



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:04 PM UTC

PDB ID : 6FG2 / pdb_00006fg2
Title : CRYSTAL STRUCTURE OF FAB OF NATALIZUMAB IN COMPLEX
WITH FAB OF NAA84.
Authors : Bertrand, T.; Pouzieux, S.
Deposited on : 2018-01-09
Resolution : 2.79 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:

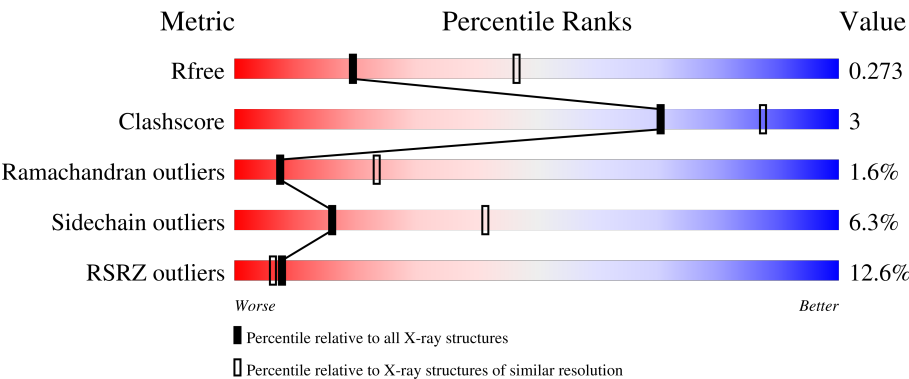
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.79 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.



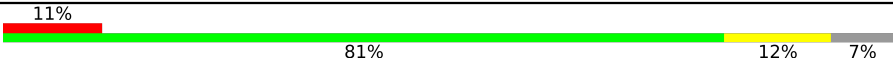
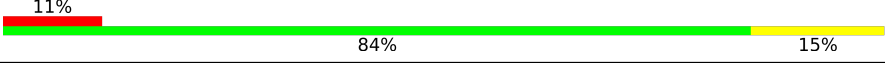
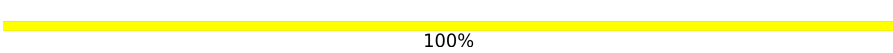
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	D	240	9% 79%12%6%
1	F	240	13% 82%12%6%
2	E	215	13% 84%12%..
2	G	215	5% 83%11%..
3	H	234	21% 75%15%9%

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Mol	Chain	Length	Quality of chain
3	I	234	
4	L	211	
4	M	211	
5	A	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13124 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 HEAVY CHAIN FAB NAA84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	225	Total	C	N	O	S	0	0	0
			1690	1067	281	335	7			
1	F	225	Total	C	N	O	S	0	0	0
			1690	1067	281	335	7			

- Molecule 2 is a protein called LIGHT CHAIN FAB NAA84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	211	Total	C	N	O	S	0	0	0
			1581	984	268	325	4			
2	G	211	Total	C	N	O	S	0	0	0
			1581	984	268	325	4			

- Molecule 3 is a protein called HEAVY CHAIN FAB NATALIZUMAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	212	Total	C	N	O	S	0	0	0
			1616	1021	269	318	8			
3	I	218	Total	C	N	O	S	0	0	0
			1656	1045	276	327	8			

- Molecule 4 is a protein called LIGHT CHAIN FAB NATALIZUMAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1641	1029	276	330	6			
4	M	211	Total	C	N	O	S	0	0	0
			1641	1029	276	330	6			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

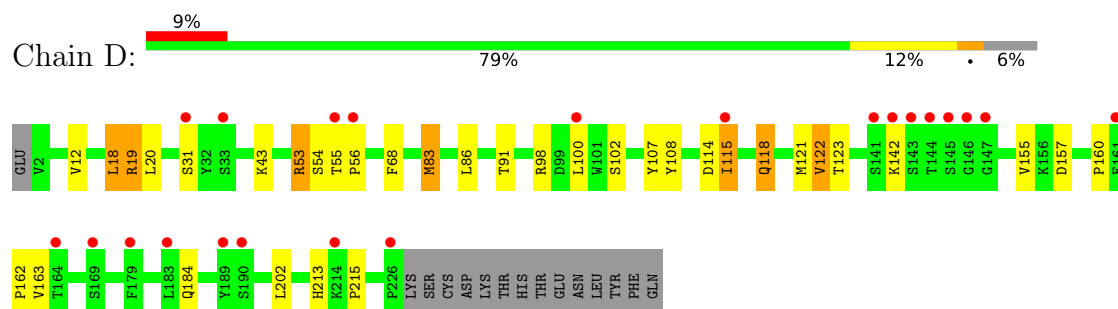


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	A	2	28	16	2	10	0	0	0

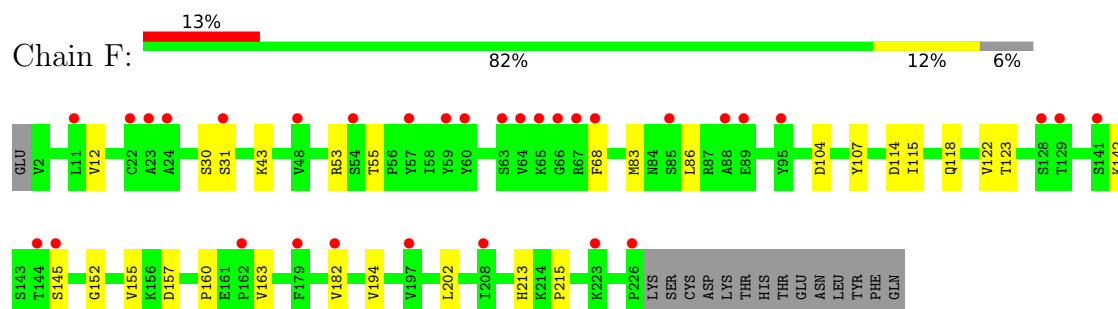
3 Residue-property plots [i](#)

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.

