

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6RU5
Title	:	human complement C3 in complex with the hC3Nb1 nanobody
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Deposited on	:	2019-05-27
Resolution	:	3.90 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	:	1.8.4, 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 3.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	$1002 \ (4.14-3.66)$
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)

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%

Mol	Chain	Length	Quality of chain		
1	А	645	83%	17%	_
2	В	992	84%	14%	•
3	С	130	87%	10%	·
4	D	5	100%		

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	MAN	D	4	Х	-	-	-
4	MAN	D	5	Х	-	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13882 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 Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	643	Total 4991	C 3177	N 848	0 951	S 15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	435	GLN	GLU	conflict	UNP P01024

• Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	980	Total 7847	C 4961	N 1335	O 1504	S 47	0	0	0

• Molecule 3 is a protein called hC3Nb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	126	Total 969	C 603	N 176	O 185	${ m S}{ m 5}$	0	0	0

• Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total 61	C 34	N 2	O 25	0	0	0



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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	А	1	Total 14	C 8	N 1	O 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. 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. 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: Complement C3

• Molecule 3: hC3Nb1



•

10%

Chain C:

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

Chain D: 100%

87%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	228.32Å 140.72Å 95.43Å	Deperitor
a, b, c, α , β , γ	90.00° 100.51° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	48.25 - 3.90	Depositor
Resolution (A)	48.25 - 3.43	EDS
% Data completeness	99.6 (48.25-3.90)	Depositor
(in resolution range)	70.6 (48.25-3.43)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	-0.17 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
P. P.	(Not available) , (Not available)	Depositor
Λ, Λ_{free}	0.266 , 0.283	DCC
R_{free} test set	1650 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	109.1	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 91.7	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13882	wwPDB-VP
Average B, all atoms $(Å^2)$	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, BMA

