



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:00 AM UTC

PDB ID : 4FA8 / pdb_00004fa8
Title : Multi-pronged modulation of cytokine signaling
Authors : He, X.; Shim, A.H.
Deposited on : 2012-05-21
Resolution : 2.20 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)
Xtrriage (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

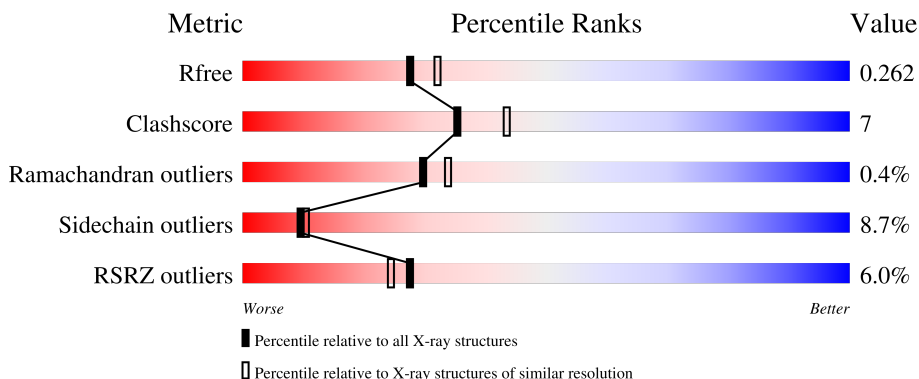
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

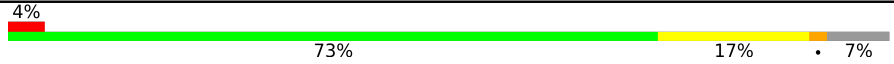
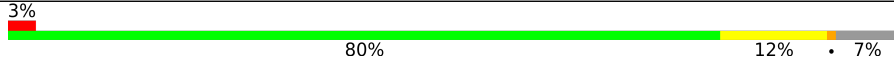



The reported resolution of this entry is 2.20 Å.

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.



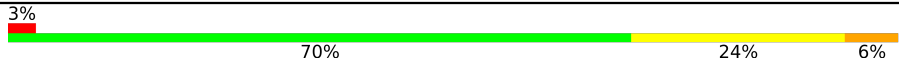

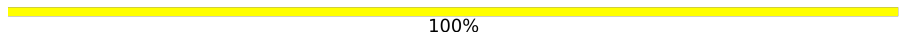
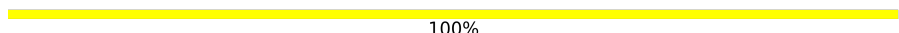
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	203	
1	B	203	
1	D	203	
2	E	147	
2	F	147	

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Mol	Chain	Length	Quality of chain
2	G	147	
3	C	3	
3	H	3	
3	I	3	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8676 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 Secreted protein BARF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	188	1497	968	255	267	7	0	0	0
1	B	189	1503	971	256	269	7	0	0	0
1	D	188	1497	968	255	267	7	0	0	0

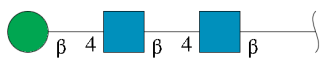
- Molecule 2 is a protein called Macrophage colony-stimulating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	145	1187	747	197	232	11	0	0	0
2	F	146	1193	750	198	234	11	0	0	0
2	G	147	1198	753	199	235	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

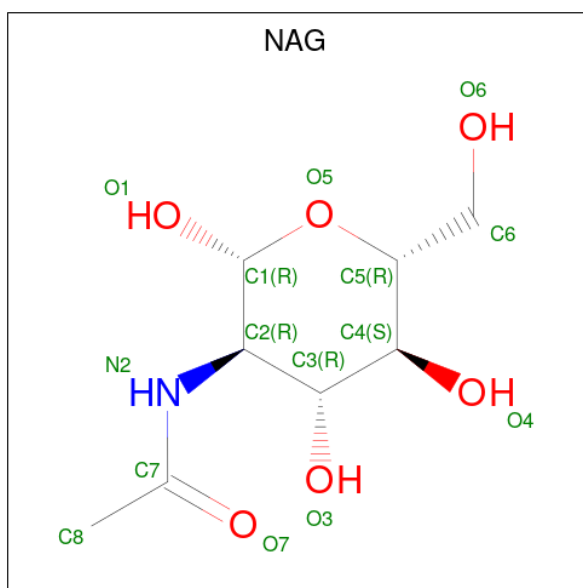
Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ASP	-	expression tag	UNP P09603
E	3	PRO	-	expression tag	UNP P09603
F	2	ASP	-	expression tag	UNP P09603
F	3	PRO	-	expression tag	UNP P09603
G	2	ASP	-	expression tag	UNP P09603
G	3	PRO	-	expression tag	UNP P09603