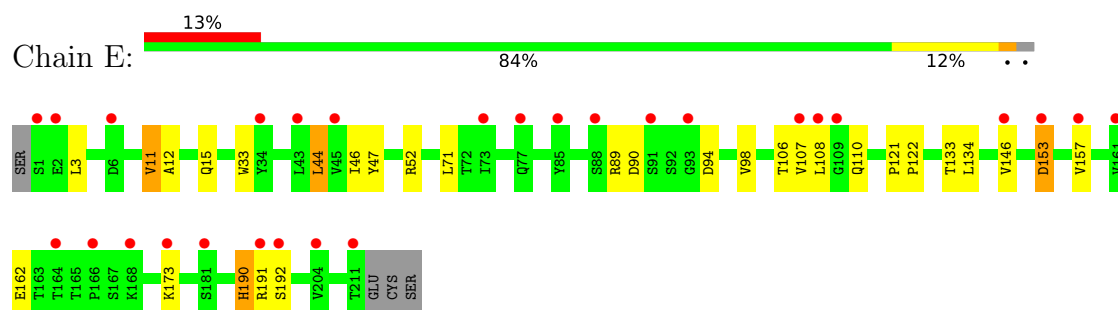
• Molecule 1: HEAVY CHAIN FAB NAA84



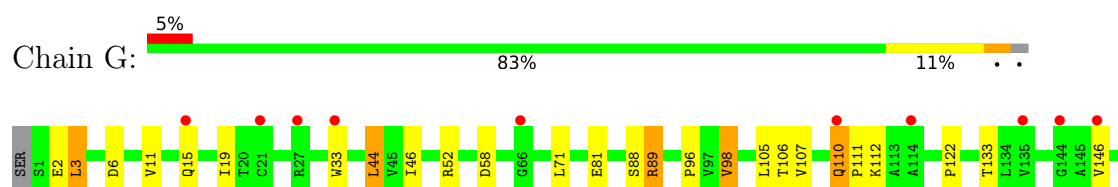
• Molecule 1: HEAVY CHAIN FAB NAA84



• Molecule 2: LIGHT CHAIN FAB NAA84

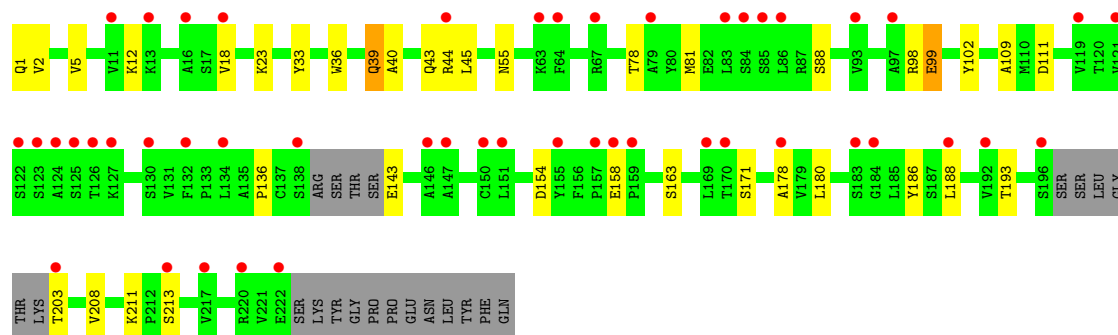
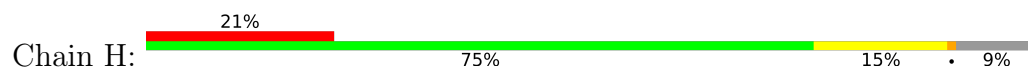


• Molecule 2: LIGHT CHAIN FAB NAA84

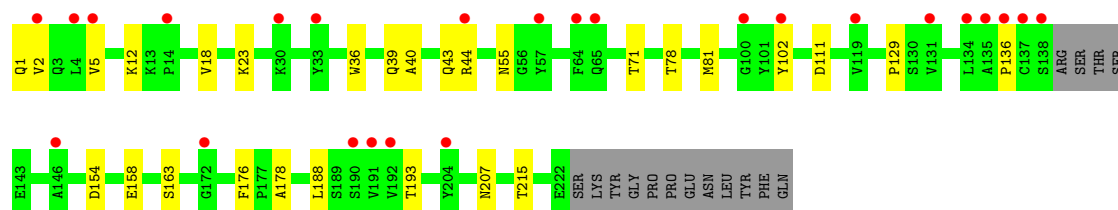
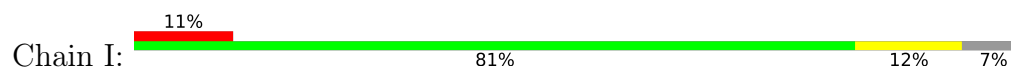




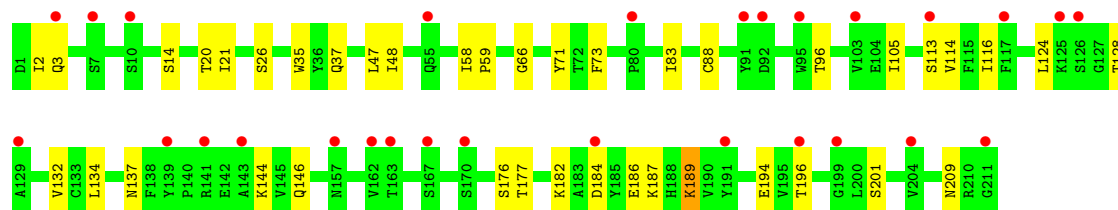
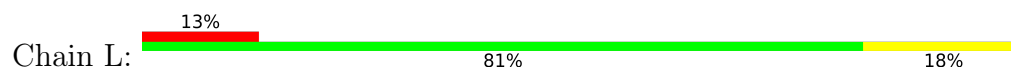
• Molecule 3: HEAVY CHAIN FAB NATALIZUMAB



