



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 02:16 AM EDT

PDB ID : 7L7R  
Title : CCHFV Gc prefusion monomer bound to ADI-36121 and ADI-37801 Fabs  
Authors : Mishra, A.K.; McLellan, J.S.  
Deposited on : 2020-12-30  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

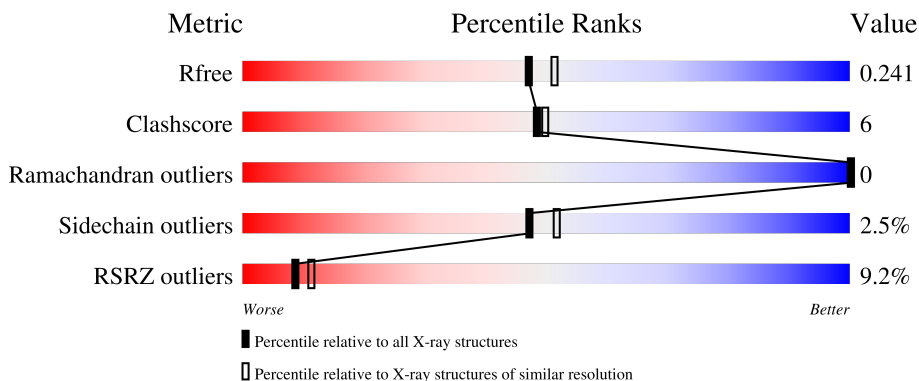
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	214	91% (green), 8% (yellow)
2	B	230	88% (green), 6% (yellow), 7% (grey)
3	C	214	25% (red), 73% (green), 21% (yellow), .. (grey)
4	D	235	7% (red), 73% (green), 15% (yellow), 11% (grey)
5	G	547	7% (red), 55% (green), 12% (yellow), 33% (grey)

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Mol	Chain	Length	Quality of chain
6	N	3	 67% 33%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9730 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 ADI-36121 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	1639	1024	276	334	5	0	0	0

- Molecule 2 is a protein called ADI-36121 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	215	1623	1031	269	317	6	0	0	0

- Molecule 3 is a protein called ADI-37801 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	205	1581	990	270	317	4	0	0	0

- Molecule 4 is a protein called ADI-37801 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	209	1579	1004	256	311	8	0	0	0

- Molecule 5 is a protein called Glycoprotein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	G	365	2873	1813	490	545	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

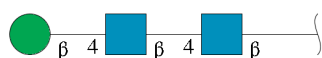
Chain	Residue	Modelled	Actual	Comment	Reference
G	1580	GLY	-	expression tag	UNP Q8JSZ3
G	1581	SER	-	expression tag	UNP Q8JSZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1582	LEU	-	expression tag	UNP Q8JSZ3
G	1583	GLU	-	expression tag	UNP Q8JSZ3
G	1584	VAL	-	expression tag	UNP Q8JSZ3
G	1585	LEU	-	expression tag	UNP Q8JSZ3
G	1586	PHE	-	expression tag	UNP Q8JSZ3
G	1587	GLN	-	expression tag	UNP Q8JSZ3

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
6	N	3	39	22	2	15	0	0	0

- Molecule 7 is water.

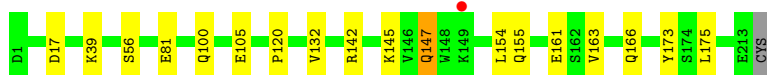
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	109	Total	O	0	0
			109	109		
7	B	119	Total	O	0	0
			119	119		
7	C	11	Total	O	0	0
			11	11		
7	D	35	Total	O	0	0
			35	35		
7	G	122	Total	O	0	0
			122	122		