- Molecule 3 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
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total	O	0	0
			117	117		

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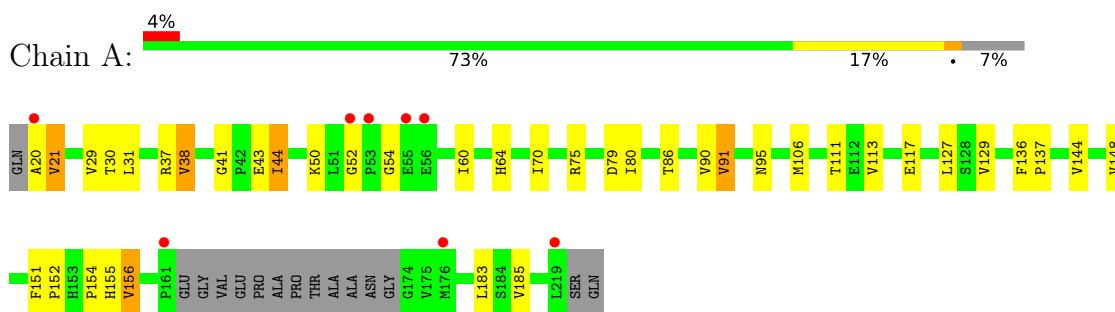
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	101	Total 101	O 101	0	0
5	D	72	Total 72	O 72	0	0
5	E	23	Total 23	O 23	0	0
5	F	63	Total 63	O 63	0	0
5	G	66	Total 66	O 66	0	0

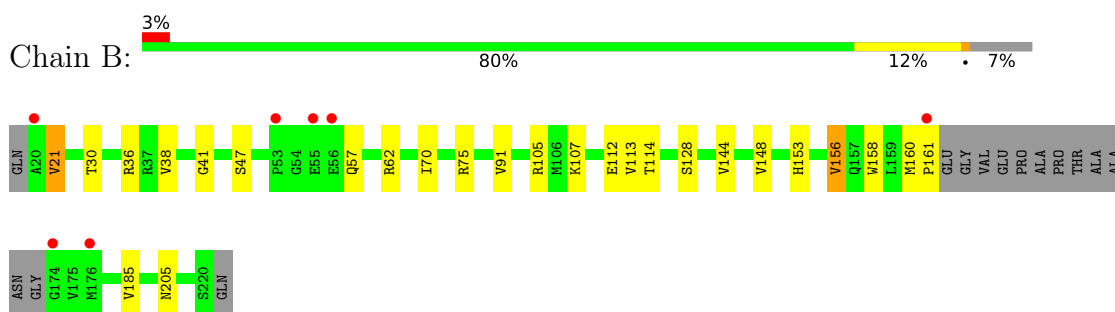
3 Residue-property plots [i](#)

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.