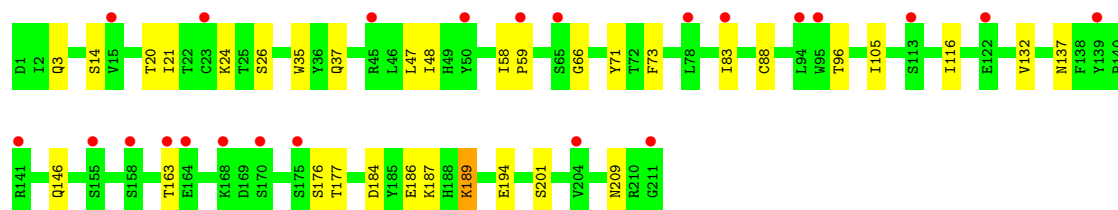
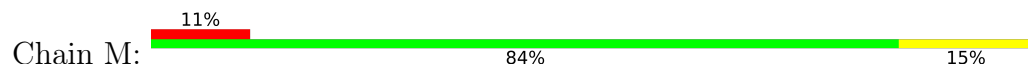
• Molecule 3: HEAVY CHAIN FAB NATALIZUMAB



• Molecule 4: LIGHT CHAIN FAB NATALIZUMAB



• Molecule 4: LIGHT CHAIN FAB NATALIZUMAB



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.40Å 66.62Å 199.50Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	55.21 – 2.79 55.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	58.6 (55.21-2.79) 58.6 (55.21-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.238 , 0.263 (Not available) , 0.273	Depositor DCC
R_{free} test set	1992 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13124	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: 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	D	0.71	0/1733	1.20	6/2362 (0.3%)
1	F	0.67	0/1733	1.16	3/2362 (0.1%)
2	E	0.71	0/1619	1.14	3/2212 (0.1%)
2	G	0.69	0/1619	1.16	5/2212 (0.2%)
3	H	0.71	0/1655	1.13	6/2253 (0.3%)
3	I	0.67	0/1696	1.13	3/2309 (0.1%)
4	L	0.77	0/1678	1.13	3/2280 (0.1%)
4	M	0.74	0/1678	1.12	2/2280 (0.1%)
All	All	0.71	0/13411	1.15	31/18270 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	18	LEU	CA-C-N	8.88	137.68	121.70
1	D	18	LEU	C-N-CA	8.88	137.68	121.70
2	G	190	HIS	CA-C-N	7.83	135.80	121.70
2	G	190	HIS	C-N-CA	7.83	135.80	121.70
2	E	190	HIS	CA-C-N	7.77	135.69	121.70
2	E	190	HIS	C-N-CA	7.77	135.69	121.70
1	F	160	PRO	CA-C-N	6.27	128.86	120.58
1	F	160	PRO	C-N-CA	6.27	128.86	120.58
1	D	160	PRO	CA-C-N	6.26	128.85	120.58
1	D	160	PRO	C-N-CA	6.26	128.85	120.58
4	L	189	LYS	CG-CD-CE	-6.23	96.97	111.30
2	G	153	ASP	CA-CB-CG	6.14	118.74	112.60
3	H	111	ASP	CA-CB-CG	5.53	118.13	112.60
1	F	68	PHE	CA-CB-CG	5.52	119.32	113.80
1	D	122	VAL	N-CA-CB	5.36	118.81	111.41
2	G	58	ASP	CA-C-N	5.35	127.45	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	58	ASP	C-N-CA	5.35	127.45	120.28
4	M	59	PRO	CA-C-N	5.30	127.91	120.28
4	M	59	PRO	C-N-CA	5.30	127.91	120.28
1	D	68	PHE	CA-CB-CG	5.25	119.06	113.80
2	E	153	ASP	CA-CB-CG	5.19	117.79	112.60
3	H	213	SER	CA-C-N	5.14	130.96	121.70
3	H	213	SER	C-N-CA	5.14	130.96	121.70
3	I	55	ASN	CA-CB-CG	5.14	117.74	112.60
3	I	102	TYR	CA-C-N	5.13	125.68	119.98
3	I	102	TYR	C-N-CA	5.13	125.68	119.98
3	H	143	GLU	CA-C-N	5.10	127.06	120.44
3	H	143	GLU	C-N-CA	5.10	127.06	120.44
4	L	59	PRO	CA-C-N	5.09	127.82	120.38
4	L	59	PRO	C-N-CA	5.09	127.82	120.38
3	H	55	ASN	CA-CB-CG	5.02	117.62	112.60

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	D	1690	0	1642	13	0
1	F	1690	0	1642	8	0
2	E	1581	0	1517	13	0
2	G	1581	0	1518	16	0
3	H	1616	0	1564	10	0
3	I	1656	0	1609	9	0
4	L	1641	0	1595	14	0
4	M	1641	0	1595	12	0
5	A	28	0	25	0	0
All	All	13124	0	12707	87	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 3.

