



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:47 AM UTC

PDB ID : 6EHG / pdb_00006ehg
Title : complement component C3b in complex with a nanobody
Authors : Jensen, R.K.; Andersen, K.R.; Gadeberg, T.A.F.; Laursen, N.S.; Andersen, G.R.
Deposited on : 2017-09-13
Resolution : 2.65 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

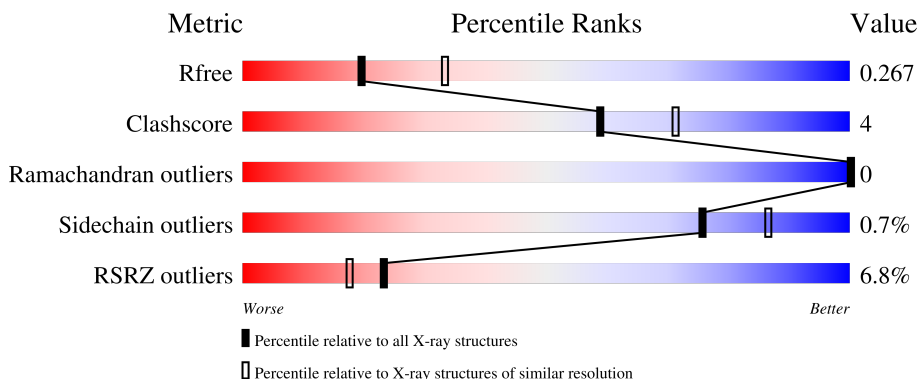
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 $\leq 5\%$. 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	643	3% 88% 11% .
2	B	915	10% 87% 12% .
3	C	130	7% 89% 6% 5%
4	D	3	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13184 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	A	638	Total	C	N	O	S	0	0	0
			4970	3165	843	947	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	GLU	ASP	conflict	UNP P01024
A	431	ILE	LEU	conflict	UNP P01024

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	4	0	0
			7211	4570	1213	1390	38			

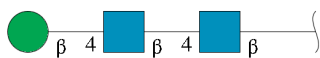
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	conflict	UNP P01024
B	1380	ASN	ALA	conflict	UNP P01024

- Molecule 3 is a protein called hC3Nb1.

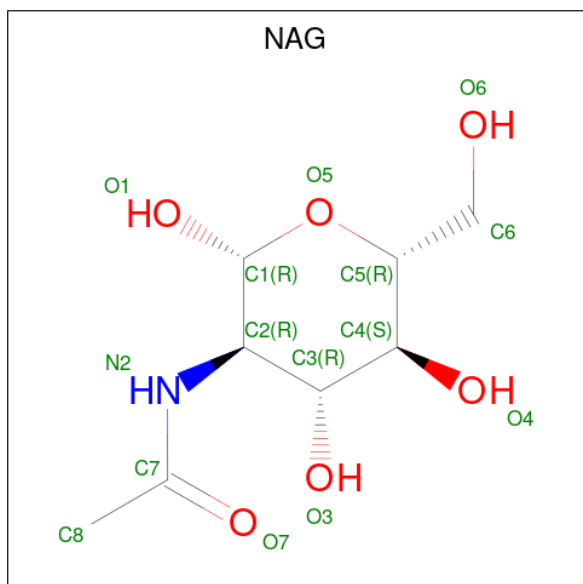
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	124	Total	C	N	O	S	1	0	0
			950	591	170	184	5			

