Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2021 – 03:08 pm BST

PDB ID	:	7A59
Title	:	Crimean-Congo Hemorrhagic Fever Virus Envelope Glycoprotein Gc W1191H/W1197A/W1199A Mutant in Postfusion Conformation (Orthorhombic Crystal Form)
Authors	:	Hellert, J.; Guardado-Calvo, P.; Rey, F.A.
Deposited on	:	2020-08-20
Resolution	:	2.20 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 following versions of software and data (see references (i)) were used in the production of this report:

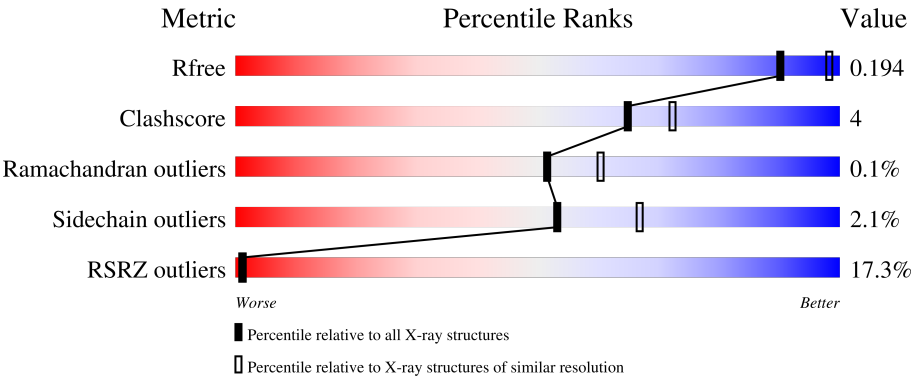
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	538	19% 83% 10% 7%
1	B	538	16% 81% 14% 5%
1	C	538	14% 82% 11% 7%
2	D	5	40% 20% 40%

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
2	BMA	D	3	-	-	-	X
2	MAN	D	4	-	-	-	X
2	FUC	D	5	-	-	-	X
3	NAG	A	1601	-	-	-	X
3	NAG	B	1601	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12589 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3874	2430	659	750	35			
1	B	513	Total	C	N	O	S	0	0	0
			3998	2511	680	772	35			
1	C	501	Total	C	N	O	S	0	0	0
			3889	2439	662	753	35			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
A	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
A	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
A	1562	GLU	-	expression tag	UNP Q8JSZ3
A	1563	ASN	-	expression tag	UNP Q8JSZ3
A	1564	LEU	-	expression tag	UNP Q8JSZ3
A	1565	TYR	-	expression tag	UNP Q8JSZ3
A	1566	PHE	-	expression tag	UNP Q8JSZ3
A	1567	GLN	-	expression tag	UNP Q8JSZ3
A	1568	SER	-	expression tag	UNP Q8JSZ3
A	1569	ALA	-	expression tag	UNP Q8JSZ3
A	1570	GLY	-	expression tag	UNP Q8JSZ3
A	1571	TRP	-	expression tag	UNP Q8JSZ3
A	1572	SER	-	expression tag	UNP Q8JSZ3
A	1573	HIS	-	expression tag	UNP Q8JSZ3
A	1574	PRO	-	expression tag	UNP Q8JSZ3
A	1575	GLN	-	expression tag	UNP Q8JSZ3
A	1576	PHE	-	expression tag	UNP Q8JSZ3
A	1577	GLU	-	expression tag	UNP Q8JSZ3
A	1578	LYS	-	expression tag	UNP Q8JSZ3
B	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
B	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
B	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3

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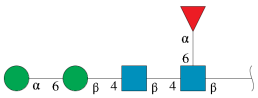
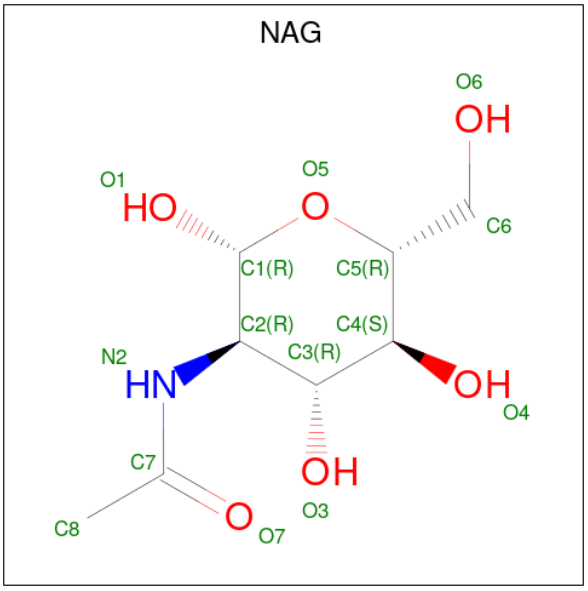
Chain	Residue	Modelled	Actual	Comment	Reference
B	1562	GLU	-	expression tag	UNP Q8JSZ3
B	1563	ASN	-	expression tag	UNP Q8JSZ3
B	1564	LEU	-	expression tag	UNP Q8JSZ3
B	1565	TYR	-	expression tag	UNP Q8JSZ3
B	1566	PHE	-	expression tag	UNP Q8JSZ3
B	1567	GLN	-	expression tag	UNP Q8JSZ3
B	1568	SER	-	expression tag	UNP Q8JSZ3
B	1569	ALA	-	expression tag	UNP Q8JSZ3
B	1570	GLY	-	expression tag	UNP Q8JSZ3
B	1571	TRP	-	expression tag	UNP Q8JSZ3
B	1572	SER	-	expression tag	UNP Q8JSZ3
B	1573	HIS	-	expression tag	UNP Q8JSZ3
B	1574	PRO	-	expression tag	UNP Q8JSZ3
B	1575	GLN	-	expression tag	UNP Q8JSZ3
B	1576	PHE	-	expression tag	UNP Q8JSZ3
B	1577	GLU	-	expression tag	UNP Q8JSZ3
B	1578	LYS	-	expression tag	UNP Q8JSZ3
C	1191	HIS	TRP	engineered mutation	UNP Q8JSZ3
C	1197	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1199	ALA	TRP	engineered mutation	UNP Q8JSZ3
C	1562	GLU	-	expression tag	UNP Q8JSZ3
C	1563	ASN	-	expression tag	UNP Q8JSZ3
C	1564	LEU	-	expression tag	UNP Q8JSZ3
C	1565	TYR	-	expression tag	UNP Q8JSZ3
C	1566	PHE	-	expression tag	UNP Q8JSZ3
C	1567	GLN	-	expression tag	UNP Q8JSZ3
C	1568	SER	-	expression tag	UNP Q8JSZ3
C	1569	ALA	-	expression tag	UNP Q8JSZ3
C	1570	GLY	-	expression tag	UNP Q8JSZ3
C	1571	TRP	-	expression tag	UNP Q8JSZ3
C	1572	SER	-	expression tag	UNP Q8JSZ3
C	1573	HIS	-	expression tag	UNP Q8JSZ3
C	1574	PRO	-	expression tag	UNP Q8JSZ3
C	1575	GLN	-	expression tag	UNP Q8JSZ3
C	1576	PHE	-	expression tag	UNP Q8JSZ3
C	1577	GLU	-	expression tag	UNP Q8JSZ3
C	1578	LYS	-	expression tag	UNP Q8JSZ3

