



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 2CH8 / pdb_00002ch8
Title : Structure of the Epstein-Barr Virus Oncogene BARF1
Authors : Tarbouriech, N.; Ruggiero, F.; deTurenne-Tessier, M.; Ooka, T.; Burmeister, W.P.
Deposited on : 2006-03-13
Resolution : 2.30 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

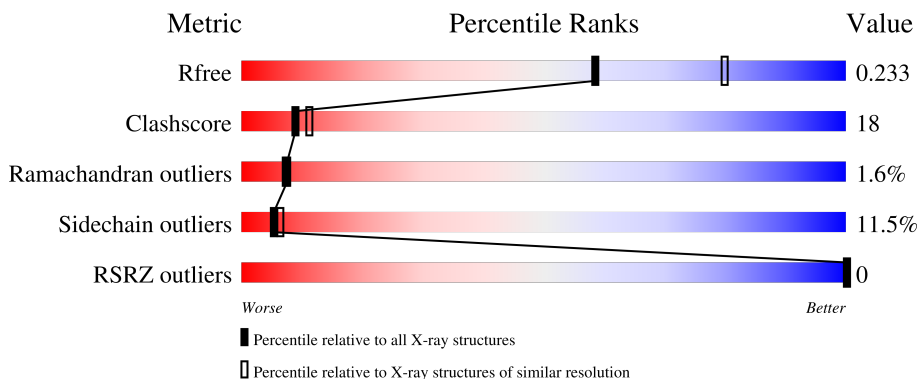
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	201	61% 23% 7% • 6%
1	B	201	62% 23% 6% • 7%
1	C	201	66% 22% • 7%
1	D	201	66% 20% 5% • 7%
2	E	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	3	 100%
2	G	3	 33% 67%
2	H	3	 33% 67%

2 Entry composition [i](#)

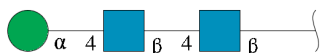
There are 4 unique types of molecules in this entry. The entry contains 6701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 33 KDA EARLY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	188	Total 1505	C 972	N 257	O 269	S 7	0	2	0
1	B	186	Total 1496	C 967	N 256	O 266	S 7	0	2	0
1	C	186	Total 1502	C 969	N 258	O 268	S 7	0	3	0
1	D	186	Total 1497	C 968	N 255	O 267	S 7	0	2	0

- Molecule 2 is an oligosaccharide called alpha-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			
2	E	3	Total 39	C 22	N 2	O 15	0	0	0
2	F	3	Total 39	C 22	N 2	O 15	0	0	0
2	G	3	Total 39	C 22	N 2	O 15	0	0	0
2	H	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Pt 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Pt 3	0	0
3	C	3	Total 3	Pt 3	0	0
3	D	3	Total 3	Pt 3	0	0

- Molecule 4 is water.

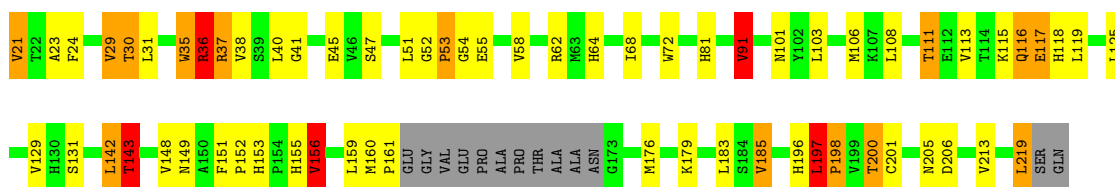
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total 128	O 128	0	0
4	B	131	Total 131	O 131	0	0
4	C	145	Total 145	O 145	0	0
4	D	129	Total 129	O 129	0	0

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.

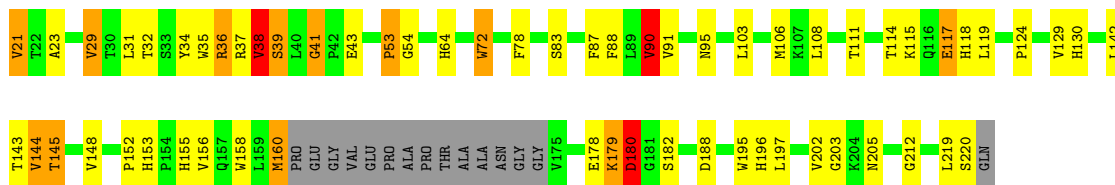
- Molecule 1: 33 KDA EARLY PROTEIN

Chain A: 



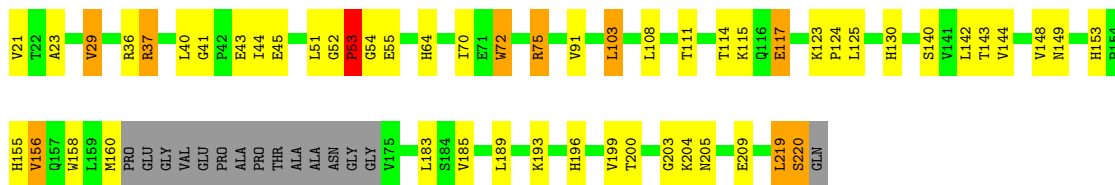
- Molecule 1: 33 KDA EARLY PROTEIN

Chain B: 



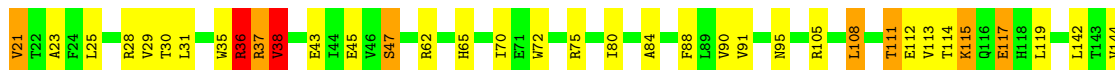
- Molecule 1: 33 KDA EARLY PROTEIN

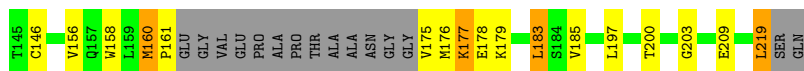
Chain C: 



- Molecule 1: 33 KDA EARLY PROTEIN

Chain D: 





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

Chain E: 33% 67%



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

Chain F: 100%



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

Chain G: 33% 67%



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

Chain H: 33% 67%



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	179.25Å 179.25Å 95.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.30) 100.0 (30.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.233 0.175 , 0.233	Depositor DCC
R_{free} test set	2583 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6701	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, PT, 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	1.35	8/1560 (0.5%)	1.29	9/2122 (0.4%)
1	B	1.21	5/1550 (0.3%)	1.23	4/2107 (0.2%)
1	C	1.28	4/1561 (0.3%)	1.19	6/2122 (0.3%)
1	D	1.18	4/1552 (0.3%)	1.16	6/2112 (0.3%)
All	All	1.26	21/6223 (0.3%)	1.22	25/8463 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ARG	N-CA	7.78	1.56	1.46
1	B	202	VAL	CA-CB	7.73	1.63	1.54
1	C	143	THR	CA-CB	7.00	1.62	1.53
1	B	54	GLY	C-N	-6.56	1.24	1.33
1	A	58	VAL	CA-CB	6.49	1.61	1.54
1	B	90	VAL	CA-CB	6.39	1.61	1.54
1	C	144	VAL	CA-CB	6.25	1.61	1.54
1	A	143	THR	CA-CB	6.20	1.62	1.53
1	D	80	ILE	CA-CB	5.88	1.63	1.54
1	A	91	VAL	CA-CB	5.69	1.60	1.54
1	D	84	ALA	CA-CB	5.68	1.62	1.53
1	C	44	ILE	CA-CB	5.66	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	38	VAL	CA-CB	5.50	1.61	1.54
1	D	72	TRP	C-O	-5.46	1.19	1.24
1	B	38	VAL	CA-CB	5.39	1.60	1.54
1	B	72	TRP	C-O	-5.28	1.19	1.24
1	A	111	THR	CA-CB	5.25	1.62	1.53
1	A	206	ASP	C-O	-5.22	1.19	1.24
1	A	117	GLU	CA-C	5.12	1.58	1.52
1	C	53	PRO	CA-C	5.12	1.59	1.52
1	A	159	LEU	CA-C	5.03	1.58	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LEU	CA-C-N	12.54	135.51	119.84
1	A	197	LEU	C-N-CA	12.54	135.51	119.84
1	A	37	ARG	N-CA-C	8.08	125.79	113.51
1	B	53	PRO	O-C-N	7.86	132.73	123.06
1	C	52	GLY	CA-C-N	7.74	129.52	119.84
1	C	52	GLY	C-N-CA	7.74	129.52	119.84
1	D	36	ARG	CA-C-N	7.33	134.89	121.70
1	D	36	ARG	C-N-CA	7.33	134.89	121.70
1	D	144	VAL	CB-CA-C	6.72	119.98	110.84
1	A	143	THR	CB-CA-C	6.25	120.54	109.72
1	B	180	ASP	N-CA-C	6.02	123.62	110.80
1	B	39	SER	N-CA-C	5.82	123.20	110.80
1	B	41	GLY	N-CA-C	5.77	124.11	112.34
1	D	36	ARG	N-CA-C	5.72	122.97	110.80
1	A	91	VAL	CB-CA-C	5.67	118.75	110.98
1	C	53	PRO	N-CA-C	5.62	124.05	112.47
1	A	156	VAL	CB-CA-C	-5.45	101.96	110.69
1	A	36	ARG	CA-C-N	5.41	135.36	126.86
1	A	36	ARG	C-N-CA	5.41	135.36	126.86
1	C	75	ARG	CG-CD-NE	-5.40	100.12	112.00
1	C	123	LYS	CA-C-N	5.21	125.21	119.90
1	C	123	LYS	C-N-CA	5.21	125.21	119.90
1	A	201	CYS	CA-CB-SG	-5.12	102.63	114.40
1	D	72	TRP	CA-C-N	-5.08	114.38	119.56
1	D	72	TRP	C-N-CA	-5.08	114.38	119.56