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

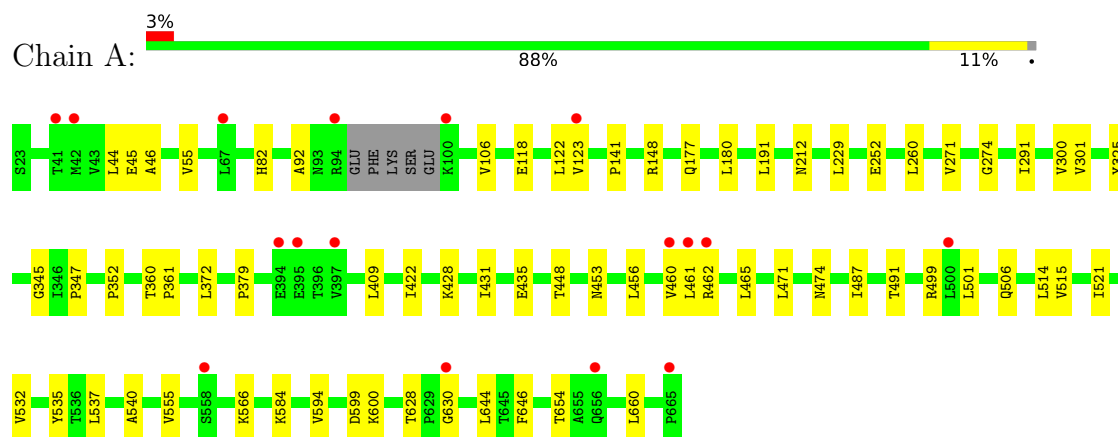


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

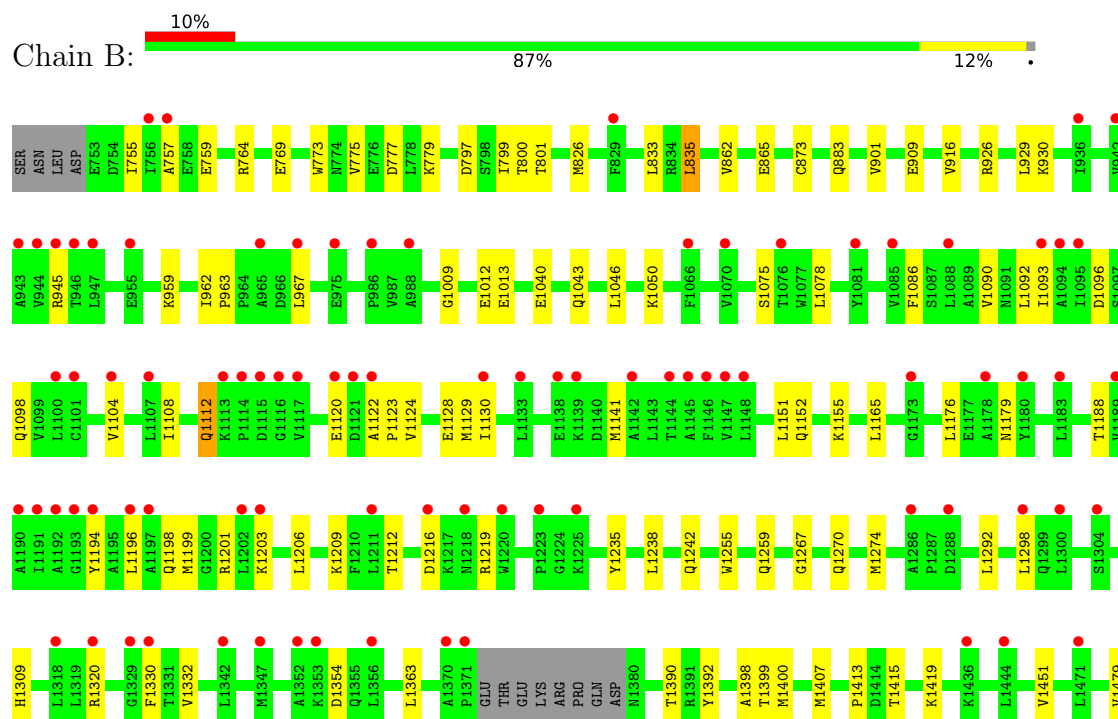
3 Residue-property plots [i](#)

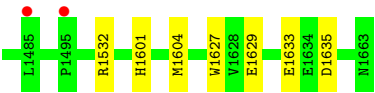
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Complement C3

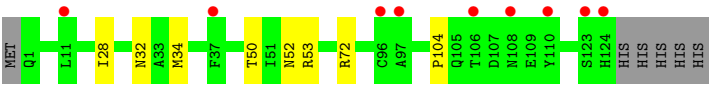
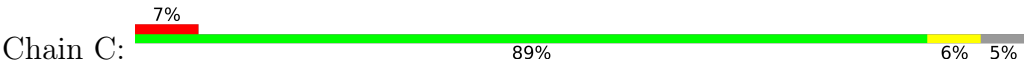