### 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.

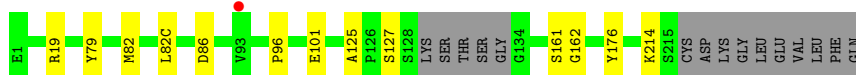
- Molecule 1: ADI-36121 Fab light chain

Chain A:  91% 8%




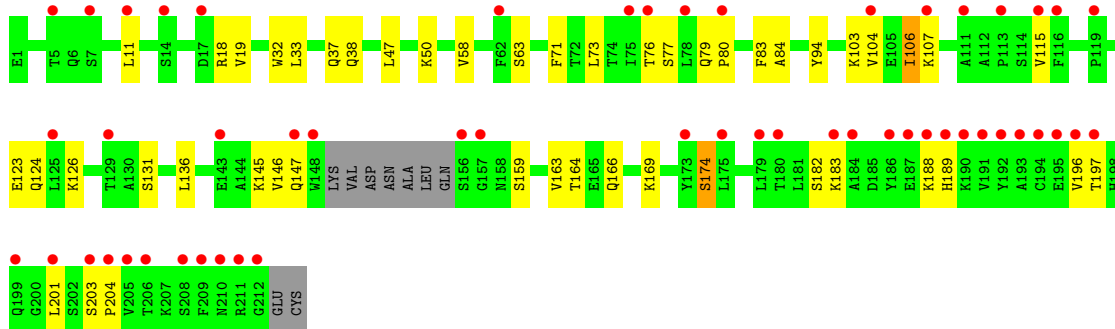
- Molecule 2: ADI-36121 Fab heavy chain

Chain B:  88% 6% 7%




- Molecule 3: ADI-37801 Fab light chain

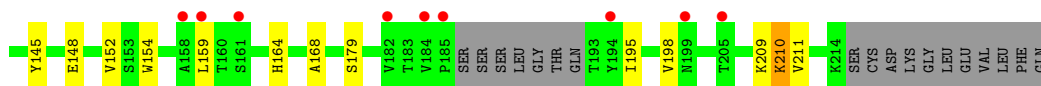
Chain C:  25% 73% 21%



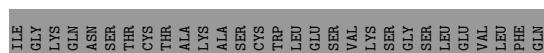
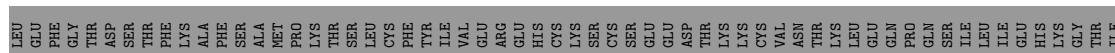
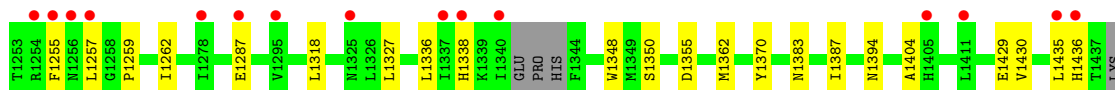
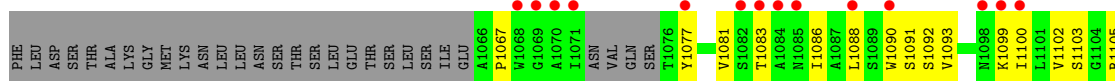
- Molecule 4: ADI-37801 Fab heavy chain

Chain D:  7% 73% 15% 11%





• Molecule 5: Glycoprotein C



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.20Å 95.18Å 323.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.05 – 2.10 43.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.05-2.10) 98.2 (43.05-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19_4080	Depositor
R, $R_{free}$	0.219 , 0.243 0.217 , 0.241	Depositor DCC
$R_{free}$ test set	5453 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtrriage
Anisotropy	0.571	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.