All (87) 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:G:110:GLN:HB3	2:G:111:PRO:HA	1.49	0.91
1:D:53:ARG:HG3	1:D:102:SER:HB2	1.69	0.74
2:G:190:HIS:HA	2:G:191:ARG:HB2	1.71	0.71
2:E:190:HIS:HA	2:E:191:ARG:HB2	1.79	0.65
3:H:178:ALA:HB2	3:H:188:LEU:HD23	1.81	0.62
2:G:110:GLN:HB3	2:G:111:PRO:CA	2.26	0.60
2:G:81:GLU:HB2	2:G:107:VAL:HG22	1.85	0.59
1:F:182:VAL:CG1	2:G:164:THR:HG23	2.32	0.59
2:E:44:LEU:HD21	2:E:47:TYR:HB3	1.86	0.57
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.86	0.57
4:M:37:GLN:HB2	4:M:47:LEU:HD11	1.86	0.57
3:I:163:SER:HB3	3:I:207:ASN:HB2	1.87	0.56
1:D:18:LEU:HA	1:D:19:ARG:HB2	1.88	0.56
3:H:40:ALA:HB3	3:H:43:GLN:HB2	1.88	0.55
1:F:182:VAL:HG12	2:G:164:THR:HG23	1.87	0.55
3:I:40:ALA:HB3	3:I:43:GLN:HB2	1.89	0.55
1:D:184:GLN:HG2	2:E:162:GLU:HG3	1.88	0.54
1:F:114:ASP:HA	2:G:44:LEU:HD12	1.90	0.52
1:F:213:HIS:CD2	1:F:215:PRO:HD2	2.44	0.52
2:G:110:GLN:CB	2:G:111:PRO:HA	2.33	0.52
1:D:213:HIS:CD2	1:D:215:PRO:HD2	2.44	0.52
3:H:23:LYS:HA	3:H:78:THR:HG22	1.91	0.51
1:D:114:ASP:HA	2:E:44:LEU:HD12	1.92	0.51
2:E:46:ILE:HD13	2:E:52:ARG:HB3	1.93	0.51
4:L:132:VAL:HG22	4:L:177:THR:HG23	1.94	0.50
4:M:132:VAL:HG22	4:M:177:THR:HG23	1.93	0.50
4:L:47:LEU:HD23	4:L:58:ILE:HD12	1.94	0.49
3:I:23:LYS:HA	3:I:78:THR:HG22	1.94	0.49
2:G:46:ILE:HD13	2:G:52:ARG:HB3	1.94	0.49
1:F:83:MET:HB3	1:F:86:LEU:HD21	1.95	0.48
3:I:178:ALA:HB2	3:I:188:LEU:HD23	1.95	0.48
3:H:39:GLN:HG3	3:H:45:LEU:HD23	1.96	0.48
4:M:47:LEU:HD23	4:M:58:ILE:HD12	1.95	0.47
4:M:146:GLN:HB3	4:M:194:GLU:HB3	1.95	0.47
1:D:118:GLN:H	1:D:118:GLN:HG3	1.47	0.47
2:G:19:ILE:HD11	2:G:105:LEU:HD13	1.97	0.47
1:D:91:THR:HG23	1:D:123:THR:HA	1.97	0.47
2:G:122:PRO:HB3	2:G:133:THR:H	1.80	0.46
4:L:146:GLN:HB3	4:L:194:GLU:HB3	1.95	0.46
3:I:178:ALA:HA	3:I:188:LEU:HB3	1.96	0.46
2:G:3:LEU:HD21	2:G:98:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:PRO:HB3	2:E:133:THR:H	1.80	0.45
4:M:66:GLY:HA3	4:M:71:TYR:HA	1.98	0.45
1:D:12:VAL:HG11	1:D:86:LEU:HD13	1.99	0.45
1:D:155:VAL:HG11	1:D:163:VAL:HG21	1.98	0.45
2:E:190:HIS:CA	2:E:191:ARG:HB2	2.47	0.44
3:I:12:LYS:HG3	3:I:18:VAL:HB	2.00	0.44
2:G:110:GLN:HG2	2:G:112:LYS:HG3	1.99	0.44
1:F:182:VAL:HG13	2:G:164:THR:HG23	2.00	0.44
3:I:176:PHE:CD2	4:M:163:THR:HG23	2.53	0.44
2:E:190:HIS:HA	2:E:191:ARG:CB	2.47	0.43
4:L:184:ASP:HA	4:L:187:LYS:HE3	2.00	0.43
4:L:66:GLY:HA3	4:L:71:TYR:HA	1.99	0.43
4:M:184:ASP:HA	4:M:187:LYS:HE3	2.00	0.43
4:M:189:LYS:HE2	4:M:209:ASN:HB2	1.99	0.43
4:L:21:ILE:HD12	4:L:73:PHE:HD2	1.83	0.43
1:D:108:TYR:O	2:E:89:ARG:HG3	2.18	0.43
3:H:12:LYS:HG3	3:H:18:VAL:HB	2.01	0.42
3:I:36:TRP:CE2	3:I:81:MET:HB2	2.54	0.42
4:L:189:LYS:HE2	4:L:209:ASN:HB2	2.01	0.42
4:L:3:GLN:HB2	4:L:26:SER:HB3	2.01	0.42
1:D:83:MET:HB2	1:D:86:LEU:HD21	2.01	0.42
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.55	0.42
1:F:155:VAL:HG11	1:F:163:VAL:HG21	2.00	0.42
4:M:35:TRP:CZ3	4:M:88:CYS:HB3	2.55	0.42
3:H:36:TRP:CE2	3:H:81:MET:HB2	2.55	0.42
1:D:98:ARG:HH11	1:D:115:ILE:HD13	1.85	0.41
2:E:121:PRO:HA	2:E:134:LEU:HD23	2.03	0.41
4:L:144:LYS:HB3	4:L:196:THR:HB	2.02	0.41
4:M:3:GLN:HB2	4:M:26:SER:HB3	2.03	0.41
4:M:47:LEU:HA	4:M:58:ILE:HG13	2.02	0.41
2:E:11:VAL:HG12	2:E:12:ALA:H	1.86	0.41
2:E:108:LEU:HD23	2:E:110:GLN:HB2	2.02	0.41
3:H:178:ALA:HA	3:H:188:LEU:HB3	2.02	0.41
3:I:129:PRO:HD2	3:I:215:THR:HG21	2.00	0.41
4:M:21:ILE:HD12	4:M:73:PHE:HD2	1.85	0.41
3:H:33:TYR:HB2	3:H:99:GLU:HB3	2.02	0.41
1:D:121:MET:HG2	1:D:162:PRO:HD3	2.03	0.41
4:L:47:LEU:HA	4:L:58:ILE:HG13	2.02	0.41
2:G:89:ARG:HA	2:G:96:PRO:O	2.21	0.41
3:H:102:TYR:HE2	3:H:109:ALA:HB3	1.85	0.41
4:L:124:LEU:HB3	4:L:182:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:33:TRP:CE2	2:G:71:LEU:HB2	2.57	0.40
3:H:180:LEU:HA	3:H:186:TYR:HA	2.03	0.40
4:L:114:VAL:HA	4:L:134:LEU:O	2.22	0.40
2:E:33:TRP:CE2	2:E:71:LEU:HB2	2.56	0.40
1:F:152:GLY:HA3	1:F:194:VAL:HG12	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	D	223/240 (93%)	206 (92%)	11 (5%)	6 (3%)	4	12
1	F	223/240 (93%)	204 (92%)	14 (6%)	5 (2%)	5	17
2	E	209/215 (97%)	194 (93%)	11 (5%)	4 (2%)	6	19
2	G	209/215 (97%)	197 (94%)	7 (3%)	5 (2%)	4	15
3	H	206/234 (88%)	195 (95%)	8 (4%)	3 (2%)	8	25
3	I	214/234 (92%)	201 (94%)	11 (5%)	2 (1%)	14	37
4	L	209/211 (99%)	192 (92%)	16 (8%)	1 (0%)	24	52
4	M	209/211 (99%)	192 (92%)	16 (8%)	1 (0%)	24	52
All	All	1702/1800 (95%)	1581 (93%)	94 (6%)	27 (2%)	7	23