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

Mal	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/5092	0.49	0/6923	
2	В	0.28	0/8000	0.47	0/10816	
3	С	0.30	0/992	0.51	0/1341	
All	All	0.28	0/14084	0.48	0/19080	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	А	4991	0	5038	74	0
2	В	7847	0	7776	88	0
3	С	969	0	918	6	0
4	D	61	0	52	0	0
5	А	14	0	13	0	0
All	All	13882	0	13797	164	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 6.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash	
	Atom-2	distance (Å)	overlap (Å)	
1:A:563:LEU:HA	1:A:586:GLU:O	1.76	0.86	
1:A:29:ILE:HG22	1:A:646:PHE:HA	1.58	0.83	
1:A:594:VAL:HG12	2:B:775:VAL:HG12	1.64	0.79	
1:A:97:LYS:HD2	1:A:102:ARG:HD2	1.65	0.76	
1:A:563:LEU:HD13	2:B:808:SER:HB3	1.68	0.75	
2:B:1303:ARG:HH11	2:B:1307:ILE:HG13	1.50	0.75	
2:B:717:GLY:HA3	2:B:720:CYS:HB2	1.66	0.75	
2:B:1501:LYS:HE2	2:B:1588:ILE:HD11	1.69	0.74	
2:B:1136:ASN:HB2	2:B:1139:LYS:HE3	1.70	0.74	
2:B:1583:THR:H	2:B:1618:LEU:HB3	1.54	0.72	
2:B:937:ARG:NH2	2:B:1347:MET:SD	2.62	0.72	
2:B:1190:ALA:HA	2:B:1210:PHE:HE1	1.56	0.71	
2:B:1520:ILE:HD12	2:B:1627:TRP:HA	1.74	0.70	
3:C:98:ALA:HB3	3:C:112:TYR:HB2	1.75	0.68	
2:B:932:VAL:HG11	2:B:1440:ASP:HA	1.77	0.67	
2:B:1004:ILE:HG22	2:B:1006:THR:H	1.60	0.67	
1:A:59:VAL:HG12	1:A:108:VAL:HG12	1.78	0.66	
1:A:496:ASN:ND2	1:A:524:ASP:O	2.30	0.65	
2:B:996:ASP:OD2	2:B:999:ARG:NH1	2.30	0.64	
2:B:728:CYS:SG	2:B:729:ASN:N	2.73	0.62	
2:B:1126:HIS:H	2:B:1129:MET:HE3	1.65	0.62	
2:B:1360:LYS:HG3	2:B:1487:GLU:HG2	1.82	0.62	
1:A:368:MET:SD	1:A:455:TYR:HB2	2.40	0.61	
1:A:232:PHE:HB3	1:A:259:PHE:HD1	1.66	0.60	
2:B:1015:MET:HG3	2:B:1081:TYR:HE2	1.67	0.60	
2:B:994:ALA:HA	2:B:1000:LEU:HD13	1.83	0.60	
1:A:291:ILE:HD13	1:A:300:VAL:HB	1.84	0.59	
1:A:606:ASN:HD21	1:A:610:LYS:HG2	1.68	0.58	
2:B:1356:LEU:HG	2:B:1357:THR:HG23	1.85	0.58	
2:B:1470:GLU:HG2	2:B:1504:LYS:HE3	1.84	0.58	
1:A:42:MET:HB3	1:A:86:VAL:HG23	1.86	0.58	
1:A:493:LEU:HD23	1:A:500:LEU:HD11	1.85	0.58	
2:B:1013:GLN:HG2	2:B:1482:TYR:CZ	2.38	0.57	
2:B:1417:ASP:O	2:B:1421:LEU:HG	2.05	0.57	
2:B:1604:MET:HA	2:B:1627:TRP:O	2.04	0.57	
1:A:29:ILE:HA	1:A:645:THR:O	2.05	0.57	
1:A:522:THR:HG23	1:A:524:ASP:H	1.70	0.57	
2:B:1548:ARG:HH21	2:B:1550:VAL:HG22	1.70	0.56	
1:A:29:ILE:CG2	1:A:646:PHE:HD1	2.18	0.56	
2:B:679:ARG:NH2	2:B:754:ASP:OD1	2.34	0.56	
2:B:699:ARG:NH2	2:B:758:GLU:OE1	2.38	0.56	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:127:SER:O	1:A:161:ARG:NH1	2.35	0.56
2:B:981:LEU:HB3	2:B:1343:SER:HB2	1.86	0.55
2:B:1130:ILE:O	2:B:1139:LYS:HE2	2.06	0.55
2:B:1004:ILE:HD13	2:B:1269:THR:HG22	1.88	0.55
2:B:844:GLN:HB2	2:B:1470:GLU:HB2	1.88	0.55
2:B:1097:SER:O	2:B:1101:CYS:HB2	2.06	0.55
2:B:957:VAL:HG11	2:B:1335:GLU:HG3	1.89	0.54
1:A:271:VAL:HG11	1:A:300:VAL:HG11	1.89	0.54
1:A:41:THR:HB	1:A:500:LEU:HB3	1.90	0.52
3:C:47:PHE:HE1	3:C:50:THR:HG1	1.57	0.52
1:A:77:THR:HG22	1:A:79:ALA:H	1.74	0.52
2:B:760:ASN:O	2:B:760:ASN:ND2	2.43	0.52
1:A:148:ARG:HG2	1:A:190:PRO:HA	1.91	0.51
1:A:156:LEU:HD11	1:A:620:VAL:HG21	1.93	0.51
1:A:267:GLY:HA2	1:A:333:HIS:CG	2.45	0.51
1:A:517:LEU:HD12	1:A:518:PRO:HD2	1.93	0.51
2:B:1371:PRO:HG2	2:B:1374:GLU:HB2	1.91	0.51
1:A:94:ARG:NH1	1:A:98:SER:O	2.44	0.51
2:B:831:ILE:HG23	2:B:925:VAL:HG23	1.94	0.50
1:A:354:GLN:HB2	1:A:377:THR:HG23	1.94	0.50
1:A:454:ASN:ND2	1:A:545:GLU:OE1	2.45	0.50
3:C:30:SER:HA	3:C:53:ARG:HH21	1.76	0.50
2:B:1501:LYS:HD3	2:B:1591:ARG:HH21	1.77	0.50
1:A:315:ARG:HD2	1:A:318:ASP:HB2	1.94	0.50
2:B:1281:GLN:O	2:B:1284:LYS:HG3	2.12	0.50
1:A:29:ILE:HD11	1:A:493:LEU:HD22	1.94	0.49
3:C:99:GLY:HA2	3:C:110:TYR:HA	1.94	0.49
2:B:1007:PRO:HG3	2:B:1445:ILE:HG12	1.93	0.49
1:A:592:ARG:HG2	2:B:777:ASP:HB3	1.94	0.48
2:B:863:ARG:NH1	2:B:883:GLN:OE1	2.46	0.48
1:A:389:VAL:HA	1:A:426:THR:HA	1.96	0.48
2:B:679:ARG:HE	2:B:698:MET:HB3	1.78	0.48
1:A:236:VAL:HG21	1:A:328:ALA:HB3	1.96	0.47
2:B:969:ASP:OD1	2:B:969:ASP:N	2.46	0.47
1:A:186:LEU:HD12	1:A:592:ARG:HG3	1.96	0.47
2:B:1554:LEU:HB2	2:B:1591:ARG:NH1	2.29	0.47
1:A:566:LYS:HD2	1:A:584:LYS:HD2	1.96	0.47
1:A:44:LEU:HD11	1:A:55:VAL:HG11	1.96	0.47
2:B:962:ILE:HG21	2:B:1344:VAL:HG21	1.96	0.47
2:B:1228:TYR:CE1	2:B:1484:ASN:HB2	2.49	0.47
2:B:1332:VAL:HG21	2:B:1342:LEU:HD21	1.97	0.47