## 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, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/1674	0.56	0/2271
2	B	0.33	0/1663	0.54	0/2266
3	C	0.33	0/1615	0.60	0/2190
4	D	0.37	0/1619	0.61	0/2208
5	G	0.33	0/2946	0.58	0/4006
All	All	0.34	0/9517	0.58	0/12941

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	A	1639	0	1592	10	0
2	B	1623	0	1601	9	0
3	C	1581	0	1545	30	0
4	D	1579	0	1537	24	0
5	G	2873	0	2762	39	0
6	N	39	0	34	0	0
7	A	109	0	0	2	0
7	B	119	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	11	0	0	0	0
7	D	35	0	0	5	0
7	G	122	0	0	3	0
All	All	9730	0	9071	110	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 (110) 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)
4:D:103:TRP:O	7:D:301:HOH:O	1.90	0.88
2:B:86:ASP:OD1	7:B:301:HOH:O	1.93	0.85
5:G:1169:CYS:SG	7:G:1706:HOH:O	2.41	0.78
1:A:161:GLU:OE1	7:A:301:HOH:O	2.01	0.78
2:B:162:GLY:O	7:B:302:HOH:O	2.03	0.76
5:G:1166:THR:O	7:G:1601:HOH:O	2.02	0.76
5:G:1192:ARG:HH11	5:G:1362:MET:HE1	1.52	0.73
2:B:79:TYR:OH	7:B:303:HOH:O	2.06	0.72
5:G:1091:SER:N	5:G:1103:SER:O	2.24	0.70
5:G:1338:HIS:O	5:G:1338:HIS:ND1	2.23	0.70
3:C:123:GLU:HA	3:C:126:LYS:HZ3	1.57	0.68
3:C:18:ARG:HG3	3:C:76:THR:HA	1.74	0.68
4:D:101:ASP:OD2	7:D:302:HOH:O	2.12	0.68
2:B:19:ARG:O	7:B:304:HOH:O	2.13	0.66
3:C:146:VAL:HG12	3:C:196:VAL:HG22	1.75	0.66
4:D:83:THR:HG22	4:D:85:ALA:H	1.60	0.66
1:A:17:ASP:OD1	7:A:302:HOH:O	2.12	0.66
2:B:125:ALA:O	7:B:305:HOH:O	2.15	0.65
3:C:79:GLN:HG3	3:C:80:PRO:HD2	1.79	0.65
5:G:1067:PRO:HD3	5:G:1248:LEU:HD21	1.80	0.64
5:G:1105:ARG:HG2	5:G:1429:GLU:HG2	1.80	0.64
3:C:145:LYS:NZ	3:C:147:GLN:OE1	2.28	0.63
5:G:1135:VAL:HG22	5:G:1237:VAL:HG12	1.80	0.62
5:G:1119:SER:HB3	5:G:1134:THR:HG22	1.82	0.61
4:D:11:LEU:O	7:D:303:HOH:O	2.16	0.60
5:G:1083:THR:HG21	5:G:1118:ILE:HG22	1.85	0.59
3:C:47:LEU:HA	3:C:58:VAL:HG21	1.84	0.58
4:D:35:TYR:HB2	4:D:95:ASP:HB3	1.85	0.58
3:C:164:THR:HG22	3:C:174:SER:H	1.68	0.58
4:D:138:LEU:HB2	4:D:211:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG22	1:A:175:LEU:HD12	1.85	0.58