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	5	Total C N O 60 34 2 24	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

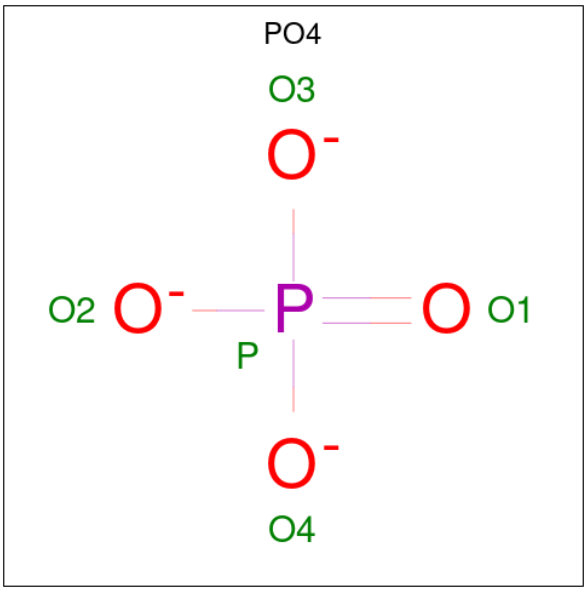


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

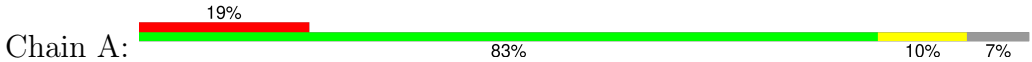
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	241	Total O 241 241	0	0
6	B	245	Total O 245 245	0	0
6	C	243	Total O 243 243	0	0

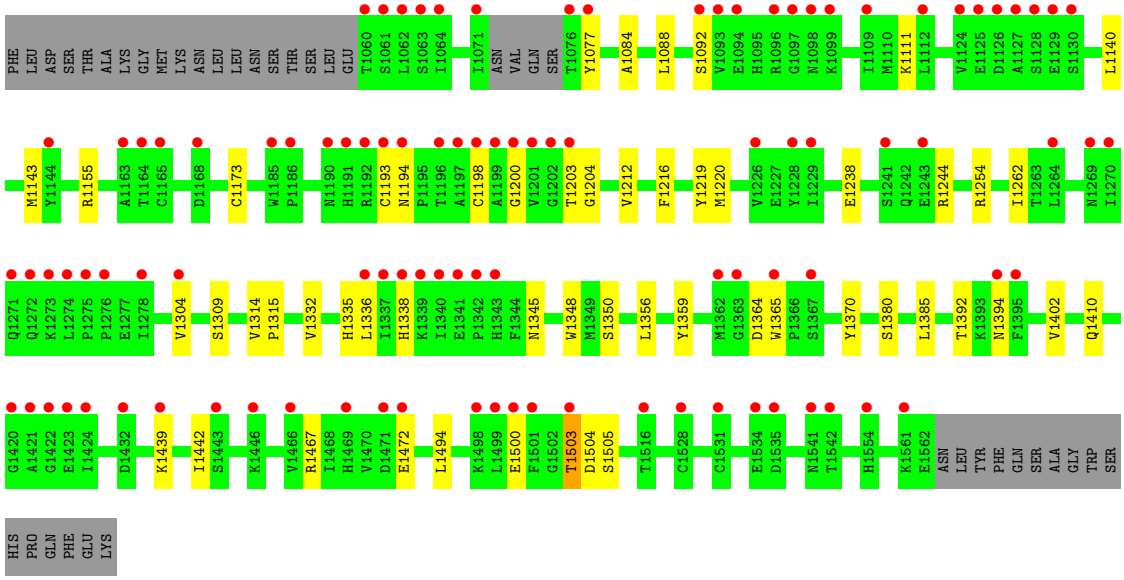
3 Residue-property plots (i)

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: Envelopment polyprotein

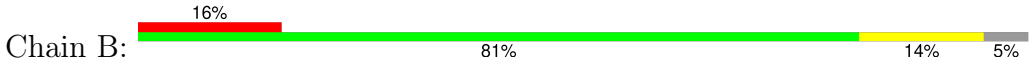
Chain A:

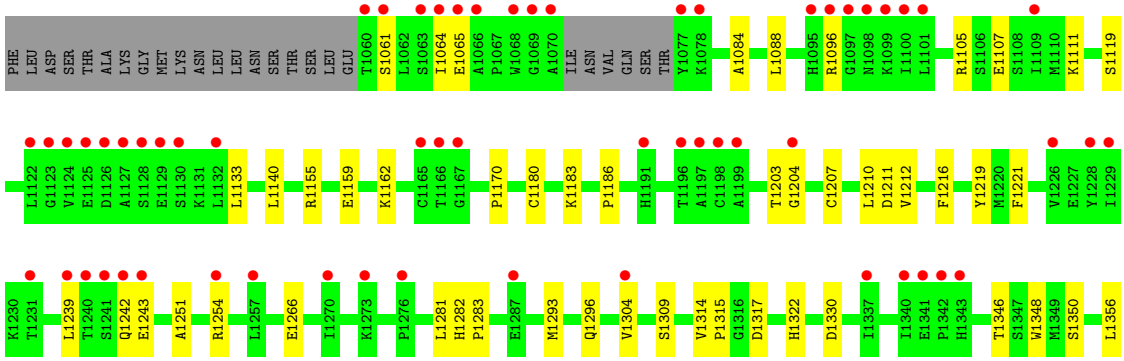


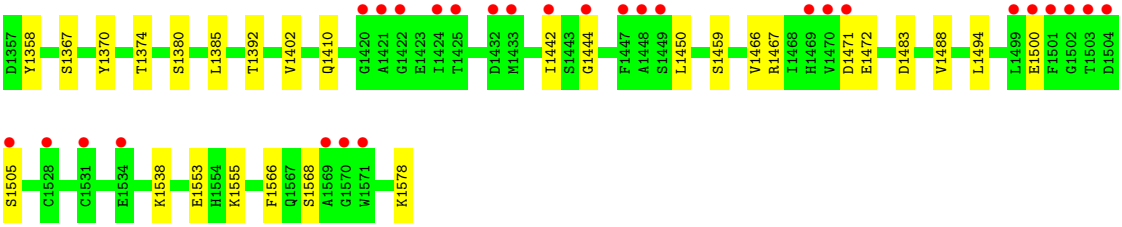


• Molecule 1: Envelopment polyprotein

Chain B:

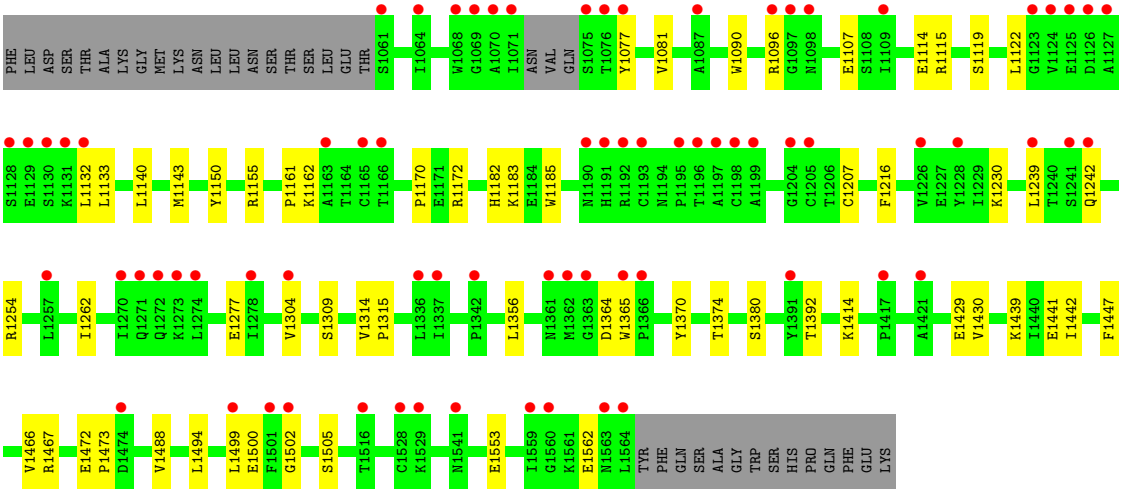






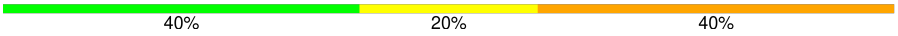
• Molecule 1: Envelopment polyprotein

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.96Å 216.08Å 274.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.20 49.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-2.20) 92.1 (49.37-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.161 , 0.194 0.161 , 0.194	Depositor DCC
R_{free} test set	1997 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12589	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: CL, BMA, PO4, MAN, NAG, FUC

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	0.37	0/3960	0.54	0/5369
1	B	0.37	1/4091 (0.0%)	0.56	1/5545 (0.0%)
1	C	0.38	1/3975 (0.0%)	0.55	0/5389
All	All	0.37	2/12026 (0.0%)	0.55	1/16303 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1207	CYS	CB-SG	-5.44	1.73	1.81
1	C	1207	CYS	CB-SG	-5.24	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1317	ASP	CB-CG-OD1	5.77	123.49	118.30

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	3874	0	3769	29	0
1	B	3998	0	3872	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3889	0	3784	35	0
2	D	60	0	52	1	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	0	0
6	A	241	0	0	1	0
6	B	245	0	0	4	0
6	C	243	0	0	2	0
All	All	12589	0	11503	96	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 4.