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	LEU	Peptide
1	A	35	TRP	Peptide
1	A	36	ARG	Peptide
1	B	53	PRO	Peptide

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	1505	0	1474	63	0
1	B	1496	0	1474	56	0
1	C	1502	0	1475	41	0
1	D	1497	0	1468	55	0
2	E	39	0	35	3	0
2	F	39	0	35	6	0
2	G	39	0	35	1	0
2	H	39	0	35	2	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
3	C	3	0	0	1	0
3	D	3	0	0	0	0
4	A	128	0	0	8	0
4	B	131	0	0	7	0
4	C	145	0	0	13	0
4	D	129	0	0	14	0
All	All	6701	0	6031	220	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 18.

All (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:HD21	2:F:1:NAG:C1	1.11	1.59
1:B:160:MET:SD	3:B:1222:PT:PT	1.03	1.39
1:C:160:MET:SD	3:C:1222:PT:PT	1.06	1.31
1:C:36[B]:ARG:CZ	4:C:2017:HOH:O	1.80	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ALA:CB	1:D:29:VAL:HG21	1.65	1.25
1:B:87:PHE:CE2	1:B:106:MET:HE3	1.71	1.25
1:B:36:ARG:N	1:B:37:ARG:HA	1.61	1.14
1:B:36:ARG:H	1:B:37:ARG:CA	1.52	1.14
1:D:23:ALA:HB2	1:D:29:VAL:HG21	1.08	1.03
1:C:160:MET:SD	4:C:2132:HOH:O	2.20	1.00
1:A:23:ALA:HB2	1:A:29:VAL:HG21	1.41	0.98
1:B:36:ARG:H	1:B:37:ARG:HA	0.82	0.98
1:C:36[B]:ARG:NH1	4:C:2017:HOH:O	1.90	0.98
1:A:23:ALA:HB2	1:A:29:VAL:CG2	1.94	0.97
1:B:87:PHE:HE2	1:B:106:MET:HE3	1.13	0.94
1:D:23:ALA:HB2	1:D:29:VAL:CG2	1.97	0.94
1:B:87:PHE:HE2	1:B:106:MET:CE	1.80	0.94
1:D:115:LYS:HG3	4:D:2013:HOH:O	1.68	0.93
1:D:117[B]:GLU:HB2	4:D:2078:HOH:O	1.69	0.93
1:C:36[B]:ARG:NH2	4:C:2020:HOH:O	1.95	0.91
1:A:156:VAL:HG22	1:A:185:VAL:CG1	2.00	0.91
1:D:177:LYS:HE3	4:D:2113:HOH:O	1.70	0.91
1:A:156:VAL:HG22	1:A:185:VAL:HG12	1.49	0.91
2:E:2:NAG:C4	2:E:3:MAN:C1	2.50	0.89
1:B:34:TYR:C	1:B:106:MET:HE1	1.96	0.89
1:B:87:PHE:CD2	1:B:106:MET:HE3	2.09	0.88
2:G:2:NAG:HO4	2:G:3:MAN:C1	1.85	0.87
1:B:35:TRP:HA	1:B:36:ARG:HB2	1.55	0.87
1:A:143:THR:HG23	4:A:2098:HOH:O	1.74	0.85
1:B:29:VAL:HG11	1:B:119:LEU:HD11	1.58	0.84
1:D:156:VAL:HG23	1:D:185:VAL:HG13	1.61	0.83
1:A:36:ARG:HG3	1:A:37:ARG:HB2	1.62	0.81
1:D:117[A]:GLU:HB2	4:D:2078:HOH:O	1.79	0.81
1:A:155:HIS:HD2	4:A:2115:HOH:O	1.63	0.81
1:C:117:GLU:HB2	4:C:2091:HOH:O	1.81	0.80
1:A:160:MET:SD	1:A:196:HIS:ND1	2.56	0.79
1:D:23:ALA:HB1	1:D:29:VAL:HG21	1.63	0.79
1:A:160:MET:HB3	1:A:196:HIS:CE1	2.18	0.78
1:A:72:TRP:HE3	4:A:2049:HOH:O	1.66	0.78
1:B:34:TYR:HE1	1:B:37:ARG:HG3	1.47	0.78
1:C:156:VAL:CG2	1:C:185:VAL:HG13	2.15	0.76
1:D:29:VAL:HG11	1:D:119:LEU:HD11	1.67	0.75
1:C:36[B]:ARG:NH2	4:C:2017:HOH:O	1.98	0.75
1:A:160:MET:HB3	1:A:196:HIS:HE1	1.51	0.75
1:A:161:PRO:HD3	1:A:198:PRO:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:CG2	4:B:2003:HOH:O	2.35	0.73
1:A:29:VAL:HG12	1:A:91:VAL:HG13	1.71	0.73
1:B:29:VAL:HG12	1:B:91:VAL:CG1	2.17	0.72
1:B:95:ASN:CG	2:F:1:NAG:C1	2.61	0.72
1:C:219:LEU:O	1:C:220:SER:HB2	1.88	0.72
1:D:29:VAL:HG11	1:D:119:LEU:CD1	2.19	0.72
1:A:51:LEU:HD21	1:A:103:LEU:HD22	1.71	0.71
1:C:204:LYS:HE3	1:C:209:GLU:HB2	1.71	0.71
1:B:23:ALA:HB2	1:B:29:VAL:HG21	1.72	0.71
1:D:177:LYS:HG2	1:D:183:LEU:CD1	2.21	0.71
1:D:177:LYS:HG2	1:D:183:LEU:HD12	1.71	0.71
1:A:40:LEU:HD12	1:A:108:LEU:HD11	1.73	0.71
1:B:29:VAL:HG23	4:B:2009:HOH:O	1.91	0.70
1:C:54:GLY:O	1:C:55:GLU:HB2	1.92	0.69
1:A:23:ALA:CB	1:A:29:VAL:HG21	2.19	0.69
1:B:36:ARG:N	1:B:37:ARG:CA	2.37	0.69
1:A:156:VAL:CG2	1:A:185:VAL:CG1	2.70	0.69
1:B:155:HIS:HD2	4:B:2117:HOH:O	1.75	0.69
2:F:2:NAG:C4	2:F:3:MAN:C1	2.70	0.69
1:C:51:LEU:HD21	1:C:103:LEU:HD22	1.74	0.69
1:A:23:ALA:CB	1:A:29:VAL:CG2	2.71	0.68
1:B:87:PHE:CE2	1:B:106:MET:CE	2.58	0.68
1:B:180:ASP:HB3	1:B:182:SER:H	1.60	0.68
1:C:156:VAL:HG23	1:C:185:VAL:HG13	1.76	0.67
1:B:35:TRP:HA	1:B:36:ARG:CB	2.25	0.66
1:A:148:VAL:HG23	1:A:156:VAL:HG13	1.78	0.65
1:D:200:THR:HG22	4:D:2106:HOH:O	1.96	0.65
1:A:29:VAL:HG13	1:A:30:THR:N	2.11	0.64
1:B:145:THR:HB	1:B:188:ASP:OD2	1.97	0.64
1:D:105:ARG:CG	1:D:114:THR:HG22	2.26	0.64
1:D:38:VAL:HG23	4:D:2022:HOH:O	1.97	0.64
1:D:35:TRP:HH2	1:D:111:THR:HG23	1.63	0.64
2:F:2:NAG:O4	2:F:3:MAN:C2	2.44	0.64
1:B:29:VAL:HG11	1:B:119:LEU:CD1	2.26	0.64
1:A:29:VAL:CG1	1:A:91:VAL:HG13	2.27	0.64
1:D:29:VAL:HG22	4:D:2010:HOH:O	1.96	0.63
1:D:105:ARG:HG2	1:D:114:THR:HG22	1.80	0.63
1:A:36:ARG:HB3	1:A:37:ARG:CA	2.29	0.63
1:A:161:PRO:HD2	1:A:196:HIS:CE1	2.34	0.62
1:B:29:VAL:HG12	1:B:91:VAL:HG11	1.79	0.62
1:B:29:VAL:HG12	1:B:91:VAL:HG12	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ALA:HB2	1:C:29:VAL:HG11	1.81	0.62
2:H:2:NAG:C4	2:H:3:MAN:C1	2.78	0.62
1:D:23:ALA:CB	1:D:29:VAL:CG2	2.60	0.61
1:D:21:VAL:HG13	1:D:31:LEU:CD2	2.30	0.61
1:C:155:HIS:HD2	4:C:2134:HOH:O	1.83	0.61
1:B:29:VAL:HG22	4:B:2012:HOH:O	2.00	0.60
1:D:37:ARG:O	1:D:38:VAL:C	2.43	0.60
1:D:36:ARG:HG2	4:D:2018:HOH:O	2.01	0.59
1:A:47:SER:HB3	1:A:62:ARG:HG2	1.84	0.59
1:A:131:SER:HB2	1:A:142:LEU:HD22	1.85	0.59
1:D:115:LYS:CG	4:D:2013:HOH:O	2.37	0.58
2:E:2:NAG:H4	2:E:3:MAN:C1	2.34	0.57
1:A:219:LEU:C	1:A:219:LEU:HD12	2.30	0.57
1:D:115:LYS:CD	1:D:117[B]:GLU:OE1	2.52	0.57
1:B:34:TYR:O	1:B:106:MET:HE1	2.04	0.56
1:C:51:LEU:HD11	1:C:103:LEU:HD13	1.86	0.56
1:D:47:SER:HB3	1:D:62:ARG:HG2	1.87	0.56
1:A:106:MET:HE3	1:A:113:VAL:HG23	1.88	0.56
1:A:148:VAL:CG2	1:A:156:VAL:HG13	2.36	0.56
1:A:156:VAL:CG2	1:A:185:VAL:HG12	2.30	0.56
1:B:32:THR:HG22	1:B:88:PHE:CD1	2.41	0.56
1:C:36[A]:ARG:HG3	1:C:37:ARG:N	2.22	0.55
