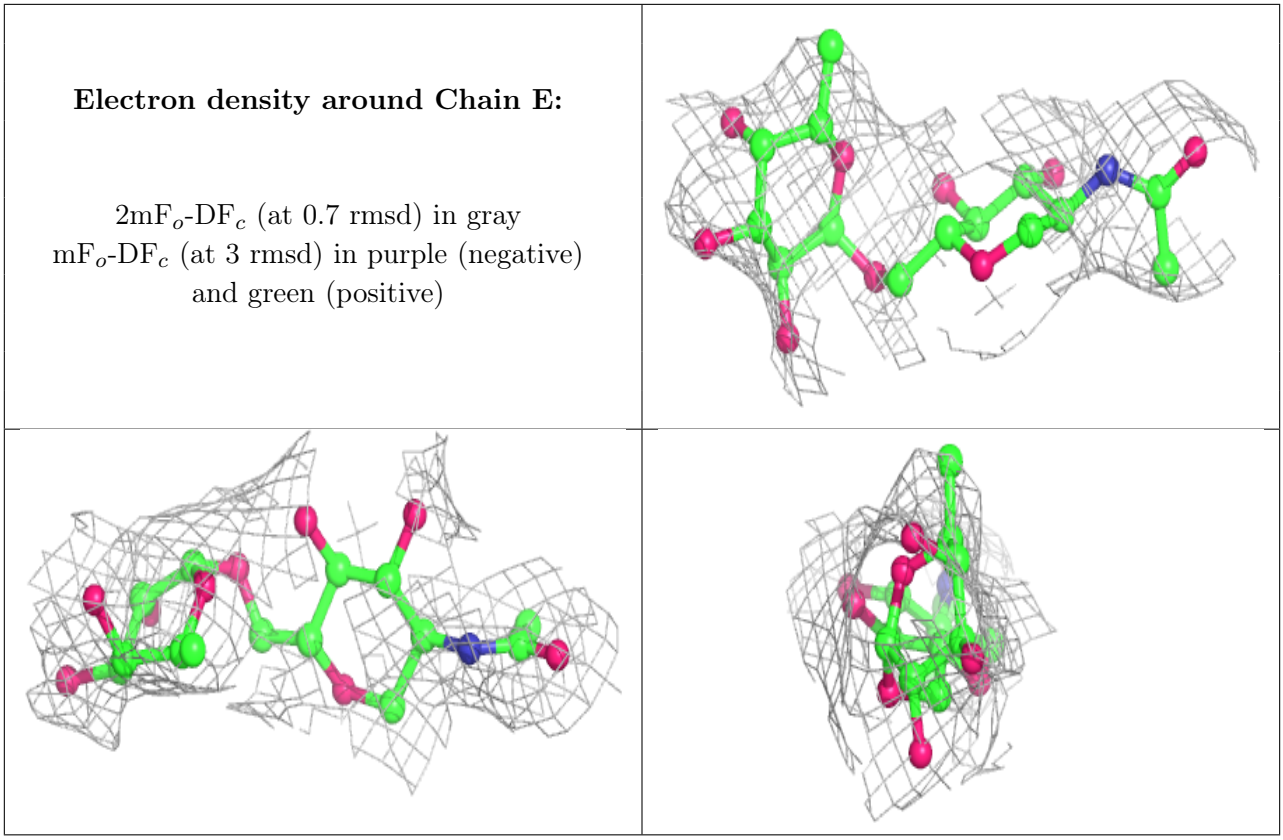






Electron density around Chain E:

$2mF_o$-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	C	1004	14/15	0.68	0.36	200,204,209,212	0
4	NAG	B	1001	14/15	0.78	0.20	170,181,183,184	0

6.5 Other polymers

There are no such residues in this entry.