5:G:1100:ILE:HD12	5:G:1127:ALA:HB2	1.87	0.57
5:G:1255:PHE:HB2	5:G:1262:ILE:HB	1.87	0.57
4:D:123:PRO:HB3	4:D:211:VAL:HG22	1.86	0.56
4:D:138:LEU:HD12	4:D:211:VAL:HB	1.87	0.56
5:G:1153:GLY:HA3	5:G:1216:PHE:HB3	1.88	0.56
5:G:1090:TRP:HZ3	5:G:1430:VAL:HG11	1.70	0.56
5:G:1133:LEU:HD21	5:G:1262:ILE:HD11	1.88	0.55
4:D:123:PRO:CD	4:D:209:LYS:HE2	2.35	0.54
4:D:152:VAL:HG13	4:D:198:VAL:HG22	1.89	0.54
5:G:1215:LEU:HD21	5:G:1336:LEU:HD23	1.89	0.54
2:B:176:TYR:OH	7:B:306:HOH:O	2.17	0.54
4:D:69:ILE:O	7:D:304:HOH:O	2.19	0.54
5:G:1099:LYS:HA	5:G:1436:HIS:HB3	1.90	0.54
2:B:214:LYS:NZ	7:B:310:HOH:O	2.41	0.53
1:A:145:LYS:HE2	1:A:147:GLN:OE1	2.09	0.53
3:C:188:LYS:HE2	3:C:189:HIS:CE1	2.44	0.53
5:G:1090:TRP:CZ3	5:G:1430:VAL:HG11	2.45	0.52
3:C:124:GLN:OE1	3:C:131:SER:N	2.42	0.52
5:G:1327:LEU:HD11	5:G:1404:ALA:HB1	1.92	0.52
3:C:197:THR:HG23	3:C:204:PRO:HG3	1.92	0.51
3:C:11:LEU:HD21	3:C:19:VAL:HG11	1.92	0.51
1:A:39:LYS:NZ	1:A:81:GLU:O	2.39	0.51
5:G:1088:LEU:HG	5:G:1122:LEU:HD22	1.93	0.51
5:G:1348:TRP:CH2	5:G:1350:SER:HB2	2.47	0.50
5:G:1077:TYR:CE1	5:G:1138:MET:HG3	2.47	0.50
4:D:195:ILE:HG12	4:D:210:LYS:CG	2.42	0.49
5:G:1092:SER:O	5:G:1102:VAL:HA	2.13	0.49
3:C:115:VAL:HG22	3:C:136:LEU:HD22	1.93	0.49
1:A:142:ARG:CZ	1:A:163:VAL:HG21	2.43	0.48
3:C:123:GLU:HA	3:C:126:LYS:NZ	2.27	0.48
5:G:1161:PRO:O	5:G:1162:LYS:HG3	2.12	0.48
3:C:201:LEU:HD13	3:C:203:SER:C	2.33	0.48
1:A:166:GLN:HG3	1:A:173:TYR:CZ	2.48	0.48
2:B:82:MET:HE2	2:B:82(C):LEU:HD21	1.96	0.48
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.95	0.48
5:G:1287:GLU:N	7:G:1610:HOH:O	2.47	0.48
3:C:38:GLN:O	3:C:84:ALA:HB1	2.14	0.47
3:C:94:TYR:OH	5:G:1191:TRP:HA	2.15	0.47
5:G:1081:VAL:HG11	5:G:1119:SER:OG	2.15	0.47
3:C:33:LEU:HD13	3:C:71:PHE:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1394:ASN:OD1	5:G:1394:ASN:N	2.44	0.46
4:D:96:ARG:O	4:D:100(C):GLY:HA3	2.15	0.46
5:G:1086:ILE:HD12	5:G:1119:SER:O	2.15	0.46
5:G:1239:LEU:HD23	5:G:1242:GLN:OE1	2.16	0.46
5:G:1383:ASN:O	5:G:1387:ILE:HG12	2.16	0.46
4:D:121:VAL:O	4:D:122:PHE:HD1	1.99	0.46