1:A:200:THR:HB	1:A:213:VAL:HG22	1.87	0.55
1:D:29:VAL:HB	1:D:91:VAL:CG1	2.37	0.55
1:C:36[B]:ARG:CG	1:C:37:ARG:N	2.70	0.55
1:C:37:ARG:HD3	4:C:2024:HOH:O	2.06	0.54
1:A:55:GLU:OE2	1:A:55:GLU:HA	2.07	0.54
1:B:95:ASN:ND2	2:F:1:NAG:C2	2.66	0.54
1:A:36:ARG:HB3	1:A:37:ARG:C	2.32	0.54
1:D:25:LEU:HD12	1:D:95:ASN:HA	1.90	0.53
1:D:36:ARG:HB3	1:D:37:ARG:HB2	1.90	0.53
1:A:24:PHE:HZ	1:D:219:LEU:HD22	1.73	0.53
1:A:36:ARG:HB3	1:A:38:VAL:N	2.23	0.53
1:B:148:VAL:HG23	1:B:156:VAL:HG22	1.91	0.53
1:B:43:GLU:O	1:B:64:HIS:HE1	1.92	0.53
1:B:144:VAL:HG23	1:B:158:TRP:CZ2	2.44	0.53
1:C:196:HIS:HB3	4:C:2132:HOH:O	2.07	0.53
1:D:156:VAL:CG2	1:D:185:VAL:HG13	2.35	0.53
1:A:143:THR:CG2	4:A:2098:HOH:O	2.42	0.52
1:D:108:LEU:O	1:D:111:THR:HG22	2.10	0.52
1:A:153:HIS:H	1:A:205:ASN:ND2	2.07	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:C	1:A:219:LEU:CD1	2.82	0.52
1:C:36[B]:ARG:HG3	1:C:37:ARG:N	2.21	0.52
1:D:28:ARG:O	1:D:29:VAL:HG23	2.09	0.52
1:B:31:LEU:HD13	1:B:117:GLU:HB3	1.92	0.52
1:A:35:TRP:HD1	1:A:36:ARG:HB2	1.75	0.51
1:A:36:ARG:CG	1:A:37:ARG:HB2	2.38	0.51
1:D:105:ARG:HG3	1:D:114:THR:HG22	1.92	0.51
1:D:30:THR:HG21	1:D:88:PHE:HD1	1.74	0.51
1:D:115:LYS:HD3	1:D:117[B]:GLU:OE1	2.10	0.50
1:A:81:HIS:HE1	4:A:2056:HOH:O	1.92	0.50
1:D:21:VAL:CG1	1:D:31:LEU:HD23	2.41	0.50
1:B:23:ALA:HB2	1:B:29:VAL:CG2	2.41	0.50
1:C:45:GLU:HG2	1:C:64:HIS:CE1	2.47	0.50
1:D:35:TRP:CH2	1:D:111:THR:HG23	2.45	0.50
1:B:35:TRP:N	1:B:106:MET:HE1	2.28	0.49
1:C:72:TRP:NE1	4:C:2059:HOH:O	2.13	0.49
1:A:152:PRO:HD2	1:A:205:ASN:HD21	1.77	0.49
1:B:29:VAL:HG23	4:B:2003:HOH:O	2.10	0.49
1:B:130[B]:HIS:CE1	1:C:124:PRO:HB2	2.47	0.49
2:F:2:NAG:H4	2:F:3:MAN:C1	2.42	0.49
1:A:29:VAL:HG21	1:A:119:LEU:HD11	1.96	0.48
1:A:101:ASN:ND2	1:A:118:HIS:ND1	2.62	0.48
1:A:155:HIS:CD2	4:A:2115:HOH:O	2.50	0.48
1:B:35:TRP:HD1	1:B:38:VAL:O	1.97	0.48
1:D:28:ARG:C	1:D:29:VAL:HG23	2.39	0.48
1:A:156:VAL:CG2	1:A:185:VAL:HG13	2.43	0.47
1:C:158:TRP:CZ3	1:C:199:VAL:HG13	2.50	0.47
1:A:21:VAL:HG13	1:A:31:LEU:CD2	2.45	0.46
1:D:36:ARG:HA	4:D:2018:HOH:O	2.15	0.46
1:C:54:GLY:O	1:C:55:GLU:CB	2.63	0.46
1:A:125:LEU:HD12	1:A:125:LEU:C	2.41	0.46
1:C:53:PRO:HB2	1:C:54:GLY:HA3	1.97	0.46
1:C:36[A]:ARG:HG2	4:C:2018:HOH:O	2.15	0.46
1:C:70:ILE:HB	1:C:75:ARG:HD2	1.96	0.46
1:A:52:GLY:O	1:A:53:PRO:C	2.58	0.46
1:D:43:GLU:OE2	1:D:65:HIS:NE2	2.47	0.46
1:A:23:ALA:CB	1:A:29:VAL:HG23	2.46	0.46
2:E:2:NAG:HO4	2:E:3:MAN:C1	2.20	0.46
1:A:53:PRO:HB2	1:A:54:GLY:CA	2.46	0.46
1:B:143:THR:HG22	4:B:2098:HOH:O	2.15	0.46
1:D:29:VAL:HG11	1:D:119:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:CD1	1:A:116:GLN:HG2	2.46	0.45
1:A:54:GLY:O	1:A:55:GLU:HB2	2.17	0.45
1:C:125:LEU:HA	1:C:149:ASN:O	2.17	0.45
1:A:35:TRP:CD1	1:A:36:ARG:HB2	2.51	0.44
1:A:45:GLU:HG2	1:A:64:HIS:CD2	2.52	0.44
1:B:153:HIS:H	1:B:205:ASN:ND2	2.14	0.44
1:C:29:VAL:HG12	4:C:2009:HOH:O	2.18	0.44
1:C:156:VAL:HG22	1:C:185:VAL:HG13	1.99	0.44
1:C:36[B]:ARG:NH1	4:C:2014:HOH:O	2.49	0.44
1:D:36:ARG:CB	4:D:2022:HOH:O	2.65	0.44
1:D:160:MET:N	1:D:161:PRO:HD3	2.33	0.44
1:D:175:VAL:HG12	1:D:176:MET:N	2.33	0.44
1:D:115:LYS:CB	4:D:2013:HOH:O	2.66	0.44
1:C:148:VAL:HG21	1:C:203:GLY:HA3	1.99	0.44
1:A:24:PHE:CZ	1:D:219:LEU:HD22	2.51	0.44
1:D:115:LYS:HB2	4:D:2013:HOH:O	2.17	0.43
1:B:91:VAL:O	1:B:91:VAL:HG13	2.18	0.43
1:B:145:THR:CG2	4:B:2099:HOH:O	2.66	0.43
1:D:29:VAL:CG2	4:D:2010:HOH:O	2.60	0.43
1:D:70:ILE:HB	1:D:75:ARG:HD2	1.99	0.43
1:A:115:LYS:HE2	1:A:117:GLU:HG2	1.99	0.43
1:B:103:LEU:HD11	1:B:114:THR:HG22	1.99	0.43
1:B:160:MET:SD	1:B:196:HIS:ND1	2.91	0.43
1:A:125:LEU:HA	1:A:149:ASN:O	2.18	0.43
1:C:153:HIS:H	1:C:205:ASN:ND2	2.16	0.43
2:H:2:NAG:O4	2:H:3:MAN:C2	2.64	0.43
1:B:129:VAL:HG11	1:B:212:GLY:HA3	2.01	0.43
1:A:196:HIS:HB2	4:A:2113:HOH:O	2.19	0.43
1:B:148:VAL:HG21	1:B:203:GLY:HA3	2.00	0.42
1:A:151:PHE:CD1	1:A:152:PRO:HA	2.54	0.42
1:B:124:PRO:HB2	1:C:130[B]:HIS:CE1	2.55	0.42
1:A:196:HIS:CG	4:A:2113:HOH:O	2.72	0.42
1:A:35:TRP:HE1	1:A:36:ARG:NH2	2.18	0.41
1:B:35:TRP:CG	1:B:36:ARG:HB3	2.56	0.41
1:C:37:ARG:HD2	1:C:40:LEU:HG	2.01	0.41
1:A:161:PRO:HD2	1:A:196:HIS:ND1	2.34	0.41
1:B:21:VAL:N	1:B:118:HIS:O	2.53	0.41
1:D:21:VAL:CG1	1:D:31:LEU:CD2	2.95	0.41
1:D:29:VAL:HB	1:D:91:VAL:HG12	2.02	0.41
1:D:203:GLY:O	1:D:209:GLU:HA	2.21	0.41
1:B:179:LYS:HD2	1:B:179:LYS:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:CYS:HB2	1:D:158:TRP:CZ2	2.55	0.41
1:C:189:LEU:CD2	1:C:199:VAL:HG21	2.51	0.41
1:B:152:PRO:HD2	1:B:205:ASN:HD21	1.84	0.41
1:B:160:MET:C	1:B:196:HIS:HE1	2.29	0.41
1:C:204:LYS:HB3	1:C:204:LYS:HE2	1.77	0.41
1:D:25:LEU:CD1	1:D:95:ASN:HA	2.50	0.41
1:C:140:SER:HB2	1:C:193:LYS:HD2	2.03	0.41
1:C:103:LEU:HG	1:C:114:THR:CG2	2.51	0.40
1:B:78:PHE:HA	1:B:90:VAL:O	2.21	0.40
1:A:40:LEU:HD12	1:A:108:LEU:CD1	2.47	0.40
1:B:35:TRP:CD2	1:B:36:ARG:CB	3.05	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	186/201 (92%)	174 (94%)	8 (4%)	4 (2%)	5	4
1	B	184/201 (92%)	173 (94%)	7 (4%)	4 (2%)	5	4
1	C	185/201 (92%)	177 (96%)	6 (3%)	2 (1%)	11	13
1	D	184/201 (92%)	175 (95%)	7 (4%)	2 (1%)	11	13
All	All	739/804 (92%)	699 (95%)	28 (4%)	12 (2%)	7	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	PRO
1	A	198	PRO
1	B	39	SER
1	B	195	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	53	PRO
1	D	36	ARG
1	A	36	ARG
1	B	36	ARG
1	B	41	GLY
1	D	38	VAL
1	A	41	GLY
1	C	41	GLY