• Molecule 2: Complement C3





• Molecule 3: hC3Nb1



• Molecule 4: 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 2	Depositor
Cell constants a, b, c, α , β , γ	255.31Å 64.88Å 144.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.88 – 2.65 62.88 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.88-2.65) 90.3 (62.88-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.25 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	(Not available) , (Not available) 0.242 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13184	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.12	0/5070	0.33	1/6890 (0.0%)
2	B	0.12	0/7355	0.29	0/9958
3	C	0.10	0/971	0.29	0/1313
All	All	0.12	0/13396	0.31	1/18161 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	ALA	N-CA-C	11.46	123.33	111.07

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	4970	0	5033	42	0
2	B	7211	0	7136	78	1
3	C	950	0	904	6	0
4	D	39	0	34	0	0
5	B	14	0	13	0	0
All	All	13184	0	13120	116	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (116) 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)
2:B:1152:GLN:OE1	2:B:1199:MET:SD	2.46	0.74
2:B:1046:LEU:HG	2:B:1093:ILE:HD11	1.74	0.68
1:A:594:VAL:HG12	2:B:775:VAL:HG22	1.79	0.65
1:A:431:ILE:HG23	1:A:435:GLU:HB2	1.81	0.62
2:B:1198:GLN:O	2:B:1199:MET:HG3	1.99	0.61
2:B:1128:GLU:HB3	2:B:1267:GLY:HA2	1.81	0.61
2:B:865:GLU:HB2	2:B:883:GLN:HG2	1.83	0.60
2:B:1203:LYS:HB2	2:B:1206:LEU:HG	1.83	0.60
2:B:1152:GLN:CD	2:B:1199:MET:SD	2.84	0.60
1:A:177:GLN:N	2:B:1320:ARG:HH12	1.99	0.60
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.67	0.58
3:C:28:ILE:HD11	3:C:34:MET:HG3	1.86	0.57
1:A:141:PRO:O	2:B:930:LYS:NZ	2.38	0.57
2:B:1354:ASP:OD1	2:B:1354:ASP:N	2.37	0.57
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.41	0.56
1:A:461:LEU:HG	1:A:462:ARG:N	2.22	0.55
2:B:862:VAL:HG22	2:B:916:VAL:HG12	1.89	0.55
2:B:1151:LEU:HB3	2:B:1165:LEU:HD11	1.88	0.55
2:B:1601:HIS:ND1	2:B:1633:GLU:OE2	2.38	0.54
2:B:1050:LYS:HG3	2:B:1093:ILE:HD13	1.89	0.54
1:A:361:PRO:HB3	1:A:630:GLY:HA3	1.88	0.54
1:A:566:LYS:HE3	1:A:584:LYS:HD2	1.90	0.54
1:A:448:THR:HG21	1:A:453:ASN:H	1.72	0.54
3:C:50:THR:HG21	3:C:104:PRO:HB2	1.90	0.53
1:A:177:GLN:H	2:B:1320:ARG:HH12	1.55	0.52
1:A:291:ILE:HD13	1:A:300:VAL:HB	1.91	0.52
2:B:1216:ASP:HB3	2:B:1219:ARG:HH12	1.74	0.52
1:A:46:ALA:HB3	1:A:82:HIS:HB3	1.92	0.52
2:B:1194:TYR:O	2:B:1198:GLN:HG2	2.09	0.52
2:B:1124:VAL:HG11	2:B:1130:ILE:HD11	1.91	0.51
2:B:833:LEU:HG	2:B:835:LEU:HD13	1.91	0.51
2:B:1198:GLN:HA	2:B:1242:GLN:HG2	1.92	0.51
1:A:465:LEU:HD21	1:A:521:ILE:HG13	1.92	0.51
1:A:372:LEU:HD11	1:A:422:ILE:HG21	1.93	0.51
2:B:1298:LEU:HG	2:B:1332:VAL:HG22	1.93	0.51
2:B:1120:GLU:HG3	2:B:1122:ALA:H	1.76	0.51
2:B:1216:ASP:CB	2:B:1219:ARG:HH12	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.92	0.50
2:B:909:GLU:OE2	2:B:926:ARG:HD2	2.12	0.50
3:C:32:ASN:HA	3:C:53:ARG:HB2	1.92	0.50
1:A:474:ASN:HB3	1:A:514:LEU:HD11	1.94	0.50
2:B:1201:ARG:HD3	2:B:1201:ARG:H	1.77	0.49
1:A:260:LEU:O	2:B:801:THR:OG1	2.28	0.49
2:B:1363:LEU:HD22	2:B:1479:VAL:HG23	1.95	0.48
2:B:835:LEU:HG	2:B:929:LEU:HD23	1.94	0.48
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.96	0.48