All (96) 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:B:1578:LYS:HG2	1:C:1172:ARG:HG2	1.62	0.79
1:A:1309:SER:HB2	1:C:1314:VAL:HG21	1.67	0.76
1:B:1254:ARG:NH1	6:B:1701:HOH:O	2.22	0.73
1:B:1315:PRO:HD3	1:B:1380:SER:HB3	1.72	0.70
1:A:1494:LEU:HD22	1:A:1505:SER:HB3	1.75	0.69
1:C:1467:ARG:NH2	1:C:1502:GLY:O	2.26	0.69
1:B:1467:ARG:HH11	1:B:1500:GLU:HB2	1.57	0.69
1:B:1578:LYS:HE3	1:C:1182:HIS:HE1	1.57	0.68
1:A:1314:VAL:HG21	1:B:1309:SER:HB2	1.76	0.66
1:A:1467:ARG:HE	1:A:1500:GLU:HG3	1.66	0.61
1:C:1364:ASP:OD1	1:C:1365:TRP:N	2.33	0.60
1:B:1555:LYS:NZ	6:B:1702:HOH:O	2.30	0.60
1:A:1238:GLU:HG2	1:A:1244:ARG:HG3	1.83	0.59
1:B:1314:VAL:HG21	1:C:1309:SER:HB2	1.86	0.58
3:B:1601:NAG:H83	3:B:1601:NAG:H3	1.86	0.58
1:A:1088:LEU:HD11	1:B:1105:ARG:HD2	1.86	0.57
1:A:1092:SER:HB2	1:C:1090:TRP:HB2	1.86	0.56
1:C:1494:LEU:HD22	1:C:1505:SER:HB3	1.87	0.56
1:B:1096:ARG:NH2	6:B:1705:HOH:O	2.32	0.56
1:C:1239:LEU:HD23	1:C:1242:GLN:HG3	1.88	0.55
1:A:1315:PRO:HD3	1:A:1380:SER:HB3	1.89	0.53
1:B:1578:LYS:HE3	1:C:1182:HIS:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1143:MET:HE1	1:C:1414:LYS:NZ	2.24	0.53
1:C:1356:LEU:HD22	1:C:1370:TYR:CD2	2.44	0.53
1:B:1239:LEU:HD23	1:B:1242:GLN:HG3	1.91	0.52
1:C:1374:THR:HG23	1:C:1553:GLU:HG2	1.92	0.52
1:A:1364:ASP:OD1	1:A:1365:TRP:N	2.38	0.52
1:C:1230:LYS:NZ	6:C:1711:HOH:O	2.43	0.52
1:A:1194:ASN:ND2	1:A:1200:GLY:O	2.39	0.52
1:B:1348:TRP:CH2	1:B:1350:SER:HB2	2.46	0.51
1:C:1162:LYS:HD3	1:C:1170:PRO:HG2	1.93	0.51
1:A:1345:ASN:OD1	1:A:1345:ASN:N	2.40	0.51
1:A:1335:HIS:ND1	1:A:1336:LEU:HG	2.26	0.50
1:B:1356:LEU:HD22	1:B:1370:TYR:CD2	2.47	0.50
1:C:1143:MET:HE1	1:C:1414:LYS:HZ2	1.77	0.49
1:B:1578:LYS:CG	1:C:1172:ARG:HG2	2.38	0.49
1:C:1277:GLU:OE1	6:C:1701:HOH:O	2.19	0.49
1:C:1466:VAL:HG11	1:C:1494:LEU:HD13	1.95	0.49
1:B:1219:TYR:CE1	1:B:1385:LEU:HD11	2.48	0.49
1:B:1293:MET:HG3	1:B:1330:ASP:OD1	2.12	0.49
1:B:1159:GLU:HG3	1:B:1210:LEU:HD13	1.94	0.49
1:C:1081:VAL:HG11	1:C:1473:PRO:HG2	1.95	0.48
1:B:1296:GLN:NE2	6:B:1713:HOH:O	2.45	0.48
1:A:1203:THR:OG1	6:A:1701:HOH:O	2.20	0.48
1:B:1084:ALA:HB1	1:B:1111:LYS:HD3	1.95	0.48
1:A:1254:ARG:HA	1:A:1262:ILE:O	2.14	0.48
1:A:1356:LEU:HD22	1:A:1370:TYR:CD2	2.49	0.48
1:C:1119:SER:HB3	1:C:1132:LEU:HD11	1.96	0.47
1:B:1488:VAL:HG21	1:C:1143:MET:HE2	1.97	0.47
1:A:1359:TYR:CG	1:B:1186:PRO:HD2	2.51	0.46
1:B:1221:PHE:HB3	1:B:1281:LEU:HD23	1.98	0.46
1:A:1220:MET:SD	1:A:1332:VAL:HG21	2.55	0.46
1:B:1162:LYS:HD3	1:B:1170:PRO:HG2	1.98	0.46
1:B:1494:LEU:HD22	1:B:1505:SER:HB3	1.98	0.45
2:D:3:BMA:H62	2:D:4:MAN:H2	1.44	0.45
1:C:1254:ARG:HA	1:C:1262:ILE:O	2.16	0.45
1:A:1203:THR:OG1	1:A:1204:GLY:N	2.50	0.45
1:B:1444:GLY:HA3	1:B:1471:ASP:OD2	2.17	0.44
1:B:1450:LEU:HB3	1:B:1538:LYS:HD3	1.99	0.44
1:C:1183:LYS:HE2	1:C:1185:TRP:CZ2	2.53	0.44
1:B:1322:HIS:HD2	1:B:1346:THR:HB	1.82	0.44
1:B:1442:ILE:HA	1:B:1472:GLU:O	2.17	0.44
1:A:1194:ASN:HB3	1:A:1198:CYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:ARG:HH21	1:A:1500:GLU:HB3	1.82	0.44
1:A:1402:VAL:HA	1:A:1410:GLN:O	2.18	0.43
1:B:1211:ASP:OD1	1:B:1212:VAL:N	2.49	0.43
1:C:1114:GLU:HG3	1:C:1115:ARG:HH21	1.83	0.43
1:B:1061:SER:O	1:B:1065:GLU:HG2	2.19	0.43
1:A:1439:LYS:H	1:A:1439:LYS:NZ	2.17	0.43
1:B:1061:SER:HA	1:B:1064:ILE:HG22	2.00	0.43
1:B:1107:GLU:HB3	1:C:1107:GLU:OE2	2.18	0.43
1:B:1566:PHE:CE2	1:B:1568:SER:HB3	2.52	0.43
1:C:1150:TYR:OH	1:C:1304:VAL:HG13	2.19	0.43
1:A:1212:VAL:O	1:A:1338:HIS:NE2	2.52	0.43
1:B:1467:ARG:HE	1:B:1500:GLU:HB2	1.84	0.43
1:A:1219:TYR:CE1	1:A:1385:LEU:HD11	2.54	0.43
1:B:1203:THR:OG1	1:B:1204:GLY:N	2.51	0.43
1:A:1143:MET:HE2	1:C:1488:VAL:HG21	2.01	0.42
1:A:1503:THR:HG22	1:A:1504:ASP:H	1.83	0.42
1:B:1466:VAL:HG11	1:B:1494:LEU:HD13	2.00	0.42
1:A:1348:TRP:CH2	1:A:1350:SER:HB2	2.55	0.42
1:B:1358:TYR:HA	1:B:1367:SER:O	2.20	0.42
1:C:1499:LEU:HD12	1:C:1500:GLU:H	1.83	0.42
1:C:1315:PRO:HD3	1:C:1380:SER:HB3	2.01	0.42
1:B:1251:ALA:HB2	1:B:1266:GLU:HB3	2.02	0.41
1:B:1282:HIS:HA	1:B:1283:PRO:HD3	1.95	0.41
1:B:1402:VAL:HA	1:B:1410:GLN:O	2.20	0.41
1:B:1119:SER:HA	1:B:1133:LEU:O	2.20	0.41
1:A:1084:ALA:HB1	1:A:1111:LYS:HD3	2.03	0.41
1:C:1442:ILE:HA	1:C:1472:GLU:O	2.20	0.41
1:A:1442:ILE:HA	1:A:1472:GLU:O	2.20	0.41
1:C:1119:SER:HA	1:C:1133:LEU:O	2.20	0.41
1:B:1088:LEU:HD11	1:C:1429:GLU:HG2	2.02	0.41
1:B:1374:THR:HG23	1:B:1553:GLU:HG2	2.02	0.41
1:C:1439:LYS:HE2	1:C:1441:GLU:HG2	2.04	0.40
1:C:1122:LEU:HD11	1:C:1430:VAL:HG21	2.03	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	495/538 (92%)	485 (98%)	10 (2%)	0	100 100
1	B	509/538 (95%)	491 (96%)	18 (4%)	0	100 100
1	C	497/538 (92%)	483 (97%)	13 (3%)	1 (0%)	47 55
All	All	1501/1614 (93%)	1459 (97%)	41 (3%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1161	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	442/477 (93%)	432 (98%)	10 (2%)	50 63
1	B	454/477 (95%)	444 (98%)	10 (2%)	52 65
1	C	444/477 (93%)	436 (98%)	8 (2%)	59 72
All	All	1340/1431 (94%)	1312 (98%)	28 (2%)	53 67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1077	TYR
1	A	1140	LEU