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	169/176 (96%)	150 (89%)	19 (11%)	6	7
1	B	169/176 (96%)	149 (88%)	20 (12%)	5	6
1	C	170/176 (97%)	153 (90%)	17 (10%)	7	9
1	D	169/176 (96%)	147 (87%)	22 (13%)	4	4
All	All	677/704 (96%)	599 (88%)	78 (12%)	5	6

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	29	VAL
1	A	30	THR
1	A	36	ARG
1	A	68	ILE
1	A	91	VAL
1	A	111	THR
1	A	116	GLN
1	A	129	VAL
1	A	142	LEU
1	A	143	THR
1	A	156	VAL
1	A	176	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	179	LYS
1	A	183	LEU
1	A	185	VAL
1	A	197	LEU
1	A	200	THR
1	A	219	LEU
1	B	21	VAL
1	B	29	VAL
1	B	38	VAL
1	B	72	TRP
1	B	83	SER
1	B	90	VAL
1	B	108	LEU
1	B	111	THR
1	B	115	LYS
1	B	117	GLU
1	B	142	LEU
1	B	144	VAL
1	B	145	THR
1	B	160	MET
1	B	178	GLU
1	B	179	LYS
1	B	180	ASP
1	B	197	LEU
1	B	219	LEU
1	B	220	SER
1	C	21	VAL
1	C	29	VAL
1	C	37	ARG
1	C	43	GLU
1	C	72	TRP
1	C	91	VAL
1	C	103	LEU
1	C	108	LEU
1	C	111	THR
1	C	115	LYS
1	C	117	GLU
1	C	142	LEU
1	C	156	VAL
1	C	183	LEU
1	C	200	THR
1	C	219	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	220	SER
1	D	21	VAL
1	D	36	ARG
1	D	37	ARG
1	D	38	VAL
1	D	45	GLU
1	D	47	SER
1	D	90	VAL
1	D	108	LEU
1	D	111	THR
1	D	112	GLU
1	D	113	VAL
1	D	115	LYS
1	D	117[A]	GLU
1	D	117[B]	GLU
1	D	142	LEU
1	D	160	MET
1	D	177	LYS
1	D	178	GLU
1	D	179	LYS
1	D	183	LEU
1	D	197	LEU
1	D	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	81	HIS
1	A	101	ASN
1	A	155	HIS
1	A	157	GLN
1	A	205	ASN
1	B	64	HIS
1	B	155	HIS
1	B	205	ASN
1	C	65	HIS
1	C	135	GLN
1	C	155	HIS
1	C	205	ASN
1	D	85	ASN