4:D:121:VAL:C	4:D:122:PHE:HD1	2.19	0.45
5:G:1237:VAL:HG21	5:G:1257:LEU:HD11	1.98	0.44
4:D:8:GLY:HA3	4:D:20:LEU:HD23	1.99	0.44
4:D:148:GLU:OE1	4:D:168:ALA:HB3	2.17	0.44
5:G:1215:LEU:HD22	5:G:1318:LEU:HD21	2.00	0.44
4:D:138:LEU:H	4:D:138:LEU:HD23	1.81	0.44
1:A:120:PRO:HD3	1:A:132:VAL:HG22	2.00	0.44
4:D:154:TRP:HB3	4:D:159:LEU:HD23	1.99	0.43
3:C:163:VAL:HG12	3:C:164:THR:H	1.84	0.43
5:G:1159:GLU:HG3	5:G:1209:GLY:O	2.18	0.43
5:G:1088:LEU:HD22	5:G:1106:SER:HB2	1.99	0.43
3:C:124:GLN:HA	4:D:122:PHE:CE2	2.54	0.43
1:A:100:GLN:H	1:A:100:GLN:CD	2.22	0.42
3:C:32:TRP:CZ3	3:C:50:LYS:HE3	2.54	0.42
2:B:96:PRO:HD3	2:B:101:GLU:HG2	2.01	0.42
4:D:119:PRO:HB3	4:D:145:TYR:HB3	2.01	0.42
3:C:145:LYS:HB3	3:C:145:LYS:HE3	1.52	0.42
3:C:188:LYS:HG2	3:C:189:HIS:CE1	2.54	0.42
5:G:1192:ARG:HA	5:G:1362:MET:HG3	2.02	0.42
3:C:103:LYS:HB2	3:C:103:LYS:HE2	1.88	0.41
3:C:33:LEU:HD13	3:C:71:PHE:CD1	2.55	0.41
3:C:106:ILE:H	3:C:166:GLN:HE22	1.67	0.41
3:C:83:PHE:HA	3:C:104:VAL:HG13	2.02	0.41
3:C:197:THR:HA	3:C:201:LEU:HD21	2.03	0.41
5:G:1093:VAL:HA	5:G:1102:VAL:HG12	2.01	0.41
3:C:79:GLN:HG3	3:C:80:PRO:CD	2.50	0.41
5:G:1242:GLN:OE1	5:G:1257:LEU:HB3	2.21	0.41
5:G:1259:PRO:O	5:G:1430:VAL:HA	2.21	0.41
3:C:63:SER:O	3:C:73:LEU:HD12	2.22	0.40
4:D:87:THR:HG23	4:D:110:THR:HA	2.03	0.40
1:A:154:LEU:HD22	1:A:155:GLN:N	2.36	0.40
4:D:6:GLU:OE1	4:D:91:TYR:HA	2.20	0.40
4:D:96:ARG:HD3	7:D:302:HOH:O	2.21	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	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	B	211/230 (92%)	209 (99%)	2 (1%)	0	100	100
3	C	201/214 (94%)	194 (96%)	7 (4%)	0	100	100
4	D	203/235 (86%)	200 (98%)	3 (2%)	0	100	100
5	G	359/547 (66%)	342 (95%)	17 (5%)	0	100	100
All	All	1185/1440 (82%)	1149 (97%)	36 (3%)	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	
1	A	188/189 (100%)	185 (98%)	3 (2%)	62	69
2	B	184/197 (93%)	182 (99%)	2 (1%)	73	79
3	C	180/188 (96%)	172 (96%)	8 (4%)	28	28
4	D	180/202 (89%)	174 (97%)	6 (3%)	38	40
5	G	324/487 (66%)	317 (98%)	7 (2%)	52	57
All	All	1056/1263 (84%)	1030 (98%)	26 (2%)	47	52