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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:160:GLY:HA3	1:A:183:GLN:HA	1.97	0.47
2:B:1616:PRO:O	2:B:1618:LEU:N	2.44	0.47
2:B:712:ARG:NH2	2:B:1455:GLU:OE2	2.48	0.46
2:B:1494:HIS:ND1	2:B:1495:PRO:HD2	2.30	0.46
1:A:104:LYS:NZ	1:A:125:LEU:HD23	2.30	0.46
1:A:647:THR:HG23	1:A:653:GLN:HB3	1.96	0.46
2:B:1013:GLN:O	2:B:1016:ILE:HG13	2.15	0.46
1:A:281:ARG:HD3	1:A:325:TYR:CE1	2.51	0.46
2:B:703:MET:HE3	2:B:1421:LEU:HD22	1.96	0.46
2:B:717:GLY:CA	2:B:720:CYS:HB2	2.41	0.46
2:B:1037:PHE:CE2	2:B:1041:LYS:HD2	2.51	0.46
1:A:29:ILE:CD1	1:A:493:LEU:HD22	2.46	0.46
1:A:170:PRO:HD3	1:A:204:TRP:CD1	2.51	0.46
2:B:714:ILE:HG21	2:B:721:LYS:HG2	1.98	0.46
1:A:340:GLN:HE21	2:B:761:ILE:HB	1.80	0.46
2:B:703:MET:O	2:B:705:PHE:N	2.49	0.46
2:B:869:ASN:HB3	2:B:872:PHE:CE2	2.51	0.46
2:B:933:PRO:HG2	2:B:1349:HIS:NE2	2.31	0.45
1:A:28:ILE:HD11	1:A:42:MET:SD	2.57	0.45
1:A:636:ALA:HB1	1:A:654:THR:HG22	1.99	0.45
2:B:1529:LEU:O	2:B:1533:LEU:HG	2.17	0.45
2:B:1300:LEU:HD12	2:B:1303:ARG:HD2	1.99	0.45
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.47	0.45
1:A:238:PRO:HA	1:A:253:VAL:HA	1.99	0.44
2:B:1199:MET:HB2	2:B:1199:MET:HE3	1.87	0.44
2:B:1506:CYS:HA	2:B:1511:CYS:HB2	1.99	0.44
1:A:365:LYS:HE3	1:A:456:LEU:O	2.17	0.44
1:A:465:LEU:HD12	1:A:555:VAL:HG13	1.98	0.44
2:B:725:LEU:HA	2:B:728:CYS:SG	2.57	0.44
2:B:831:ILE:HG22	2:B:923:ASP:OD2	2.17	0.44
1:A:29:ILE:HG22	1:A:646:PHE:CA	2.39	0.44
1:A:402:GLN:HG2	1:A:403:GLY:H	1.83	0.44
1:A:45:GLU:OE1	1:A:47:HIS:NE2	2.50	0.43
1:A:206:ILE:O	1:A:219:SER:HA	2.18	0.43
2:B:1145:ALA:HA	2:B:1176:LEU:HD11	2.00	0.43
1:A:193:TRP:CZ3	1:A:195:ILE:HG12	2.53	0.43
2:B:717:GLY:O	2:B:721:LYS:HG3	2.18	0.43
2:B:1225:LYS:HB3	2:B:1228:TYR:CD1	2.54	0.43
3:C:91:THR:HG23	3:C:120:THR:HA	2.01	0.43
1:A:497:LYS:HE3	1:A:526:ILE:O	2.18	0.43
2:B:1615:LYS:HA	2:B:1616:PRO:C	2.38	0.43