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](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.70	0	17,19,21	1.70	4 (23%)
2	NAG	E	2	2	14,14,15	1.03	1 (7%)	17,19,21	2.03	6 (35%)
2	MAN	E	3	2	11,11,12	0.87	0	15,15,17	1.62	3 (20%)
2	NAG	F	1	1,2	14,14,15	0.77	0	17,19,21	1.23	2 (11%)
2	NAG	F	2	2	14,14,15	0.80	0	17,19,21	1.95	5 (29%)
2	MAN	F	3	2	11,11,12	0.93	1 (9%)	15,15,17	1.73	3 (20%)
2	NAG	G	1	1,2	14,14,15	0.75	0	17,19,21	1.92	3 (17%)
2	NAG	G	2	2	14,14,15	0.98	1 (7%)	17,19,21	2.26	5 (29%)
2	MAN	G	3	2	11,11,12	0.94	0	15,15,17	1.82	5 (33%)
2	NAG	H	1	1,2	14,14,15	0.78	0	17,19,21	2.21	4 (23%)
2	NAG	H	2	2	14,14,15	0.93	0	17,19,21	1.66	3 (17%)
2	MAN	H	3	2	11,11,12	1.14	2 (18%)	15,15,17	1.61	3 (20%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	MAN	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	MAN	H	3	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	O5-C1	-2.22	1.40	1.43
2	F	3	MAN	O5-C1	-2.19	1.40	1.43
2	E	2	NAG	O5-C1	-2.11	1.40	1.43
2	H	3	MAN	O5-C1	-2.05	1.40	1.43
2	H	3	MAN	C4-C5	2.01	1.57	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C4-C3-C2	-7.23	100.42	111.02
2	G	1	NAG	O5-C1-C2	6.03	120.63	111.29
2	G	2	NAG	C1-C2-N2	-5.48	101.81	110.43
2	F	3	MAN	C3-C4-C5	4.60	118.57	110.23
2	G	2	NAG	O5-C1-C2	4.14	117.69	111.29
2	F	2	NAG	C2-N2-C7	-4.00	117.54	122.90
2	E	3	MAN	O4-C4-C3	-3.99	100.96	110.38
2	H	2	NAG	C1-C2-N2	-3.91	104.27	110.43
2	E	2	NAG	O4-C4-C5	-3.85	99.84	109.32
2	F	2	NAG	C1-O5-C5	-3.84	107.04	112.19
2	G	2	NAG	C4-C3-C2	-3.81	105.44	111.02
2	E	2	NAG	C1-C2-N2	-3.76	104.51	110.43
2	H	3	MAN	C3-C4-C5	3.73	116.99	110.23
2	G	3	MAN	C1-O5-C5	-3.60	107.36	112.19
2	E	1	NAG	C6-C5-C4	-3.46	104.53	113.02
2	F	2	NAG	C1-C2-N2	-3.31	105.21	110.43
2	E	2	NAG	O5-C5-C6	3.10	113.70	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C1-C2	3.09	116.08	111.29
2	H	1	NAG	C1-C2-N2	3.05	115.25	110.43
2	G	2	NAG	O5-C5-C4	-3.04	103.42	110.83
2	E	2	NAG	O5-C1-C2	3.01	115.95	111.29
2	H	2	NAG	O5-C1-C2	2.94	115.84	111.29
2	E	3	MAN	O5-C1-C2	2.91	117.73	110.79
2	H	3	MAN	O3-C3-C4	2.80	116.98	110.38
2	G	3	MAN	C1-C2-C3	-2.75	105.63	109.64
2	G	1	NAG	C6-C5-C4	-2.67	106.46	113.02
2	E	2	NAG	C3-C4-C5	2.67	115.07	110.23
2	H	3	MAN	C1-C2-C3	-2.67	105.76	109.64
2	H	1	NAG	C3-C4-C5	2.61	114.96	110.23
2	F	1	NAG	C4-C3-C2	-2.56	107.27	111.02
2	G	3	MAN	C3-C4-C5	2.54	114.84	110.23
2	F	2	NAG	C8-C7-N2	2.47	120.22	116.12
2	E	3	MAN	C6-C5-C4	2.45	119.02	113.02
2	H	1	NAG	O5-C5-C4	-2.42	104.93	110.83
2	G	2	NAG	C2-N2-C7	-2.42	119.66	122.90
2	H	2	NAG	O6-C6-C5	-2.41	103.12	111.33
2	F	1	NAG	O5-C5-C4	-2.38	105.03	110.83
2	G	3	MAN	O4-C4-C3	-2.36	104.82	110.38
2	F	2	NAG	C3-C4-C5	2.32	114.44	110.23
2	E	1	NAG	C3-C4-C5	2.30	114.40	110.23
2	G	3	MAN	O3-C3-C4	2.25	115.67	110.38
2	E	2	NAG	C4-C3-C2	-2.22	107.77	111.02
2	E	1	NAG	O5-C5-C6	2.19	111.92	107.66
2	F	3	MAN	O4-C4-C3	-2.10	105.42	110.38
2	F	3	MAN	C2-C3-C4	2.06	114.49	110.86
2	G	1	NAG	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

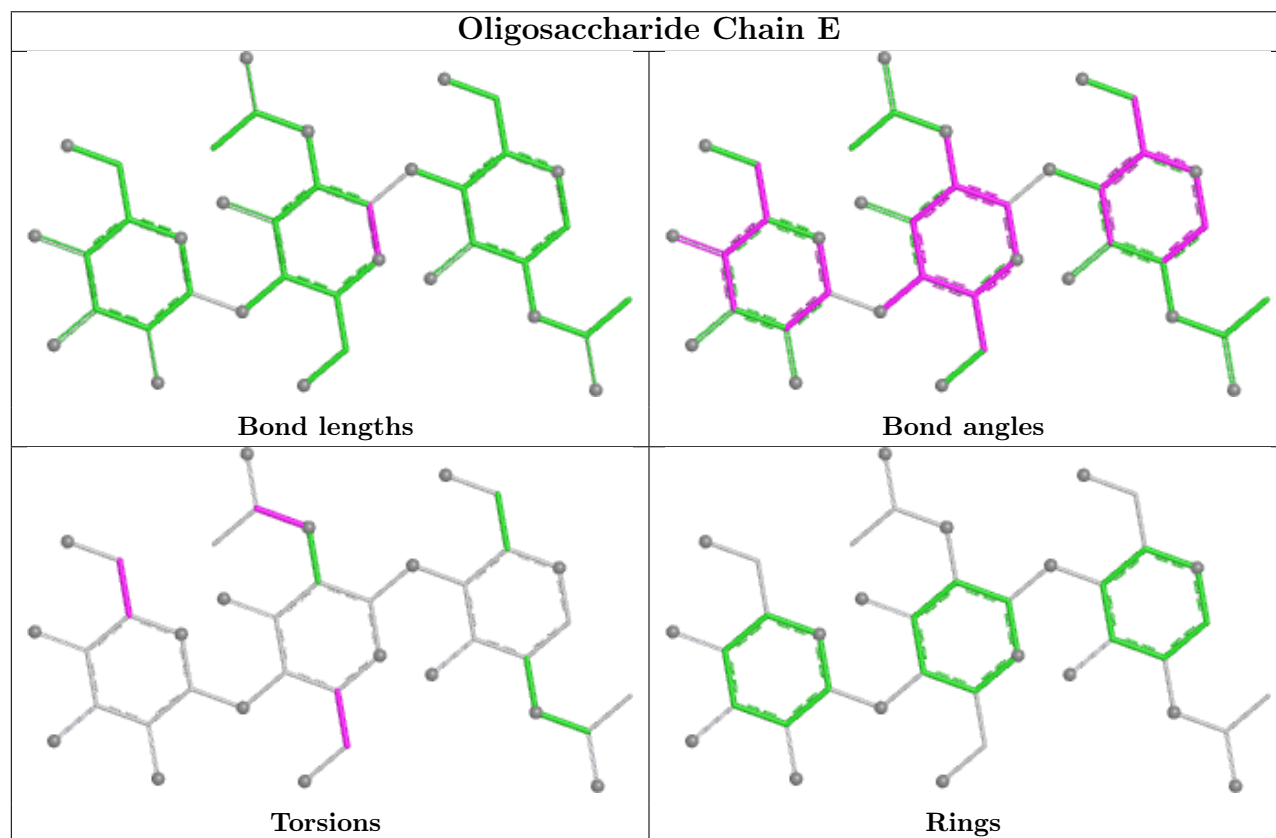
Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C3-C2-N2-C7