2:B:945:ARG:HH12	2:B:963:PRO:HD3	1.79	0.48
2:B:777:ASP:HB2	2:B:779:LYS:NZ	2.28	0.48
2:B:873:CYS:HB3	2:B:901:VAL:HB	1.96	0.48
2:B:1309:HIS:NE2	2:B:1320:ARG:HG2	2.29	0.48
1:A:487:ILE:HD11	1:A:537:LEU:HD13	1.96	0.47
1:A:252:GLU:HG2	1:A:301:VAL:HG22	1.95	0.47
1:A:352:PRO:O	1:A:379:PRO:HD3	2.15	0.47
2:B:1075:SER:HB3	2:B:1078:LEU:HB3	1.95	0.47
2:B:1075:SER:HB2	2:B:1123:PRO:HG2	1.96	0.46
2:B:1198:GLN:O	2:B:1198:GLN:HG3	2.14	0.46
1:A:372:LEU:HB2	1:A:409:LEU:HB2	1.98	0.46
2:B:1415:THR:HG22	2:B:1419:LYS:HE2	1.98	0.46
1:A:45:GLU:OE2	1:A:491:THR:HG21	2.15	0.46
2:B:1120:GLU:HG3	2:B:1122:ALA:N	2.31	0.46
1:A:499:ARG:NH2	1:A:501:LEU:HD13	2.31	0.46
2:B:799:ILE:HG23	2:B:826:MET:HA	1.98	0.46
2:B:1104:VAL:HG13	2:B:1151:LEU:HD22	1.97	0.45
2:B:1198:GLN:C	2:B:1199:MET:CG	2.89	0.45
2:B:1398:ALA:HB3	2:B:1451:VAL:HG12	1.99	0.45
2:B:777:ASP:HB2	2:B:779:LYS:HZ2	1.79	0.45
2:B:1363:LEU:HD13	2:B:1479:VAL:HG21	1.99	0.45
1:A:229:LEU:HD11	2:B:769:GLU:HG2	1.98	0.45
2:B:1155:LYS:NZ	2:B:1199:MET:HE1	2.32	0.45
2:B:1176:LEU:HB2	2:B:1196:LEU:HD21	1.99	0.45
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.52	0.44
1:A:599:ASP:OD2	2:B:800:THR:HG21	2.17	0.44
1:A:148:ARG:HG3	2:B:773:TRP:CZ2	2.52	0.44
2:B:962:ILE:HG13	2:B:1330:PHE:CE2	2.52	0.44
2:B:1198:GLN:O	2:B:1199:MET:C	2.59	0.44
2:B:1009:GLY:HA3	2:B:1013:GLU:HB3	2.00	0.44
1:A:118:GLU:OE2	2:B:1043:GLN:NE2	2.51	0.44
2:B:1141:MET:HE2	2:B:1176:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ALA:HB1	1:A:212:ASN:HB3	2.00	0.44
2:B:1012:GLU:OE2	2:B:1124:VAL:HA	2.18	0.43
1:A:271:VAL:HG11	1:A:300:VAL:HG11	2.00	0.43
2:B:1141:MET:HE1	2:B:1179:ASN:HB2	2.01	0.43
2:B:1199:MET:HE3	2:B:1199:MET:HB2	1.78	0.43
2:B:1086:PHE:O	2:B:1090:VAL:HG23	2.19	0.43
2:B:1532:ARG:NH2	2:B:1629:GLU:OE2	2.31	0.43
2:B:1235:TYR:CE1	2:B:1274:MET:HE2	2.54	0.43
2:B:1096:ASP:OD1	2:B:1098:GLN:HG2	2.19	0.43
3:C:28:ILE:HG13	3:C:34:MET:HE3	2.00	0.43
3:C:53:ARG:HA	3:C:72:ARG:NH1	2.33	0.43
2:B:1255:TRP:O	2:B:1259:GLN:HG2	2.19	0.42
2:B:1129:MET:O	2:B:1270:GLN:HG2	2.19	0.42
2:B:1399:THR:OG1	2:B:1400:MET:N	2.52	0.42
2:B:759:GLU:CD	3:C:52:ASN:HD21	2.27	0.42
2:B:1152:GLN:NE2	2:B:1199:MET:SD	2.91	0.42
1:A:106:VAL:HG13	1:A:123:VAL:HG21	2.01	0.42
1:A:428:LYS:HB3	1:A:431:ILE:HB	2.01	0.42
2:B:1604:MET:HA	2:B:1627:TRP:O	2.19	0.42
2:B:1309:HIS:CD2	2:B:1320:ARG:HG2	2.55	0.42
2:B:1108:ILE:O	2:B:1112:GLN:HB2	2.20	0.42
2:B:1209:LYS:HA	2:B:1212:THR:HG22	2.00	0.42
2:B:1194:TYR:CE1	2:B:1238:LEU:HB3	2.55	0.42
1:A:460:VAL:HG21	1:A:471:LEU:HD21	2.02	0.41
2:B:1407:MET:HE3	2:B:1413:PRO:HD3	2.02	0.41
1:A:360:THR:HG21	1:A:372:LEU:HD23	2.03	0.41
1:A:456:LEU:HB2	1:A:535:TYR:CE2	2.51	0.41
1:A:646:PHE:HB3	1:A:654:THR:HG23	2.02	0.41
1:A:600:LYS:HE2	1:A:600:LYS:HB3	1.96	0.41
1:A:122:LEU:HD21	1:A:660:LEU:HD23	2.02	0.41
2:B:1216:ASP:HB3	2:B:1219:ARG:NH1	2.36	0.40
2:B:1203:LYS:H	2:B:1206:LEU:HD12	1.86	0.40
1:A:180:LEU:HD11	1:A:191:LEU:HD21	2.03	0.40
1:A:345:GLY:O	1:A:347:PRO:HD3	2.20	0.40
1:A:506:GLN:HE21	1:A:515:VAL:HB	1.86	0.40
1:A:532:VAL:HG11	1:A:644:LEU:HD12	2.04	0.40
2:B:757:ALA:C	2:B:759:GLU:H	2.30	0.40
2:B:1390:THR:HG23	2:B:1451:VAL:HG21	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:959:LYS:NZ	2:B:1635:ASP:OD2[3_455]	1.76	0.44