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	105	GLU
1	A	147	GLN
2	B	127	SER
2	B	161	SER
3	C	77	SER
3	C	106	ILE
3	C	107	LYS
3	C	159	SER
3	C	169	LYS
3	C	174	SER
3	C	182	SER
3	C	183	LYS
4	D	30	SER
4	D	35(B)	SER
4	D	116	THR
4	D	164	HIS
4	D	179	SER
4	D	210	LYS
5	G	1107	GLU
5	G	1140	LEU
5	G	1155	ARG
5	G	1230	LYS
5	G	1355	ASP
5	G	1370	TYR
5	G	1435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	166	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

3 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
6	NAG	N	1	6,5	14,14,15	0.37	0	17,19,21	0.59	0
6	NAG	N	2	6	14,14,15	0.23	0	17,19,21	0.57	0
6	BMA	N	3	6	11,11,12	0.59	0	15,15,17	0.98	1 (6%)

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
6	NAG	N	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	1/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	3	BMA	C1-O5-C5	2.59	115.70	112.19

There are no chirality outliers.

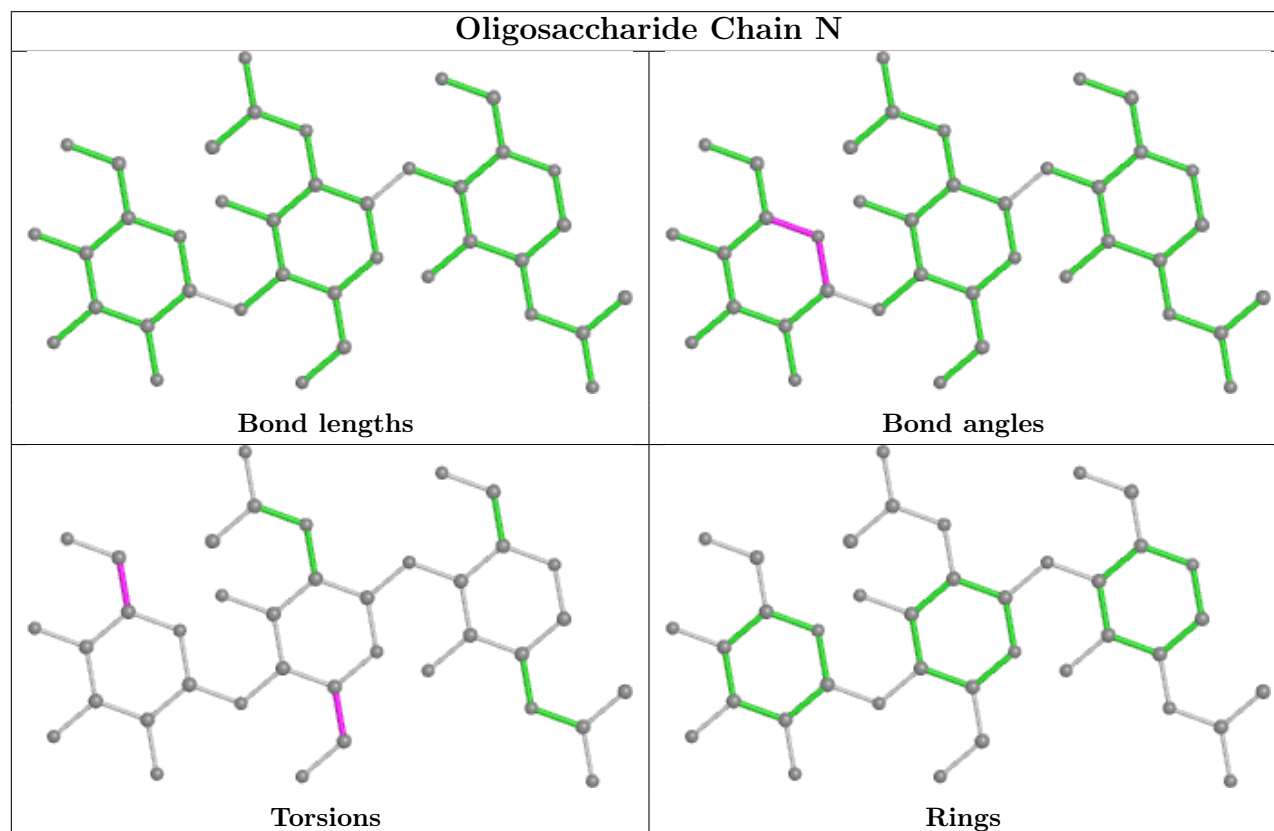
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	3	BMA	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6

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](#)

There are no ligands in this entry.