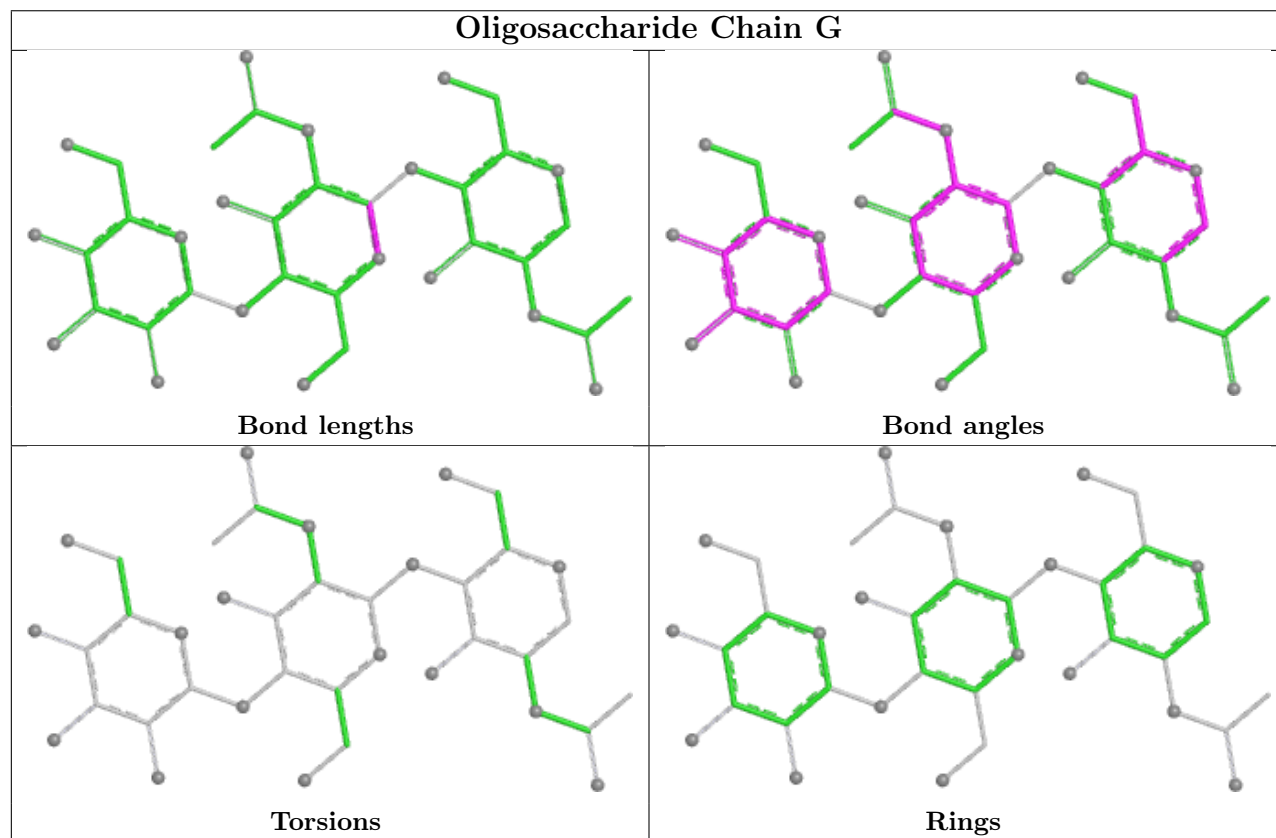
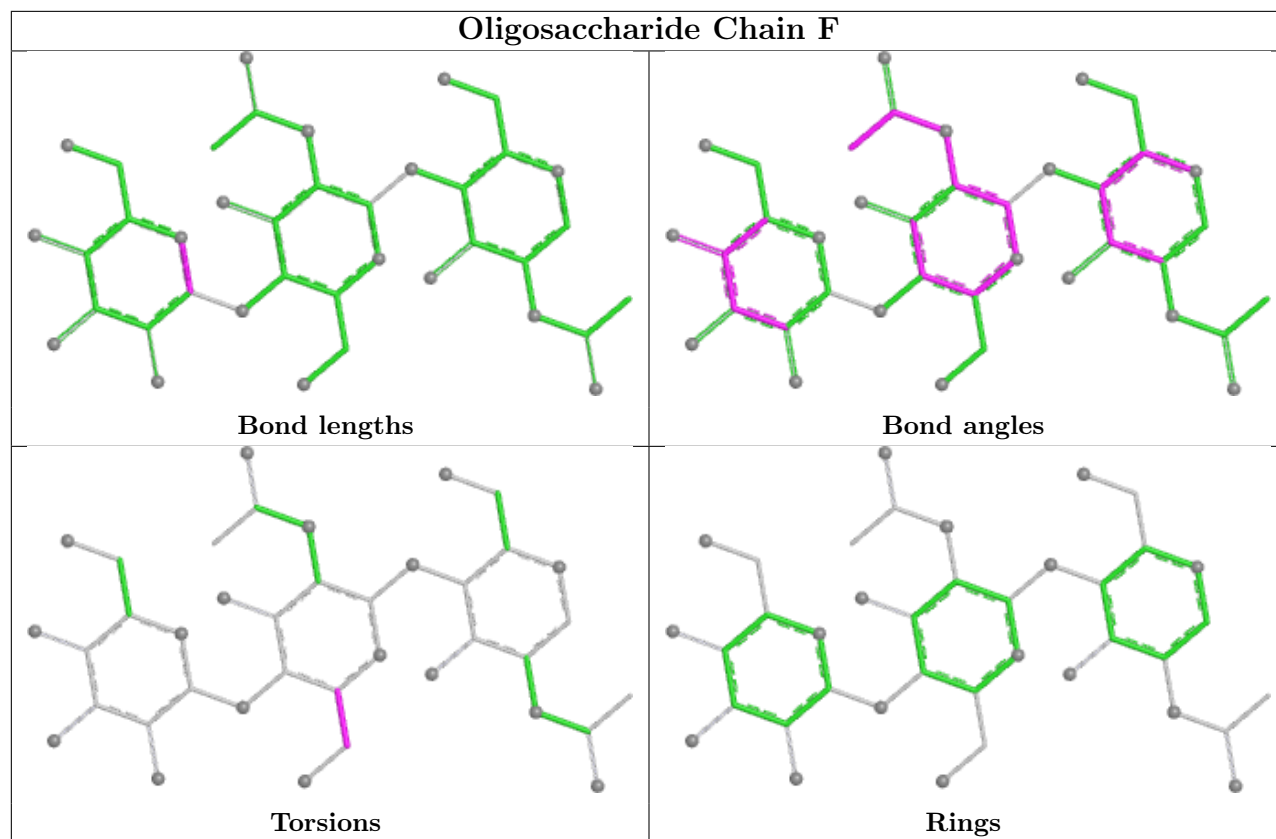
There are no ring outliers.