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	634/643 (99%)	613 (97%)	21 (3%)	0	100	100
2	B	899/915 (98%)	867 (96%)	32 (4%)	0	100	100
3	C	122/130 (94%)	120 (98%)	2 (2%)	0	100	100
All	All	1655/1688 (98%)	1600 (97%)	55 (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	562/567 (99%)	560 (100%)	2 (0%)	84	93
2	B	799/811 (98%)	791 (99%)	8 (1%)	68	81
3	C	98/104 (94%)	98 (100%)	0	100	100
All	All	1459/1482 (98%)	1449 (99%)	10 (1%)	76	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	555	VAL
1	A	628	THR
2	B	755	ILE
2	B	835	LEU
2	B	967	LEU
2	B	1040	GLU
2	B	1092	LEU
2	B	1112	GLN
2	B	1188	THR
2	B	1292	LEU

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	50	GLN
1	A	103	ASN
1	A	356	HIS
1	A	392	GLN
1	A	580	GLN
1	A	589	HIS
2	B	792	ASN
2	B	856	GLN
2	B	989	GLN
2	B	1055	GLN
2	B	1061	GLN
2	B	1349	HIS
2	B	1453	HIS
2	B	1617	ASN
2	B	1642	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.46	0	17,19,21	0.41	0
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.49	0
4	BMA	D	3	4	11,11,12	0.61	0	15,15,17	0.71	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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