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Mol	Chain	Res	Type
1	A	1155	ARG
1	A	1173	CYS
1	A	1193	CYS
1	A	1216	PHE
1	A	1304	VAL
1	A	1392	THR
1	A	1394	ASN
1	A	1503	THR
1	B	1140	LEU
1	B	1155	ARG
1	B	1180	CYS
1	B	1183	LYS
1	B	1216	PHE
1	B	1243	GLU
1	B	1304	VAL
1	B	1392	THR
1	B	1459	SER
1	B	1483	ASP
1	C	1077	TYR
1	C	1096	ARG
1	C	1140	LEU
1	C	1155	ARG
1	C	1216	PHE
1	C	1392	THR
1	C	1447	PHE
1	C	1562	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1322	HIS
1	C	1546	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)

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.29	0	17,19,21	0.77	0
2	BMA	D	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.04	1 (6%)
2	MAN	D	4	2	11,11,12	1.66	2 (18%)	15,15,17	1.63	3 (20%)
2	FUC	D	5	2	10,10,11	1.10	0	14,14,16	0.88	1 (7%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	C1-C2	4.65	1.62	1.52
2	D	3	BMA	C1-C2	2.61	1.58	1.52
2	D	4	MAN	C2-C3	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	MAN	C1-C2-C3	3.53	114.00	109.67
2	D	4	MAN	C1-O5-C5	3.51	116.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	MAN	O2-C2-C3	-2.24	105.65	110.14
2	D	5	FUC	O2-C2-C1	2.20	113.65	109.15
2	D	3	BMA	O5-C5-C6	2.19	110.64	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