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	19	ARG
1	D	157	ASP
1	F	31	SER
1	F	145	SER
1	F	157	ASP

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Mol	Chain	Res	Type
1	D	31	SER
1	D	53	ARG
1	D	54	SER
2	E	90	ASP
2	E	153	ASP
2	G	110	GLN
3	H	136	PRO
4	L	137	ASN
1	F	55	THR
2	G	153	ASP
3	H	154	ASP
3	I	154	ASP
4	M	137	ASN
1	D	56	PRO
2	E	173	LYS
1	F	12	VAL
2	G	2	GLU
2	G	191	ARG
2	G	192	SER
3	H	171	SER
2	E	107	VAL
3	I	136	PRO

5.3.2 Protein sidechains ⓘ

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	D	191/206 (93%)	180 (94%)	11 (6%)	18	45
1	F	191/206 (93%)	180 (94%)	11 (6%)	18	45
2	E	176/180 (98%)	166 (94%)	10 (6%)	18	46
2	G	176/180 (98%)	164 (93%)	12 (7%)	14	38
3	H	178/198 (90%)	164 (92%)	14 (8%)	11	31
3	I	183/198 (92%)	174 (95%)	9 (5%)	22	52
4	L	187/187 (100%)	174 (93%)	13 (7%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	187/187 (100%)	175 (94%)	12 (6%)	16	41
All	All	1469/1542 (95%)	1377 (94%)	92 (6%)	16	41

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	D	43	LYS
1	D	55	THR
1	D	83	MET
1	D	100	LEU
1	D	107	TYR
1	D	115	ILE
1	D	118	GLN
1	D	122	VAL
1	D	142	LYS
1	D	202	LEU
2	E	3	LEU
2	E	11	VAL
2	E	15	GLN
2	E	44	LEU
2	E	94	ASP
2	E	98	VAL
2	E	106	THR
2	E	146	VAL
2	E	157	VAL
2	E	192	SER
1	F	30	SER
1	F	43	LYS
1	F	53	ARG
1	F	104	ASP
1	F	107	TYR
1	F	115	ILE
1	F	118	GLN
1	F	122	VAL
1	F	123	THR
1	F	142	LYS
1	F	202	LEU
2	G	3	LEU
2	G	6	ASP
2	G	11	VAL
2	G	15	GLN

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Mol	Chain	Res	Type
2	G	44	LEU
2	G	88	SER
2	G	89	ARG
2	G	98	VAL
2	G	106	THR
2	G	146	VAL
2	G	153	ASP
2	G	181	SER
3	H	1	GLN
3	H	2	VAL
3	H	5	VAL
3	H	39	GLN
3	H	44	ARG
3	H	88	SER
3	H	98	ARG
3	H	99	GLU
3	H	158	GLU
3	H	163	SER
3	H	193	THR
3	H	203	THR
3	H	208	VAL
3	H	211	LYS
3	I	1	GLN
3	I	2	VAL
3	I	5	VAL
3	I	39	GLN
3	I	44	ARG
3	I	71	THR
3	I	111	ASP
3	I	158	GLU
3	I	193	THR
4	L	2	ILE
4	L	14	SER
4	L	20	THR
4	L	48	ILE
4	L	83	ILE
4	L	96	THR
4	L	105	ILE
4	L	113	SER
4	L	116	ILE
4	L	128	THR
4	L	176	SER