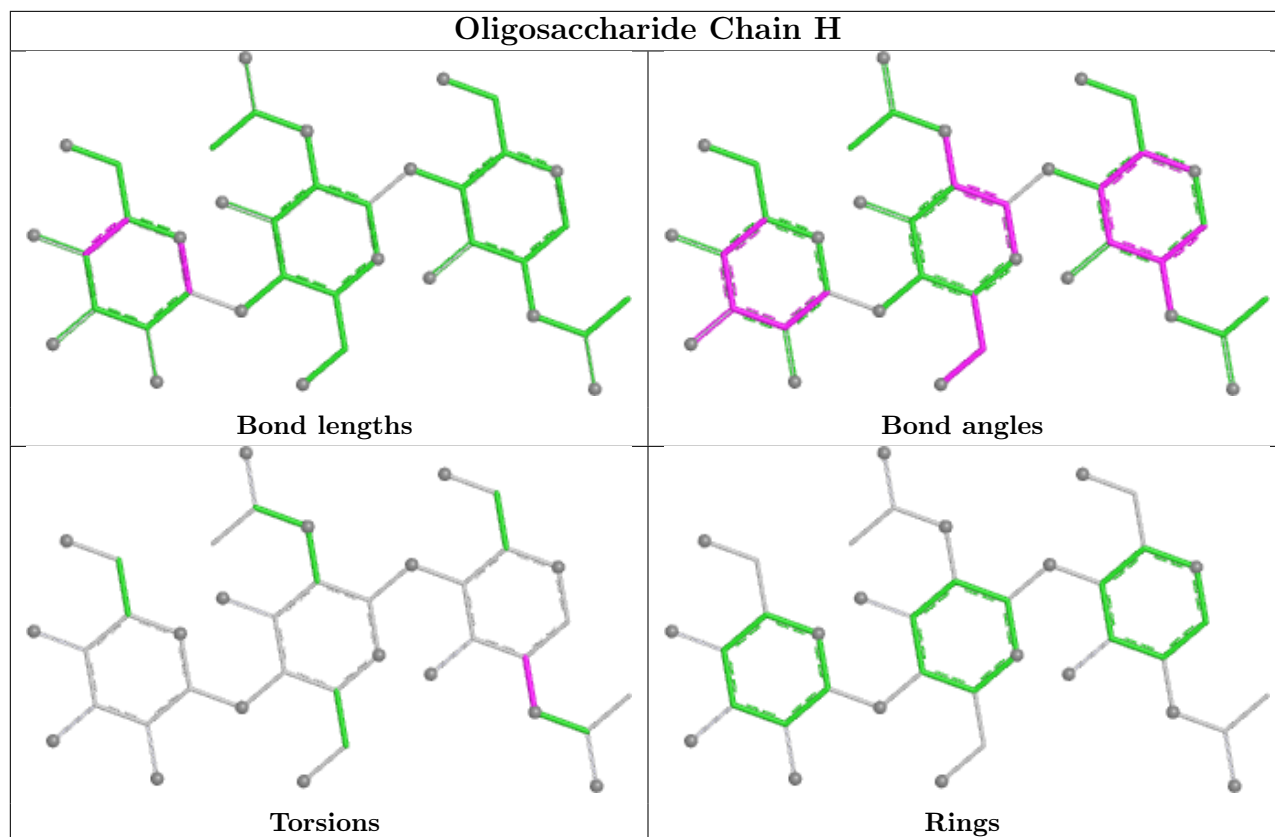
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	3	0
2	H	3	MAN	2	0
2	E	3	MAN	3	0
2	F	1	NAG	3	0
2	H	2	NAG	2	0
2	G	3	MAN	1	0
2	F	3	MAN	3	0
2	G	2	NAG	1	0
2	E	2	NAG	3	0

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







5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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](#)

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	188/201 (93%)	-1.42	0 100 100	19, 28, 40, 52	2 (1%)
1	B	186/201 (92%)	-1.43	0 100 100	19, 29, 39, 51	2 (1%)
1	C	186/201 (92%)	-1.48	0 100 100	17, 28, 38, 47	3 (1%)
1	D	186/201 (92%)	-1.41	0 100 100	18, 29, 39, 52	2 (1%)
All	All	746/804 (92%)	-1.43	0 100 100	17, 29, 40, 52	9 (1%)

There are no RSRZ outliers to report.

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.

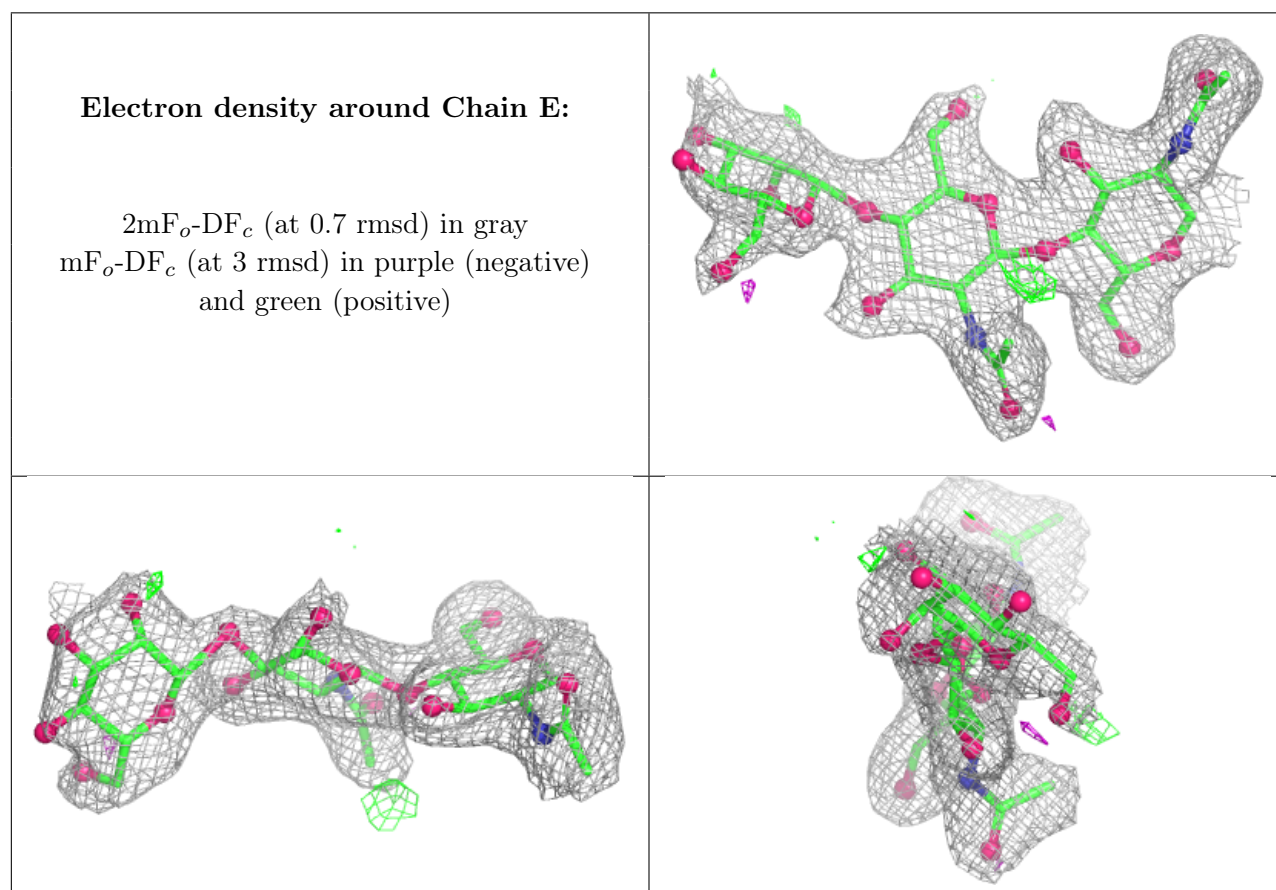
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	G	3	11/12	0.96	0.06	59,63,66,66	0
2	MAN	H	3	11/12	0.96	0.06	53,57,58,59	0
2	MAN	E	3	11/12	0.97	0.05	52,54,56,57	0
2	MAN	F	3	11/12	0.97	0.05	47,52,57,59	0
2	NAG	F	2	14/15	0.99	0.03	28,35,41,42	0
2	NAG	E	2	14/15	0.99	0.04	29,32,38,43	0
2	NAG	G	1	14/15	0.99	0.03	22,30,38,40	0
2	NAG	G	2	14/15	0.99	0.04	25,35,39,40	0
2	NAG	E	1	14/15	0.99	0.03	21,27,35,36	0

Continued on next page...