## 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/214 (99%)	-0.02	1 (0%) 91 92	35, 53, 68, 81	0
2	B	215/230 (93%)	0.06	1 (0%) 91 92	35, 52, 62, 72	0
3	C	205/214 (95%)	1.19	53 (25%) 0 0	43, 111, 144, 167	0
4	D	209/235 (88%)	0.58	16 (7%) 13 17	41, 69, 104, 110	0
5	G	365/547 (66%)	0.71	40 (10%) 5 7	32, 48, 121, 148	0
All	All	1207/1440 (83%)	0.52	111 (9%) 9 11	32, 57, 128, 167	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	209	PHE	8.1
5	G	1071	ILE	7.4
5	G	1070	ALA	7.1
5	G	1129	GLU	6.5
4	D	159	LEU	6.0
5	G	1083	THR	5.9
3	C	148	TRP	5.7
3	C	194	CYS	5.7
3	C	191	VAL	5.4
3	C	193	ALA	5.4
4	D	136	ALA	4.8
3	C	206	THR	4.7
4	D	184	VAL	4.7
5	G	1084	ALA	4.6
5	G	1126	ASP	4.5
3	C	204	PRO	4.5
3	C	208	SER	4.4
3	C	80	PRO	4.4
5	G	1088	LEU	4.3
4	D	137	ALA	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	186	TYR	4.0
5	G	1125	GLU	4.0
5	G	1128	SER	3.9
5	G	1338	HIS	3.9
3	C	195	GLU	3.8
5	G	1340	ILE	3.7
3	C	192	TYR	3.6
3	C	189	HIS	3.6
3	C	116	PHE	3.6
4	D	135	THR	3.5
4	D	185	PRO	3.5
3	C	129	THR	3.4
3	C	7	SER	3.4
3	C	157	GLY	3.4
5	G	1082	SER	3.4
3	C	197	THR	3.4
5	G	1436	HIS	3.3
3	C	183	LYS	3.3
3	C	147	GLN	3.3
5	G	1435	LEU	3.3
3	C	104	VAL	3.3
5	G	1077	TYR	3.3
3	C	76	THR	3.3
3	C	211	ARG	3.3
3	C	107	LYS	3.2
4	D	194	TYR	3.2
5	G	1337	ILE	3.2
5	G	1255	PHE	3.1
5	G	1251	ALA	3.1
4	D	116	THR	3.1
5	G	1257	LEU	3.0
3	C	188	LYS	3.0
5	G	1239	LEU	3.0
5	G	1098	ASN	3.0
3	C	201	LEU	2.9
3	C	199	GLN	2.9
3	C	78	LEU	2.9
3	C	190	LYS	2.9
3	C	203	SER	2.9
5	G	1254	ARG	2.8
3	C	111	ALA	2.8
3	C	173	TYR	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	161	SER	2.8
3	C	210	ASN	2.8
3	C	184	ALA	2.7
3	C	205	VAL	2.6
3	C	17	ASP	2.6
3	C	143	GLU	2.6
3	C	75	ILE	2.6
2	B	93	VAL	2.6
5	G	1069	GLY	2.6
3	C	179	LEU	2.6
5	G	1100	ILE	2.5
3	C	62	PHE	2.5
5	G	1252	GLY	2.5
3	C	14	SER	2.5
3	C	125	LEU	2.4
5	G	1242	GLN	2.4
3	C	196	VAL	2.4
3	C	156	SER	2.4
3	C	11	LEU	2.4
5	G	1411	LEU	2.4
3	C	113	PRO	2.4
3	C	115	VAL	2.4
5	G	1124	VAL	2.3
4	D	1	GLN	2.3
5	G	1068	TRP	2.3
3	C	119	PRO	2.3
5	G	1405	HIS	2.3
4	D	182	VAL	2.3
3	C	212	GLY	2.3
4	D	140	CYS	2.3
5	G	1287	GLU	2.3
5	G	1147	VAL	2.2
5	G	1224	TRP	2.2
5	G	1090	TRP	2.2
3	C	187	GLU	2.2
3	C	5	THR	2.2
3	C	180	THR	2.2
3	C	175	LEU	2.2
5	G	1295	VAL	2.2
4	D	138	LEU	2.1
5	G	1325	ASN	2.1
5	G	1278	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	158	ALA	2.1
4	D	199	ASN	2.1
5	G	1085	ASN	2.1
4	D	205	THR	2.1
1	A	149	LYS	2.1
5	G	1256	ASN	2.0
5	G	1099	LYS	2.0