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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:52:ASP:HB3	1:A:77:THR:HA	2.01	0.43
1:A:124:SER:HB2	1:A:660:LEU:HD11	2.00	0.43
1:A:368:MET:HG3	1:A:478:ARG:HE	1.84	0.43
1:A:456:LEU:HD23	1:A:547:VAL:HG12	2.00	0.43
1:A:596:VAL:O	1:A:596:VAL:HG13	2.18	0.43
1:A:108:VAL:O	1:A:118:GLU:HA	2.18	0.43
1:A:475:PHE:HB2	1:A:515:VAL:O	2.19	0.42
2:B:1501:LYS:HD3	2:B:1591:ARG:NH2	2.34	0.42
2:B:1551:LYS:HB3	2:B:1562:ILE:HD12	2.01	0.42
1:A:232:PHE:HB3	1:A:259:PHE:CD1	2.51	0.42
1:A:281:ARG:HD3	1:A:325:TYR:CZ	2.54	0.42
1:A:133:GLN:HB2	1:A:611:LEU:HD22	2.02	0.42
2:B:1538:GLU:HB2	2:B:1541:VAL:HG23	2.02	0.42
2:B:1206:LEU:H	2:B:1206:LEU:HD12	1.85	0.42
1:A:267:GLY:HA2	1:A:333:HIS:CD2	2.54	0.42
2:B:710:ARG:NH2	2:B:728:CYS:HB2	2.35	0.42
1:A:255:ILE:HG13	1:A:291:ILE:HD11	2.02	0.42
2:B:1553:GLN:HG3	2:B:1560:GLU:HB2	2.02	0.41
1:A:45:GLU:OE2	1:A:491:THR:HG21	2.20	0.41
1:A:169:ASN:HB2	1:A:170:PRO:HD2	2.02	0.41
2:B:1008:SER:HA	2:B:1013:GLN:HB3	2.02	0.41
1:A:105:PHE:CD2	1:A:122:LEU:HA	2.55	0.41
2:B:1498:GLU:H	2:B:1498:GLU:CD	2.21	0.41
2:B:1072:ARG:HG3	2:B:1427:ARG:HH12	1.84	0.41
2:B:1604:MET:HE3	2:B:1628:VAL:HG22	2.02	0.41
2:B:845:VAL:HG12	2:B:1469:VAL:HG22	2.02	0.41
2:B:1504:LYS:HD3	2:B:1504:LYS:HA	1.83	0.41
2:B:1549:LEU:HD23	2:B:1597:GLU:O	2.21	0.41
1:A:59:VAL:HG22	1:A:69:LEU:HB3	2.02	0.41
1:A:433:GLU:HG2	1:A:436:GLN:NE2	2.35	0.41
2:B:957:VAL:HG11	2:B:1335:GLU:HA	2.03	0.41
2:B:1582:ARG:HA	2:B:1618:LEU:HG	2.02	0.41
1:A:372:LEU:O	1:A:408:LYS:HA	2.21	0.41
2:B:1237:LEU:HD11	2:B:1249:VAL:HG13	2.02	0.41
2:B:1523:SER:O	2:B:1526:LYS:N	2.48	0.40
2:B:1546:LYS:HD3	2:B:1567:GLN:HG2	2.02	0.40
3:C:6:GLU:OE1	3:C:116:GLY:N	2.54	0.40
1:A:30:THR:OG1	1:A:31:PRO:HD2	2.22	0.40
2:B:1303:ARG:NH2	2:B:1322:GLU:OE2	2.53	0.40
2:B:1574:ASP:OD1	2:B:1574:ASP:N	2.52	0.40
1:A:29:ILE:HD11	1:A:493:LEU:CD2	2.52	0.40