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Mol	Chain	Res	Type
4	L	186	GLU
4	L	201	SER
4	M	14	SER
4	M	20	THR
4	M	24	LYS
4	M	48	ILE
4	M	83	ILE
4	M	96	THR
4	M	105	ILE
4	M	116	ILE
4	M	176	SER
4	M	186	GLU
4	M	189	LYS
4	M	201	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	74	ASN
1	D	106	ASN
1	D	212	ASN
2	E	15	GLN
2	E	40	GLN
2	E	95	HIS
2	E	110	GLN
2	E	172	ASN
2	E	196	GLN
1	F	74	ASN
1	F	84	ASN
1	F	212	ASN
2	G	15	GLN
2	G	40	GLN
2	G	110	GLN
2	G	172	ASN
3	H	1	GLN
3	I	1	GLN
4	L	55	GLN
4	L	93	ASN
4	L	209	ASN
4	M	55	GLN
4	M	93	ASN
4	M	137	ASN

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Mol	Chain	Res	Type
4	M	154	GLN

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 ⓘ

2 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	$\# Z > 2$
5	NAG	A	1	2,5	14,14,15	0.32	0	17,19,21	1.00	1 (5%)
5	NAG	A	2	5	14,14,15	0.34	0	17,19,21	0.69	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	NAG	C1-O5-C5	3.55	116.95	112.19
5	A	2	NAG	C1-O5-C5	2.07	114.95	112.19