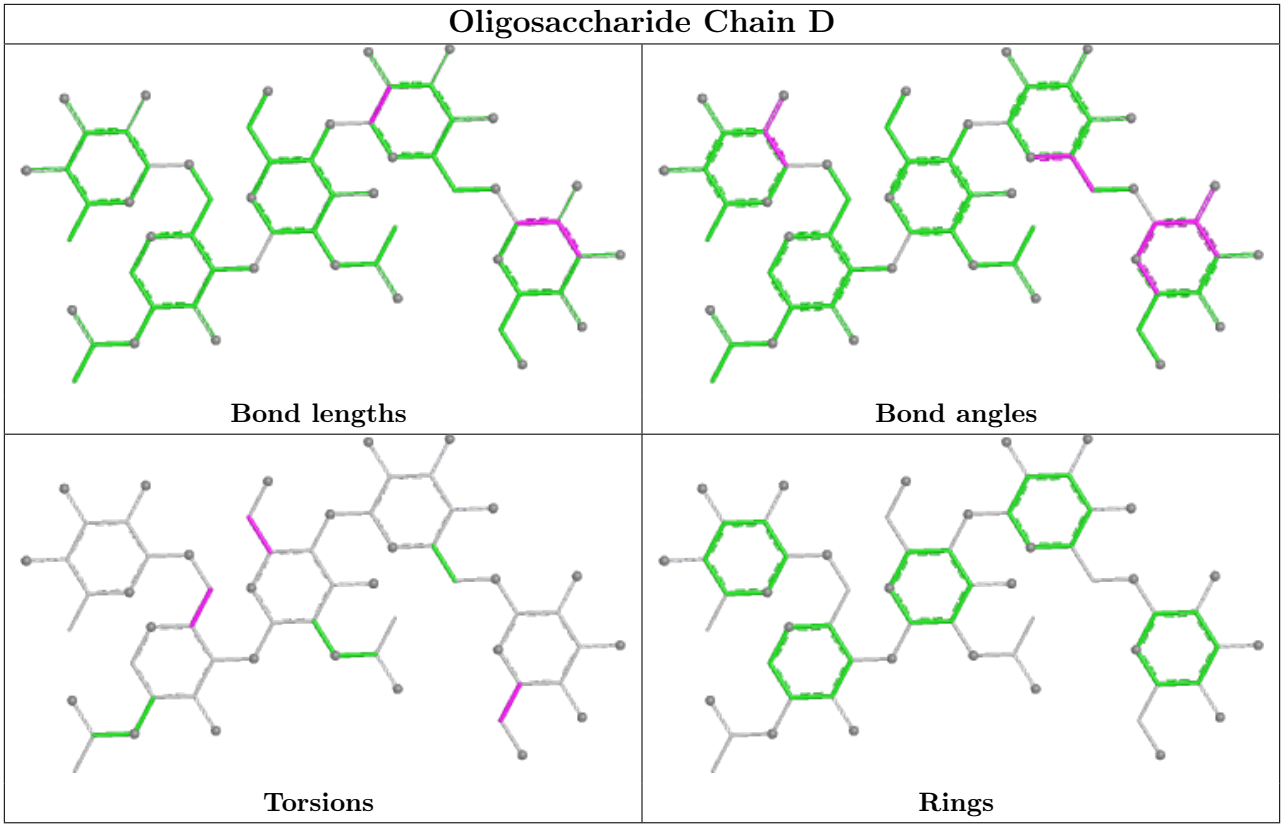
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	MAN	1	0
2	D	3	BMA	1	0

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



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
3	NAG	A	1601	1	14,14,15	0.47	0	17,19,21	0.37	0
5	PO4	A	1605	-	4,4,4	0.81	0	6,6,6	0.44	0
3	NAG	B	1601	1	14,14,15	0.87	1 (7%)	17,19,21	1.34	2 (11%)