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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	Analysed Favoured Allowed		Outliers	Perce	entiles
1	А	641/645~(99%)	596~(93%)	45 (7%)	0	100	100
2	В	976/992~(98%)	905~(93%)	71 (7%)	0	100	100
3	С	124/130~(95%)	115 (93%)	9 (7%)	0	100	100
All	All	1741/1767~(98%)	1616 (93%)	125 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	\mathbf{s}
1	А	561/567~(99%)	560 (100%)	1 (0%)	93 96	
2	В	870/879~(99%)	858~(99%)	12 (1%)	67 81	
3	С	100/104~(96%)	99~(99%)	1 (1%)	76 86	
All	All	1531/1550~(99%)	1517 (99%)	14 (1%)	78 87	

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	455	TYR
2	В	917	TYR



Mol	Chain	Res	Type
2	В	1219	ARG
2	В	1276	PHE
2	В	1325	LYS
2	В	1361	PHE
2	В	1434	LEU
2	В	1441	ARG
2	В	1450	LYS
2	В	1518	CYS
2	В	1520	ILE
2	В	1588	ILE
2	В	1590	CYS
3	С	11	LEU

Continued from previous page...

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 monosaccharides are modelled in this entry.

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

Mal Turna Chain Bag		Tink	Bond lengths			Bond angles				
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	1	2,4	14,14,15	0.90	0	17,19,21	1.20	1 (5%)
4	NAG	D	2	4	14,14,15	0.76	0	17,19,21	2.12	7 (41%)
4	BMA	D	3	4	11,11,12	0.56	0	15,15,17	1.34	3 (20%)



Mal	Mol Type Chain Bog		in Res Link		Bo	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	MAN	D	4	4	11,11,12	0.47	0	$15,\!15,\!17$	1.06	2 (13%)	
4	MAN	D	5	4	11,11,12	0.37	0	$15,\!15,\!17$	1.13	2 (13%)	

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

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

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	2	NAG	C2-N2-C7	-4.85	115.99	122.90
4	D	2	NAG	O3-C3-C2	-3.39	102.45	109.47
4	D	2	NAG	C4-C3-C2	-3.36	106.10	111.02
4	D	1	NAG	O4-C4-C3	-2.88	103.68	110.35
4	D	3	BMA	O3-C3-C4	2.76	116.74	110.35
4	D	3	BMA	O4-C4-C5	-2.65	102.72	109.30
4	D	4	MAN	C2-C3-C4	-2.62	106.35	110.89
4	D	5	MAN	C2-C3-C4	-2.34	106.84	110.89
4	D	2	NAG	O3-C3-C4	2.33	115.73	110.35
4	D	2	NAG	O4-C4-C5	-2.27	103.65	109.30
4	D	5	MAN	O2-C2-C3	-2.27	105.59	110.14
4	D	2	NAG	C1-O5-C5	-2.13	109.31	112.19
4	D	3	BMA	C1-C2-C3	-2.09	107.09	109.67
4	D	2	NAG	C3-C4-C5	-2.06	106.56	110.24
4	D	4	MAN	O2-C2-C3	-2.01	106.11	110.14

All (15) bond angle outliers are listed below:

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	4	MAN	C1
4	D	5	MAN	C1



Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	BMA	O5-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	5	MAN	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6

All (11) torsion outliers are listed below:

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.





5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	NAG	А	2000	1	14,14,15	0.40	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	А	2000	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