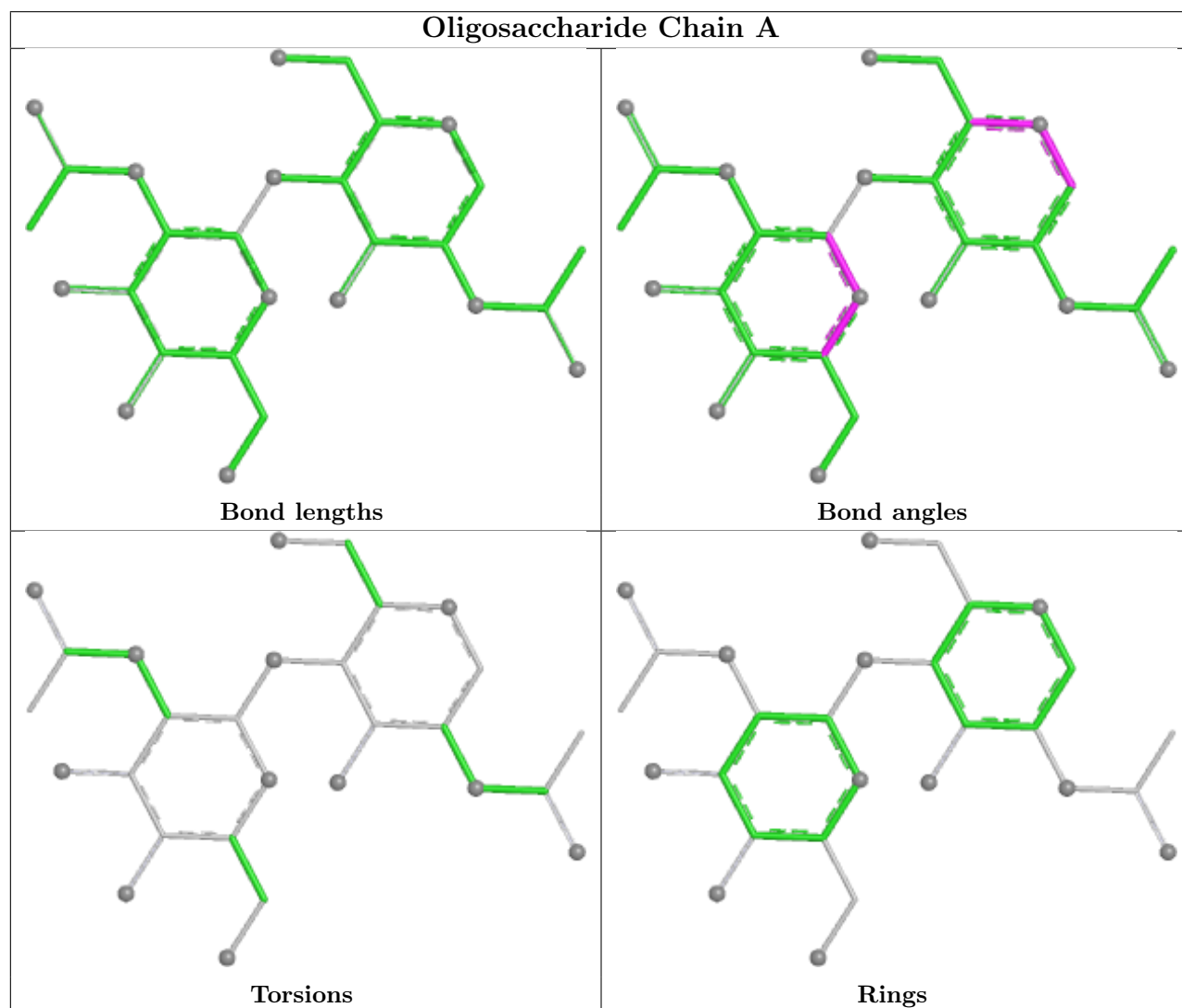
There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	D	225/240 (93%)	1.04	22 (9%) 13 10	32, 56, 76, 92	0
1	F	225/240 (93%)	1.16	32 (14%) 6 5	32, 49, 72, 82	0
2	E	211/215 (98%)	1.21	28 (13%) 7 6	36, 59, 79, 93	0
2	G	211/215 (98%)	0.86	11 (5%) 33 27	31, 46, 63, 78	0
3	H	212/234 (90%)	1.41	48 (22%) 2 1	39, 65, 82, 101	0
3	I	218/234 (93%)	1.03	25 (11%) 9 7	36, 54, 70, 96	0
4	L	211/211 (100%)	1.18	28 (13%) 7 6	36, 59, 76, 88	0
4	M	211/211 (100%)	1.08	23 (10%) 10 8	39, 57, 72, 88	0
All	All	1724/1800 (95%)	1.12	217 (12%) 8 6	31, 55, 76, 101	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	211	GLY	6.2
4	L	211	GLY	4.8
1	F	144	THR	4.8
2	E	108	LEU	4.7
1	D	144	THR	4.6
3	H	138	SER	4.6
1	D	145	SER	4.4
4	L	143	ALA	4.2
3	I	138	SER	4.2
2	G	27	ARG	4.2
3	I	64	PHE	4.1
1	F	141	SER	3.9
3	H	16	ALA	3.8
3	H	151	LEU	3.8
3	H	126	THR	3.6
2	E	109	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	G	146	VAL	3.6
1	D	226	PRO	3.6
3	I	2	VAL	3.6
3	H	122	SER	3.5
3	H	13	LYS	3.5
1	D	143	SER	3.4
2	E	153	ASP	3.4
1	F	48	VAL	3.4
3	H	85	SER	3.4
1	D	55	THR	3.4
3	H	158	GLU	3.4
1	D	142	LYS	3.3
4	L	162	VAL	3.3
3	H	203	THR	3.3
2	G	15	GLN	3.3
3	H	147	ALA	3.3
2	E	146	VAL	3.3
4	L	196	THR	3.2
4	M	164	GLU	3.1
1	F	85	SER	3.1
1	D	100	LEU	3.1
4	M	15	VAL	3.1
4	M	94	LEU	3.1
1	F	66	GLY	3.1
1	F	65	LYS	3.1
3	H	127	LYS	3.1
1	D	56	PRO	3.0
1	F	226	PRO	3.0
3	H	63	LYS	3.0
3	H	125	SER	3.0
4	L	103	VAL	3.0
1	D	147	GLY	3.0
2	G	33	TRP	2.9
3	H	157	PRO	2.9
1	F	57	TYR	2.9
1	F	89	GLU	2.9
2	E	173	LYS	2.9
2	E	88	SER	2.9
2	E	6	ASP	2.9
2	E	211	THR	2.9
3	H	97	ALA	2.9
3	I	192	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	31	SER	2.9
2	G	110	GLN	2.9
2	E	93	GLY	2.9
3	H	11	VAL	2.9
3	H	83	LEU	2.9
3	H	134	LEU	2.9
3	H	188	LEU	2.9
1	F	145	SER	2.8
3	H	178	ALA	2.8
4	L	167	SER	2.8
2	E	85	TYR	2.8
2	E	2	GLU	2.8
1	D	146	GLY	2.8
4	L	184	ASP	2.8
3	H	79	ALA	2.8
3	H	169	LEU	2.8
2	E	45	VAL	2.8
1	F	31	SER	2.7
1	F	129	THR	2.7
4	L	117	PHE	2.7
1	D	33	SER	2.7
4	L	95	TRP	2.7
3	H	217	VAL	2.7
3	I	136	PRO	2.7
1	F	128	SER	2.7
1	F	197	VAL	2.7
3	I	137	CYS	2.7
3	H	86	LEU	2.7
2	G	162	GLU	2.7
3	H	213	SER	2.7
1	D	164	THR	2.7
4	L	80	PRO	2.7
3	H	159	PRO	2.6
4	L	92	ASP	2.6
3	H	67	ARG	2.6
4	L	170	SER	2.6
4	L	91	TYR	2.6
2	E	77	GLN	2.6
3	H	64	PHE	2.6
4	M	155	SER	2.5
3	I	204	TYR	2.5
3	I	191	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	88	ALA	2.5
2	E	91	SER	2.5
2	E	34	TYR	2.5
3	H	146	ALA	2.5
2	G	21	CYS	2.5
2	E	192	SER	2.5
4	L	10	SER	2.5
1	F	59	TYR	2.5
4	L	3	GLN	2.5
3	I	100	GLY	2.5
1	F	162	PRO	2.5
2	E	204	VAL	2.5
3	H	183	SER	2.4
3	H	196	SER	2.4
4	M	158	SER	2.4
4	L	191	TYR	2.4
3	H	130	SER	2.4
4	M	23	CYS	2.4
1	D	214	LYS	2.4
1	F	182	VAL	2.4
1	F	63	SER	2.4
4	L	126	SER	2.4
3	H	150	CYS	2.4
1	F	64	VAL	2.4
1	D	183	LEU	2.4
1	F	11	LEU	2.4
1	F	208	ILE	2.4
1	D	141	SER	2.4
1	F	54	SER	2.4
1	F	223	LYS	2.4
4	L	125	LYS	2.4
3	I	65	GLN	2.4
2	E	107	VAL	2.4
2	E	168	LYS	2.3
3	H	184	GLY	2.3
3	I	119	VAL	2.3
3	I	135	ALA	2.3
1	D	115	ILE	2.3
1	D	189	TYR	2.3
3	I	57	TYR	2.3
4	L	163	THR	2.3
2	E	166	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
4	M	45	ARG	2.3
2	E	161	VAL	2.3
3	H	18	VAL	2.3
4	L	204	VAL	2.3
1	D	179	PHE	2.3
3	H	84	SER	2.3
4	M	170	SER	2.3
3	I	14	PRO	2.3
2	E	157	VAL	2.3
3	I	4	LEU	2.3
4	M	50	TYR	2.3
3	I	44	ARG	2.3
4	M	59	PRO	2.3
4	L	199	GLY	2.3
3	H	121	VAL	2.3
3	I	5	VAL	2.3
4	L	129	ALA	2.2
1	D	161	GLU	2.2
2	E	1	SER	2.2
2	E	73	ILE	2.2
3	H	132	PHE	2.2
2	G	114	ALA	2.2
2	E	164	THR	2.2
4	M	139	TYR	2.2
4	L	113	SER	2.2
3	I	134	LEU	2.2
1	F	24	ALA	2.2
2	E	181	SER	2.2
3	H	123	SER	2.2
4	M	168	LYS	2.2
4	M	122	GLU	2.2
3	H	155	TYR	2.2
4	L	55	GLN	2.2
4	L	7	SER	2.2
3	I	146	ALA	2.1
2	G	66	GLY	2.1
2	G	144	GLY	2.1
1	D	169	SER	2.1
3	H	192	VAL	2.1
4	M	65	SER	2.1
4	M	141	ARG	2.1
4	M	113	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	191	ARG	2.1
3	I	30	LYS	2.1
4	L	157	ASN	2.1
1	F	60	TYR	2.1
3	I	131	VAL	2.1
3	H	124	ALA	2.1
3	I	190	SER	2.1
3	H	222	GLU	2.1
3	I	172	GLY	2.1
2	G	135	VAL	2.1
1	F	68	PHE	2.1
1	F	179	PHE	2.1
1	F	67	ARG	2.0
3	H	170	THR	2.0
4	M	163	THR	2.0
1	F	22	CYS	2.0
3	H	119	VAL	2.0
4	L	139	TYR	2.0
4	M	204	VAL	2.0
3	H	44	ARG	2.0
3	H	220	ARG	2.0
4	L	141	ARG	2.0
1	F	23	ALA	2.0
1	D	190	SER	2.0
4	M	175	SER	2.0
4	M	95	TRP	2.0
2	E	43	LEU	2.0
4	M	78	LEU	2.0
4	M	83	ILE	2.0
3	H	93	VAL	2.0
1	F	95	TYR	2.0
3	I	33	TYR	2.0
3	I	102	TYR	2.0