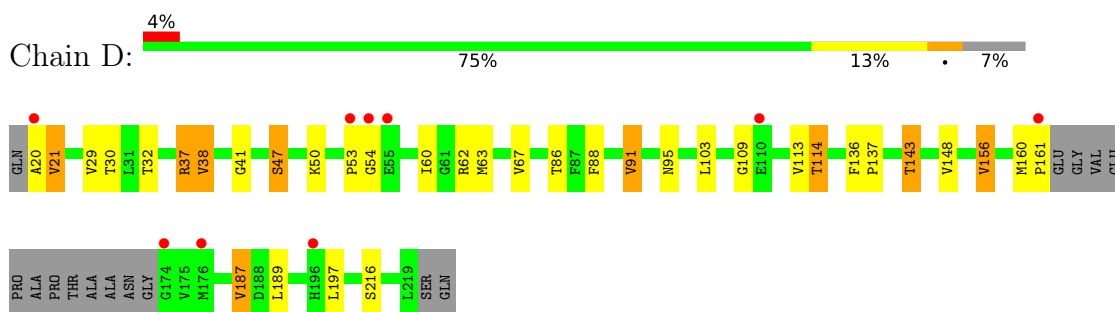
- Molecule 1: Secreted protein BARF1



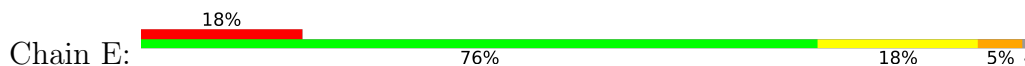
- Molecule 1: Secreted protein BARF1

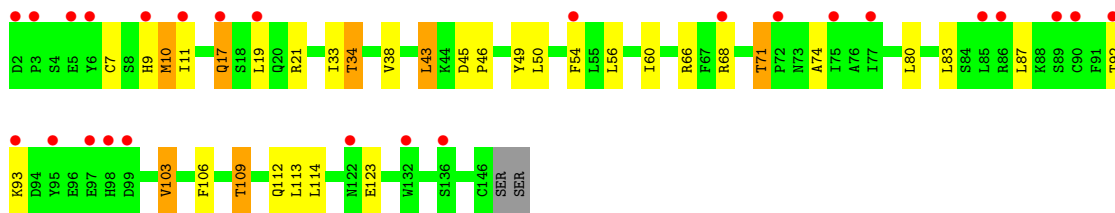


- Molecule 1: Secreted protein BARF1

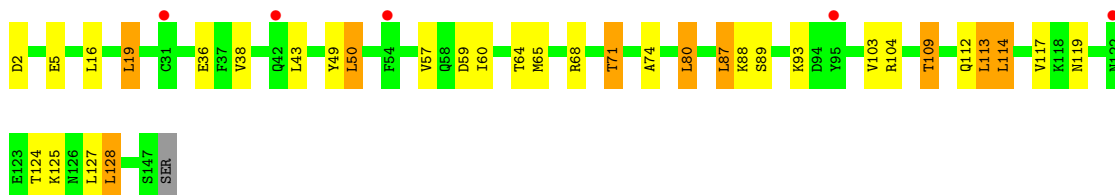
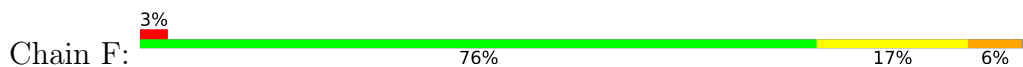


- Molecule 2: Macrophage colony-stimulating factor 1

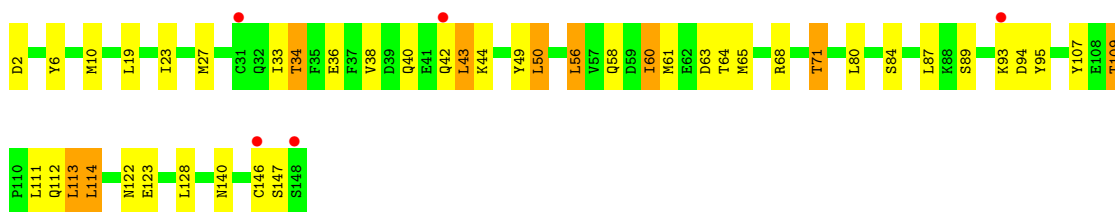




- Molecule 2: Macrophage colony-stimulating factor 1



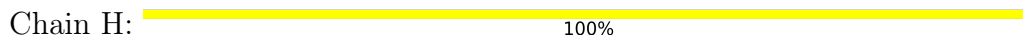
- Molecule 2: Macrophage colony-stimulating factor 1



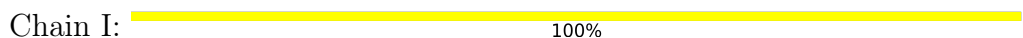
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.55Å 162.70Å 57.34Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-2.20) 97.6 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.222 , 0.260 0.222 , 0.262	Depositor DCC
R_{free} test set	4499 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtrriage
Anisotropy	0.539	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8676	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: 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	0.82	1/1541 (0.1%)	0.85	0/2097
1	B	0.80	0/1547	0.88	1/2105 (0.0%)
1	D	0.78	0/1541	0.85	0/2097
2	E	0.59	0/1208	0.89	0/1628
2	F	0.74	0/1214	0.99	2/1636 (0.1%)
2	G	0.65	1/1219 (0.1%)	0.94	0/1643
All	All	0.74	2/8270 (0.0%)	0.90	3/11206 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	ASN	C-N	6.51	1.42	1.33
2	G	122	ASN	C-N	5.67	1.41	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	ASP	CA-C-N	-6.36	114.07	120.31
2	F	2	ASP	C-N-CA	-6.36	114.07	120.31
1	B	21	VAL	N-CA-C	5.71	116.53	108.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1497	0	1471	27	0
1	B	1503	0	1476	14	0
1	D	1497	0	1471	26	0
2	E	1187	0	1150	16	0
2	F	1193	0	1154	22	0
2	G	1198	0	1156	28	0
3	C	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
4	G	14	0	13	0	0
5	A	117	0	0	1	0
5	B	101	0	0	0	0
5	D	72	0	0	3	0
5	E	23	0	0	2	0
5	F	63	0	0	2	0
5	G	66	0	0	2	0
All	All	8676	0	8019	121	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 7.