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
3	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1601	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1601	NAG	C1-C2	2.40	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1601	NAG	C2-N2-C7	4.23	128.92	122.90
3	B	1601	NAG	C1-O5-C5	2.32	115.33	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1601	NAG	O5-C5-C6-O6
3	A	1601	NAG	C4-C5-C6-O6
3	B	1601	NAG	C8-C7-N2-C2
3	B	1601	NAG	O7-C7-N2-C2
3	B	1601	NAG	O5-C5-C6-O6
3	B	1601	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1601	NAG	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	499/538 (92%)	1.05	101 (20%)	1 1	37, 67, 131, 211	0
1	B	513/538 (95%)	0.95	87 (16%)	1 1	37, 66, 130, 184	0
1	C	501/538 (93%)	0.80	74 (14%)	2 2	36, 65, 124, 184	0
All	All	1513/1614 (93%)	0.93	262 (17%)	1 1	36, 66, 128, 211	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1127	ALA	14.6
1	B	1501	PHE	11.6
1	C	1128	SER	11.5
1	B	1064	ILE	10.1
1	A	1126	ASP	9.0
1	A	1198	CYS	8.8
1	C	1501	PHE	8.4
1	C	1071	ILE	7.5
1	B	1502	GLY	7.4
1	C	1191	HIS	7.3
1	A	1096	ARG	7.1
1	B	1500	GLU	7.1
1	B	1069	GLY	7.1
1	B	1503	THR	7.0
1	A	1340	ILE	6.8
1	C	1204	GLY	6.7
1	B	1061	SER	6.7
1	C	1076	THR	6.7
1	B	1127	ALA	6.6
1	C	1199	ALA	6.4
1	B	1166	THR	6.3
1	B	1065	GLU	6.3
1	B	1126	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	1061	SER	6.0
1	A	1338	HIS	6.0
1	B	1504	ASP	5.9
1	B	1287	GLU	5.8
1	C	1064	ILE	5.8
1	C	1192	ARG	5.8
1	B	1060	THR	5.8
1	A	1341	GLU	5.6
1	C	1241	SER	5.6
1	B	1124	VAL	5.6
1	B	1570	GLY	5.4
1	C	1127	ALA	5.4
1	B	1125	GLU	5.3
1	B	1167	GLY	5.2
1	A	1199	ALA	5.1
1	A	1064	ILE	5.1
1	A	1097	GLY	5.0
1	A	1128	SER	5.0
1	B	1077	TYR	5.0
1	A	1099	LYS	4.9
1	A	1270	ILE	4.9
1	B	1499	LEU	4.9
1	B	1123	GLY	4.9
1	A	1342	PRO	4.7
1	A	1501	PHE	4.7
1	A	1060	THR	4.7
1	A	1362	MET	4.7
1	B	1198	CYS	4.6
1	A	1191	HIS	4.6
1	A	1201	VAL	4.6
1	A	1197	ALA	4.6
1	C	1077	TYR	4.6
1	A	1093	VAL	4.5
1	A	1124	VAL	4.4
1	B	1096	ARG	4.4
1	B	1165	CYS	4.4
1	C	1193	CYS	4.3
1	B	1444	GLY	4.3
1	B	1101	LEU	4.3
1	C	1124	VAL	4.3
1	A	1343	HIS	4.3
1	A	1443	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1129	GLU	4.2
1	B	1070	ALA	4.2
1	B	1241	SER	4.2
1	B	1129	GLU	4.1
1	A	1535	ASP	4.1
1	B	1270	ILE	4.1
1	A	1165	CYS	4.1
1	C	1129	GLU	4.1
1	A	1503	THR	4.0
1	A	1226	VAL	4.0
1	B	1128	SER	4.0
1	A	1542	THR	4.0
1	C	1564	LEU	4.0
1	B	1068	TRP	4.0
1	B	1343	HIS	4.0
1	B	1191	HIS	3.9
1	A	1554	HIS	3.9
1	C	1198	CYS	3.9
1	C	1270	ILE	3.9
1	C	1123	GLY	3.9
1	A	1196	THR	3.8
1	A	1528	CYS	3.8
1	C	1196	THR	3.8
1	C	1365	TRP	3.8
1	B	1239	LEU	3.8
1	A	1168	ASP	3.8
1	B	1569	ALA	3.7
1	A	1130	SER	3.7
1	B	1196	THR	3.7
1	A	1098	ASN	3.6
1	A	1194	ASN	3.6
1	B	1340	ILE	3.6
1	A	1336	LEU	3.6
1	A	1271	GLN	3.6
1	A	1200	GLY	3.6
1	C	1366	PRO	3.5
1	C	1098	ASN	3.5
1	A	1531	CYS	3.4
1	C	1342	PRO	3.4
1	A	1228	TYR	3.4
1	B	1505	SER	3.4
1	C	1362	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1239	LEU	3.3
1	C	1563	ASN	3.3
1	C	1195	PRO	3.3
1	A	1076	THR	3.3
1	A	1471	ASP	3.3
1	A	1439	LYS	3.3
1	C	1499	LEU	3.3
1	B	1432	ASP	3.2
1	A	1421	ALA	3.2
1	B	1528	CYS	3.2
1	B	1122	LEU	3.2
1	C	1336	LEU	3.2
1	C	1165	CYS	3.2
1	A	1541	ASN	3.2
1	C	1226	VAL	3.1
1	C	1271	GLN	3.1
1	B	1257	LEU	3.1
1	A	1561	LYS	3.1
1	A	1186	PRO	3.1
1	C	1075	SER	3.1
1	C	1363	GLY	3.0
1	A	1112	LEU	3.0
1	A	1190	ASN	3.0
1	A	1337	ILE	3.0
1	A	1092	SER	3.0
1	A	1498	LYS	3.0
1	C	1068	TRP	3.0
1	B	1228	TYR	3.0
1	A	1273	LYS	3.0
1	B	1063	SER	3.0
1	B	1240	THR	3.0
1	A	1193	CYS	3.0
1	A	1125	GLU	3.0
1	C	1130	SER	2.9
1	C	1132	LEU	2.9
1	C	1529	LYS	2.9
1	A	1424	ILE	2.9
1	B	1095	HIS	2.9
1	B	1132	LEU	2.9
1	B	1337	ILE	2.9
1	A	1062	LEU	2.9
1	B	1531	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1448	ALA	2.8
1	A	1063	SER	2.8
1	A	1516	THR	2.8
1	A	1363	GLY	2.8
1	A	1071	ILE	2.8
1	B	1447	PHE	2.8
1	A	1367	SER	2.8
1	B	1471	ASP	2.8
1	C	1278	ILE	2.8
1	B	1078	LYS	2.8
1	A	1202	GLY	2.8
1	C	1304	VAL	2.8
1	A	1276	PRO	2.8
1	C	1417	PRO	2.8
1	A	1077	TYR	2.8
1	B	1243	GLU	2.7
1	C	1070	ALA	2.7
1	C	1125	GLU	2.7
1	B	1571	TRP	2.7
1	C	1069	GLY	2.6
1	A	1241	SER	2.6
1	A	1420	GLY	2.6
1	A	1534	GLU	2.6
1	B	1342	PRO	2.6
1	A	1274	LEU	2.6
1	B	1421	ALA	2.6
1	B	1341	GLU	2.6
1	C	1163	ALA	2.5
1	C	1205	CYS	2.5
1	B	1130	SER	2.5
1	B	1254	ARG	2.5
1	A	1229	ILE	2.5
1	C	1474	ASP	2.5
1	A	1472	GLU	2.5
1	A	1192	ARG	2.5
1	A	1278	ILE	2.5
1	A	1422	GLY	2.5
1	C	1391	TYR	2.5
1	A	1203	THR	2.5
1	B	1470	VAL	2.4
1	A	1185	TRP	2.4
1	A	1469	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1559	ILE	2.4
1	C	1087	ALA	2.4
1	A	1304	VAL	2.4
1	A	1365	TRP	2.4
1	C	1361	ASN	2.4
1	A	1144	TYR	2.4
1	B	1304	VAL	2.4
1	C	1126	ASP	2.4
1	A	1164	THR	2.4
1	A	1275	PRO	2.4
1	C	1421	ALA	2.4
1	A	1446	LYS	2.4
1	B	1425	THR	2.4
1	C	1096	ARG	2.4
1	B	1109	ILE	2.4
1	B	1469	HIS	2.3
1	C	1131	LYS	2.3
1	B	1099	LYS	2.3
1	A	1094	GLU	2.3
1	B	1273	LYS	2.3
1	C	1560	GLY	2.3
1	B	1449	SER	2.3
1	A	1264	LEU	2.3
1	C	1273	LYS	2.3
1	C	1274	LEU	2.2
1	C	1197	ALA	2.2
1	B	1231	THR	2.2
1	C	1166	THR	2.2
1	C	1337	ILE	2.2
1	B	1242	GLN	2.2
1	B	1100	ILE	2.2
1	B	1424	ILE	2.2
1	C	1516	THR	2.2
1	A	1499	LEU	2.2
1	C	1528	CYS	2.2
1	C	1061	SER	2.2
1	C	1272	GLN	2.2
1	A	1423	GLU	2.2
1	A	1109	ILE	2.2
1	B	1229	ILE	2.2
1	B	1420	GLY	2.2
1	A	1432	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1269	ASN	2.2
1	B	1433	MET	2.2
1	B	1204	GLY	2.2
1	B	1442	ILE	2.1
1	C	1109	ILE	2.1
1	A	1394	ASN	2.1
1	B	1097	GLY	2.1
1	A	1272	GLN	2.1
1	A	1243	GLU	2.1
1	C	1541	ASN	2.1
1	C	1257	LEU	2.1
1	B	1199	ALA	2.1
1	C	1190	ASN	2.1
1	C	1097	GLY	2.1
1	A	1466	VAL	2.1
1	B	1098	ASN	2.1
1	B	1226	VAL	2.1
1	B	1276	PRO	2.1
1	B	1197	ALA	2.1
1	A	1395	PHE	2.1
1	C	1242	GLN	2.1
1	A	1339	LYS	2.1
1	C	1228	TYR	2.1
1	C	1502	GLY	2.1
1	A	1163	ALA	2.0
1	A	1500	GLU	2.0
1	B	1534	GLU	2.0
1	B	1066	ALA	2.0
1	B	1422	GLY	2.0