Continued from previous page...

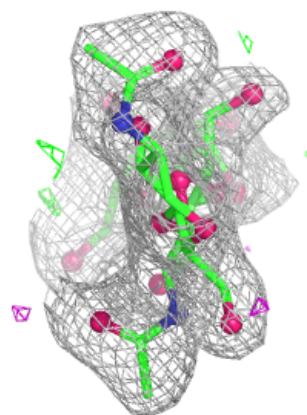
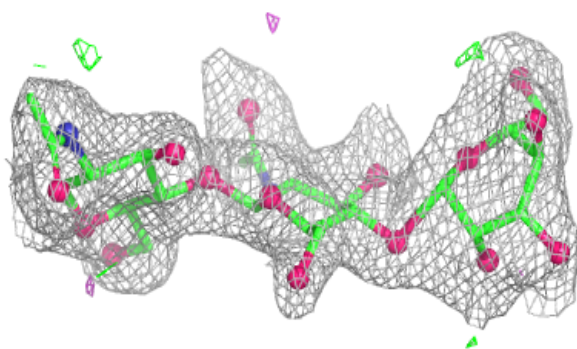
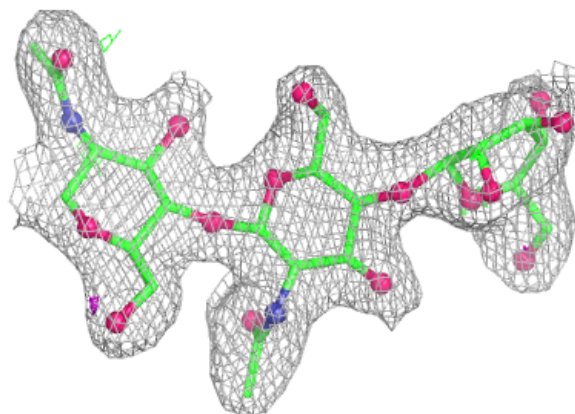
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	H	1	14/15	0.99	0.03	24,30,39,40	0
2	NAG	H	2	14/15	0.99	0.03	26,34,40,41	0
2	NAG	F	1	14/15	0.99	0.03	24,27,34,35	0

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.



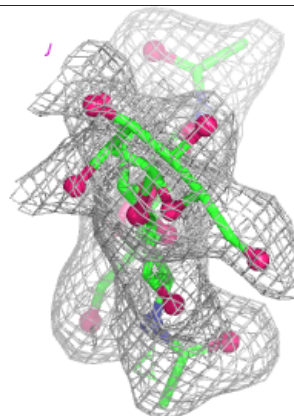
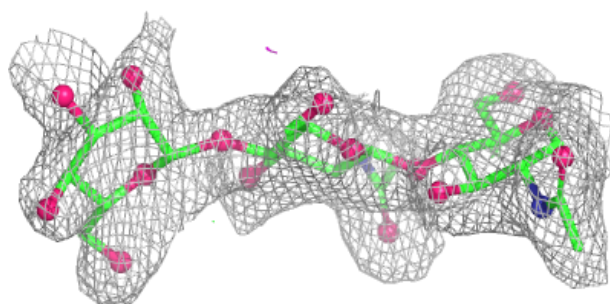
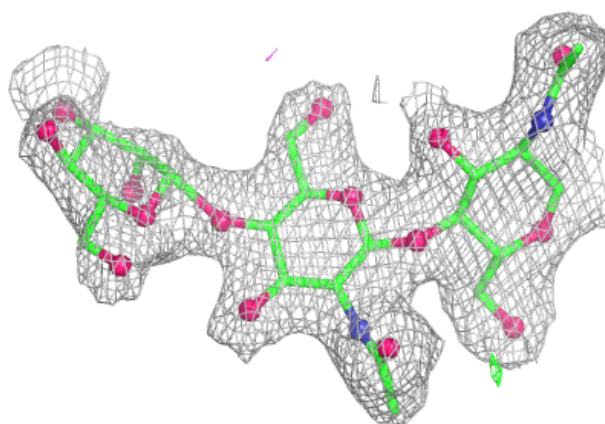
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

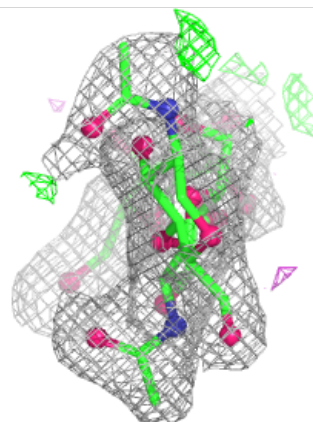
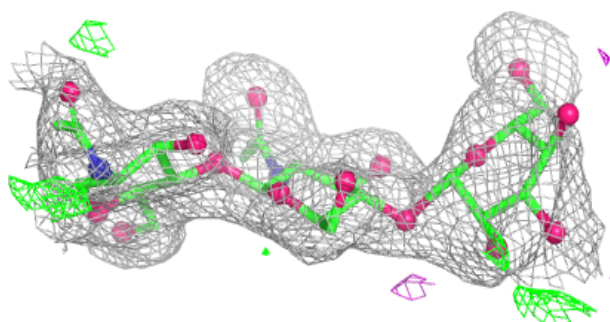
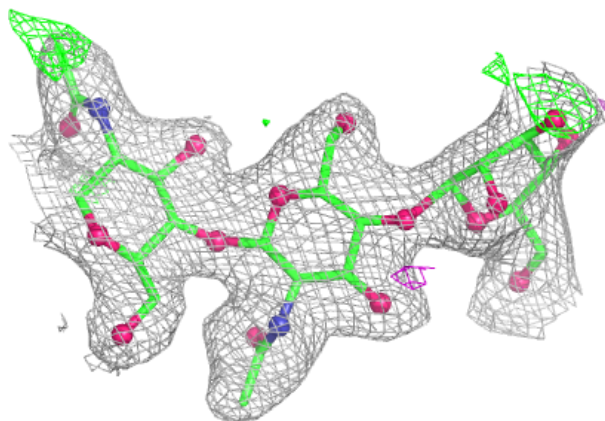


Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain H:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å ²)	Q<0.9
3	PT	D	1222	1/1	0.97	0.14	41,41,41,41	1
3	PT	A	1222	1/1	0.99	0.20	45,45,45,45	1
3	PT	B	1221	1/1	0.99	0.03	44,44,44,44	1
3	PT	B	1226	1/1	0.99	0.14	31,31,31,31	1
3	PT	C	1223	1/1	0.99	0.18	32,32,32,32	1
3	PT	A	1220	1/1	0.99	0.05	41,41,41,41	1
3	PT	C	1221	1/1	1.00	0.03	38,38,38,38	1
3	PT	C	1222	1/1	1.00	0.01	32,32,32,32	1
3	PT	B	1222	1/1	1.00	0.02	44,44,44,44	1
3	PT	D	1220	1/1	1.00	0.04	44,44,44,44	1
3	PT	D	1221	1/1	1.00	0.01	36,36,36,36	1
3	PT	A	1221	1/1	1.00	0.01	40,40,40,40	1

6.5 Other polymers [i](#)

There are no such residues in this entry.