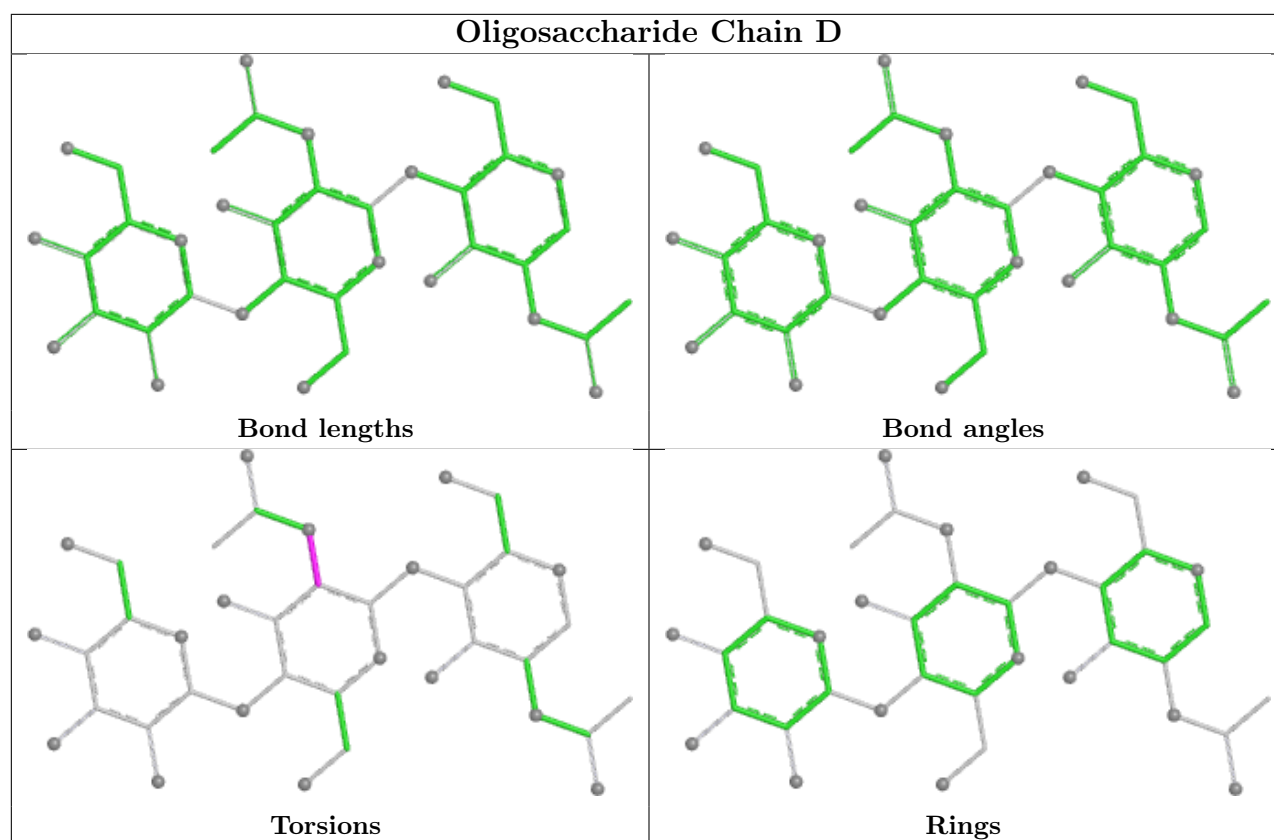
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1701	2	14,14,15	0.40	0	17,19,21	0.52	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	B	1701	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1701	NAG	C1-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, 95th 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	638/643 (99%)	0.23	17 (2%) 56 49	53, 92, 149, 203	0
2	B	903/915 (98%)	0.69	88 (9%) 13 10	54, 118, 187, 263	1 (0%)
3	C	124/130 (95%)	0.64	9 (7%) 21 15	88, 129, 176, 206	0
All	All	1665/1688 (98%)	0.51	114 (6%) 23 17	53, 108, 179, 263	1 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1104	VAL	5.3
3	C	108	ASN	4.6
2	B	1122	ALA	4.5
3	C	124	HIS	4.4
2	B	1133	LEU	4.4
2	B	1318	LEU	4.3
2	B	1100	LEU	4.3
2	B	1115	ASP	4.2
1	A	397	VAL	4.1
2	B	1190	ALA	3.9
2	B	1196	LEU	3.9
2	B	1216	ASP	3.8
1	A	461	LEU	3.6
2	B	1193	GLY	3.6
2	B	757	ALA	3.5
2	B	1142	ALA	3.5
2	B	944	VAL	3.5
2	B	942	VAL	3.5
2	B	967	LEU	3.4
2	B	1300	LEU	3.4
2	B	1371	PRO	3.3
2	B	1116	GLY	3.3
2	B	1203	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	460	VAL	3.2
1	A	462	ARG	3.2
2	B	1356	LEU	3.2
2	B	945	ARG	3.2
2	B	1148	LEU	3.1
3	C	106	THR	3.1
2	B	1189	VAL	3.1
1	A	94	ARG	3.1
2	B	1114	PRO	3.0
2	B	986	PRO	3.0
2	B	1117	VAL	3.0
2	B	1220	TRP	3.0
2	B	965	ALA	2.9
2	B	1066	PHE	2.9
2	B	1145	ALA	2.9