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

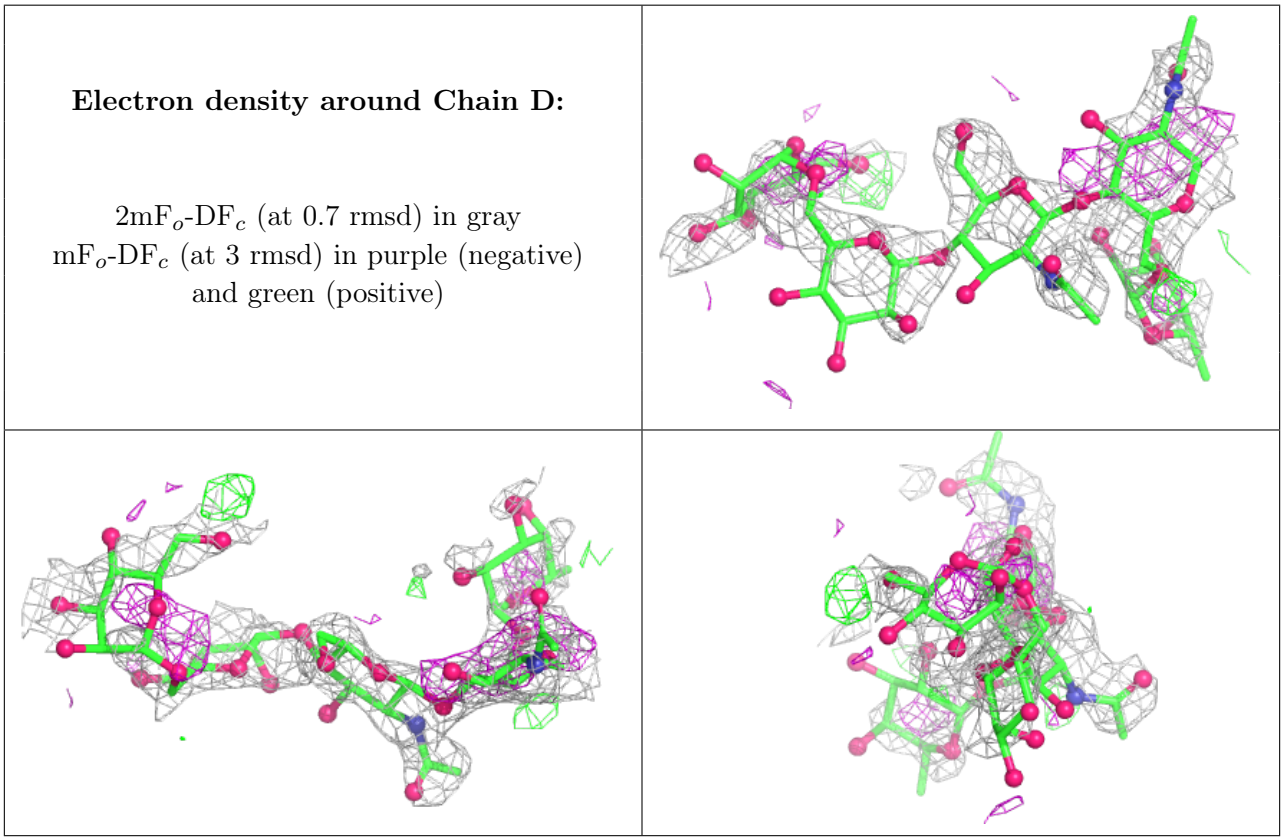
There are no non-standard protein/DNA/RNA residues in this entry.

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	MAN	D	4	11/12	0.46	0.57	131,148,154,154	0
2	FUC	D	5	10/11	0.52	0.44	136,139,142,144	0
2	NAG	D	2	14/15	0.65	0.36	111,125,136,144	0
2	BMA	D	3	11/12	0.68	0.49	150,154,157,158	0
2	NAG	D	1	14/15	0.78	0.40	72,101,116,128	0

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
3	NAG	B	1601	14/15	0.15	0.58	106,120,124,125	0
3	NAG	A	1601	14/15	0.35	0.81	117,135,139,140	0
4	CL	C	1601	1/1	0.82	0.23	94,94,94,94	0
4	CL	C	1602	1/1	0.89	0.11	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	1604	1/1	0.90	0.29	84,84,84,84	0
4	CL	B	1602	1/1	0.92	0.09	94,94,94,94	0
5	PO4	A	1605	5/5	0.93	0.12	111,112,116,116	0
4	CL	A	1603	1/1	0.97	0.16	49,49,49,49	0
4	CL	A	1602	1/1	0.99	0.26	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.