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

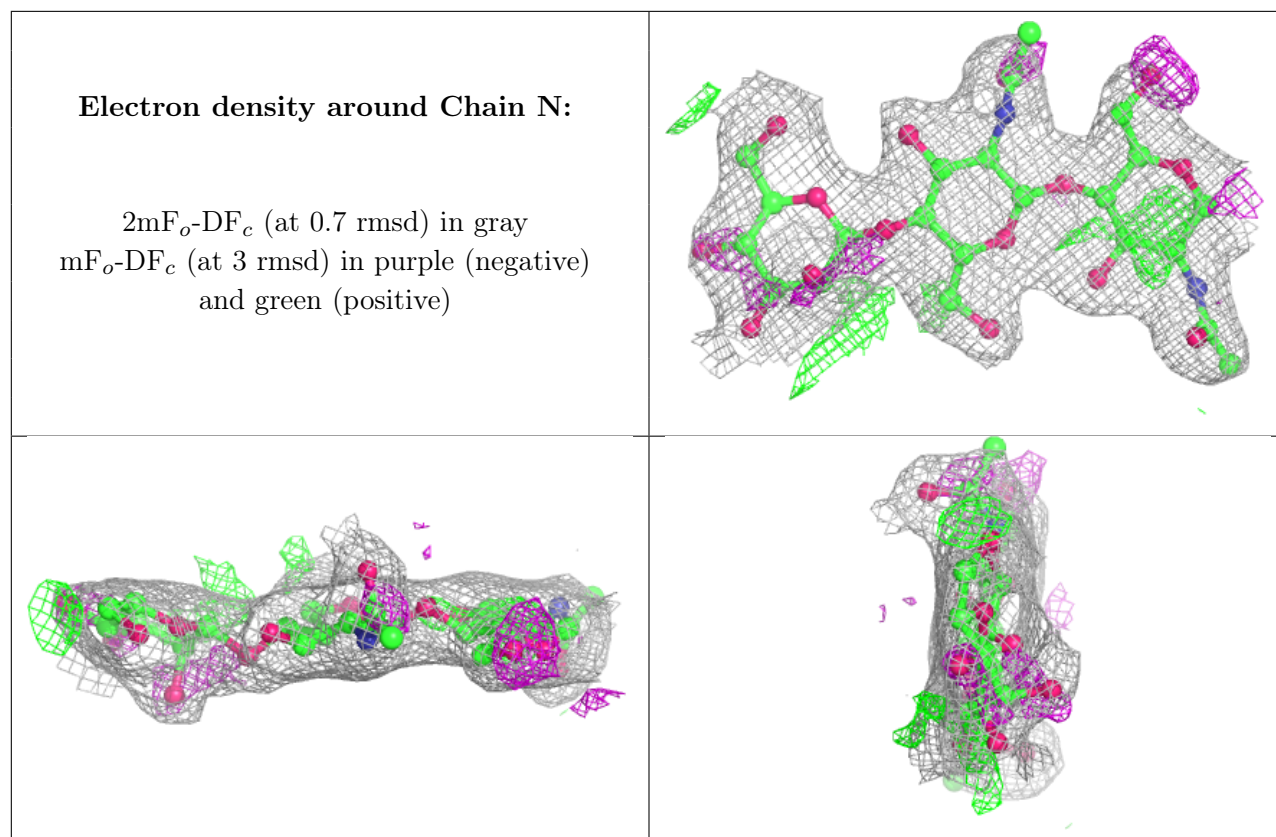
There are no non-standard protein/DNA/RNA residues in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	BMA	N	3	11/12	0.87	0.23	58,59,60,61	0
6	NAG	N	2	14/15	0.88	0.14	51,52,56,58	0
6	NAG	N	1	14/15	0.90	0.16	47,49,51,53	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.