2	B	1211	LEU	2.8
2	B	1120	GLU	2.8
2	B	1197	ALA	2.8
2	B	1139	LYS	2.8
2	B	1076	THR	2.7
2	B	1223	PRO	2.7
2	B	1070	VAL	2.7
2	B	1085	VAL	2.7
2	B	943	ALA	2.7
3	C	37	PHE	2.7
2	B	1147	VAL	2.6
2	B	1146	PHE	2.6
2	B	1088	LEU	2.6
2	B	1178	ALA	2.6
2	B	946	THR	2.6
2	B	1121	ASP	2.5
2	B	1101	CYS	2.5
2	B	1320	ARG	2.5
2	B	936	ILE	2.5
2	B	1225	LYS	2.5
2	B	1353	LYS	2.5
1	A	395	GLU	2.5
2	B	1180	TYR	2.5
2	B	1286	ALA	2.5
2	B	1330	PHE	2.5
3	C	11	LEU	2.4
1	A	558	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	1218	ASN	2.4
2	B	1304	SER	2.4
1	A	394	GLU	2.4
1	A	630	GLY	2.4
1	A	665	PRO	2.4
2	B	1194	TYR	2.3
2	B	1444	LEU	2.3
2	B	1094	ALA	2.3
2	B	1183	LEU	2.3
2	B	1130	ILE	2.3
1	A	100	LYS	2.3
2	B	955	GLU	2.3
3	C	123	SER	2.3
1	A	656	GLN	2.3
2	B	829	PHE	2.3
2	B	988	ALA	2.3
2	B	1352	ALA	2.3
2	B	1081	TYR	2.3
2	B	1329	GLY	2.3
2	B	756	ILE	2.2
2	B	1288	ASP	2.2
2	B	947	LEU	2.2
2	B	1485	LEU	2.2
2	B	1202	LEU	2.2
2	B	1192	ALA	2.2
2	B	975	GLU	2.2
2	B	1138	GLU	2.2
2	B	1495	PRO	2.2
2	B	1095	ILE	2.2
2	B	1144	THR	2.2
3	C	96	CYS	2.2
2	B	1113	LYS	2.2
2	B	1107	LEU	2.2
1	A	123	VAL	2.1
2	B	1093	ILE	2.1
2	B	1370	ALA	2.1
1	A	41	THR	2.1
2	B	1347	MET	2.1
3	C	97	ALA	2.1
1	A	42	MET	2.1
1	A	500	LEU	2.1
2	B	1298	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1342	LEU	2.1
2	B	1191	ILE	2.1
3	C	110	TYR	2.1
2	B	1436	LYS	2.0
1	A	67	LEU	2.0
2	B	1471	LEU	2.0
2	B	1173	GLY	2.0