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

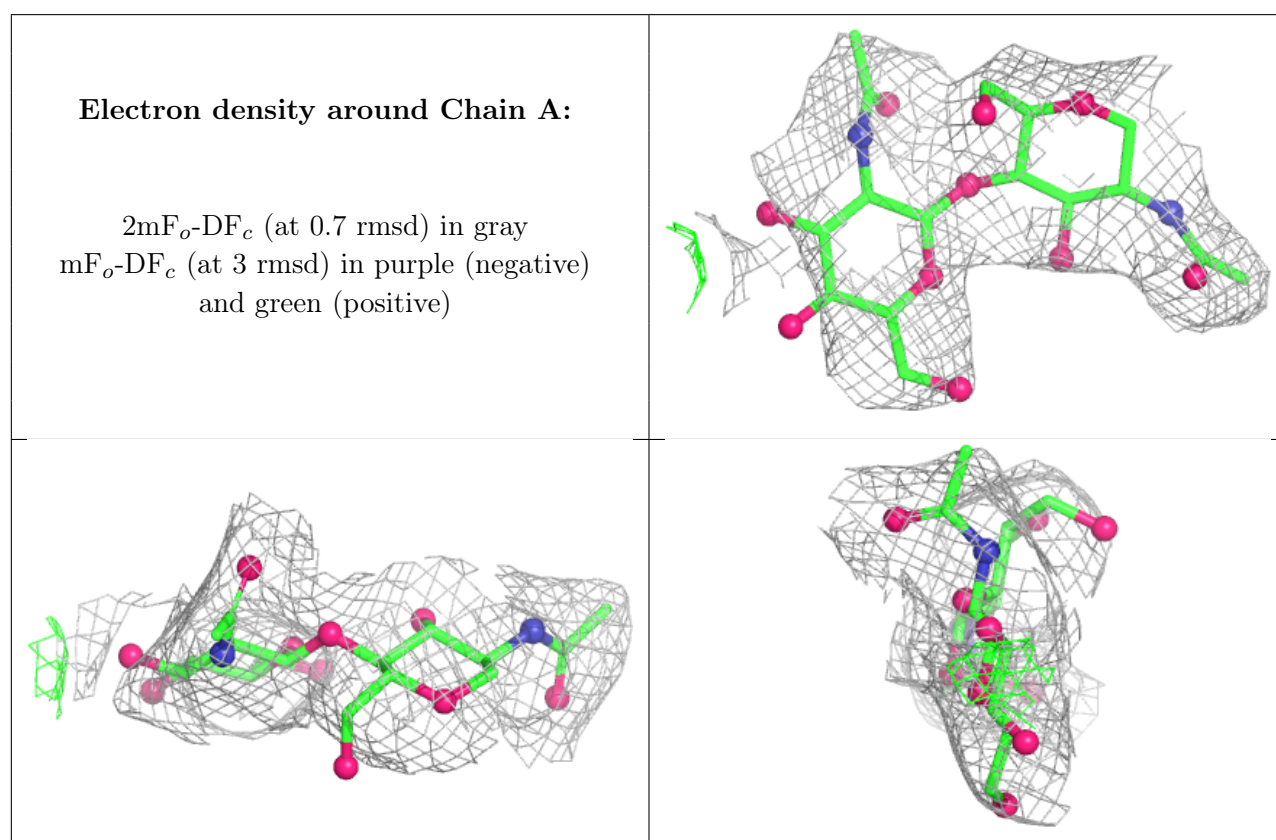
There are no non-standard protein/DNA/RNA residues in this entry.

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
5	NAG	A	1	14/15	-	-	70,79,82,85	0
5	NAG	A	2	14/15	-	-	88,89,91,91	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.