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

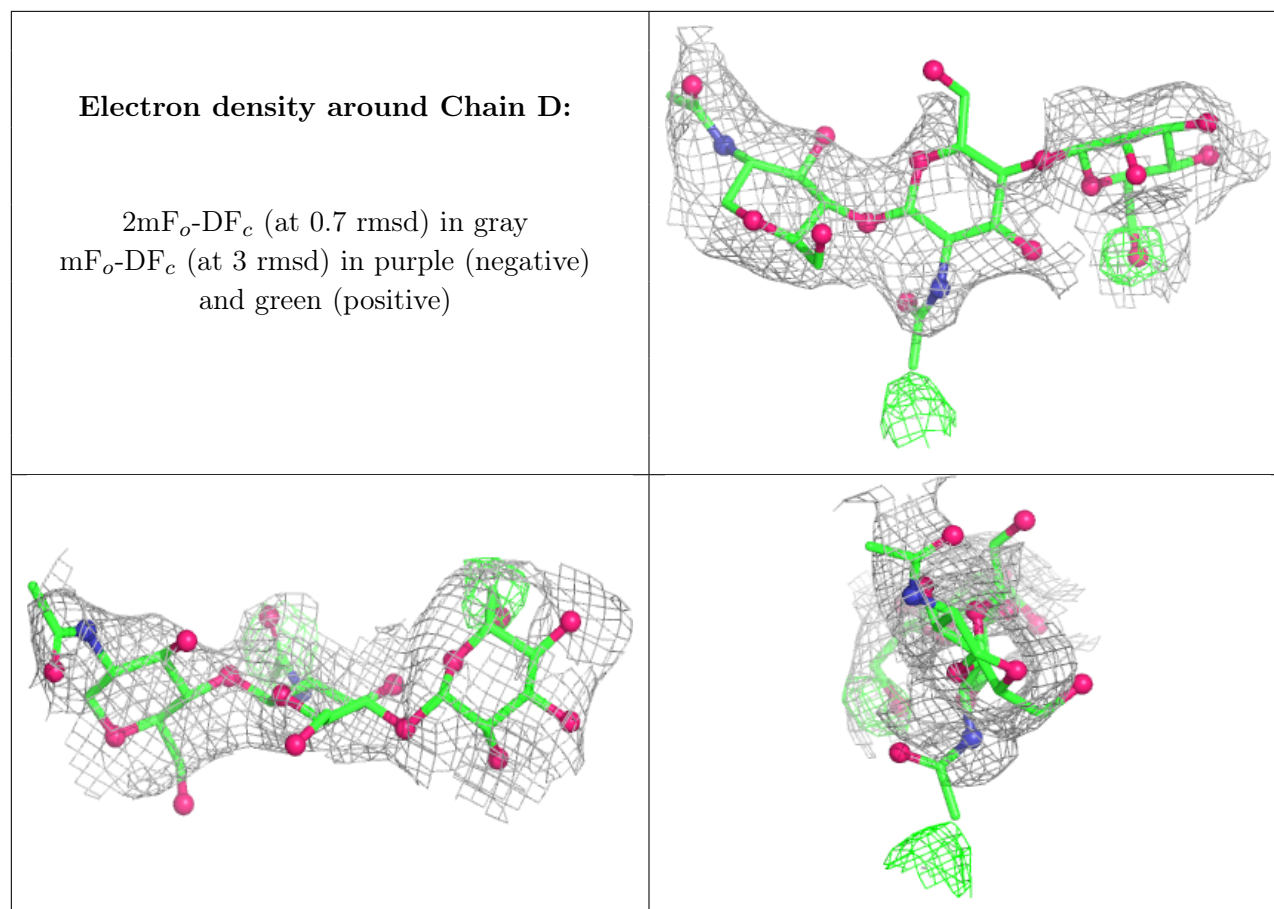
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
4	BMA	D	3	11/12	0.34	0.16	183,190,195,196	0
4	NAG	D	2	14/15	0.58	0.17	183,189,196,199	0
4	NAG	D	1	14/15	0.89	0.17	113,125,148,168	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](#)

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($\text{\AA}^2$)	Q<0.9
5	NAG	B	1701	14/15	0.83	0.14	103,122,134,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.