All (121) 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:D:20:ALA:CB	1:D:21:VAL:HA	1.76	1.13
2:F:65:MET:HE1	2:F:117:VAL:HG21	1.18	1.10
1:A:20:ALA:HB1	1:A:21:VAL:HA	1.31	1.07
1:D:20:ALA:HB1	1:D:21:VAL:CA	1.90	1.01
1:D:20:ALA:HB1	1:D:21:VAL:HA	1.03	0.99
2:F:65:MET:CE	2:F:117:VAL:HG21	2.03	0.87
1:A:156:VAL:HG22	1:A:185:VAL:HG13	1.55	0.87
1:B:156:VAL:HG22	1:B:185:VAL:HG13	1.59	0.85
2:G:95:TYR:H	2:G:140:ASN:HD21	1.27	0.82
2:F:109:THR:HG22	2:F:112:GLN:H	1.44	0.81
1:B:148:VAL:HG23	1:B:156:VAL:HG13	1.63	0.78
1:B:144:VAL:HG23	1:B:158:TRP:CZ2	2.21	0.76
1:D:143:THR:HG22	5:D:448:HOH:O	1.85	0.76
2:G:34:THR:HG22	2:G:107:TYR:HD1	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:58:GLN:HE21	2:G:84:SER:HB2	1.52	0.73
1:A:106:MET:HE3	1:A:113:VAL:HG23	1.70	0.72
2:G:43:LEU:HD13	2:G:49:TYR:HA	1.71	0.72
2:E:109:THR:HG21	5:E:314:HOH:O	1.93	0.68
2:G:61:MET:HA	2:G:65:MET:HE3	1.74	0.68
1:B:148:VAL:CG2	1:B:156:VAL:HG13	2.23	0.68
2:G:34:THR:HG22	2:G:107:TYR:CD1	2.29	0.68
1:D:37:ARG:HD3	2:G:63:ASP:OD1	1.94	0.67
1:A:50:LYS:HB2	1:A:60:ILE:HD11	1.77	0.67
1:A:20:ALA:CB	1:A:21:VAL:HA	2.09	0.66
2:F:71:THR:HG22	2:F:74:ALA:H	1.61	0.66
1:A:20:ALA:HB1	1:A:21:VAL:CA	2.19	0.65
1:A:148:VAL:HG23	1:A:156:VAL:HG13	1.79	0.65
2:E:7:CYS:HA	2:E:10:MET:HG3	1.78	0.65
1:A:156:VAL:CG2	1:A:185:VAL:HG13	2.27	0.65
1:D:86:THR:OG1	2:G:34:THR:HG23	1.99	0.63
2:G:58:GLN:NE2	2:G:84:SER:HB2	2.13	0.62
1:B:148:VAL:HG23	1:B:156:VAL:CG1	2.28	0.62
1:D:103:LEU:HD11	1:D:114:THR:HG23	1.82	0.61
2:F:43:LEU:HD13	2:F:49:TYR:HA	1.83	0.61
2:G:71:THR:HG23	5:G:306:HOH:O	1.99	0.61
1:A:29:VAL:HG12	1:A:91:VAL:HG22	1.83	0.60
2:G:109:THR:HG22	2:G:112:GLN:H	1.66	0.60
2:F:65:MET:HE1	2:F:117:VAL:CG2	2.11	0.59
1:A:155:HIS:HD2	5:A:461:HOH:O	1.85	0.59
1:B:36:ARG:NH2	2:F:59:ASP:HB3	2.18	0.59
2:G:36:GLU:HB2	2:G:60:ILE:HD11	1.86	0.58
2:F:68:ARG:O	2:F:71:THR:HB	2.03	0.58
2:G:6:TYR:CD1	2:G:10:MET:HE2	2.38	0.58
2:F:64:THR:O	2:G:27:MET:HE3	2.06	0.55
1:D:47:SER:HB3	1:D:62:ARG:HG2	1.89	0.55
1:B:47:SER:HB3	1:B:62:ARG:HG2	1.87	0.54
2:E:71:THR:HG22	2:E:74:ALA:H	1.70	0.54
2:E:109:THR:HG23	5:E:311:HOH:O	2.07	0.54
1:A:151:PHE:CD1	1:A:152:PRO:HA	2.43	0.53
1:D:143:THR:CG2	5:D:448:HOH:O	2.51	0.53
2:F:119:ASN:HB3	5:F:359:HOH:O	2.09	0.53
2:G:109:THR:HB	2:G:112:GLN:OE1	2.08	0.53
2:E:43:LEU:HD13	2:E:49:TYR:HA	1.91	0.52
1:A:127:LEU:O	1:B:128:SER:HA	2.10	0.52
1:A:86:THR:OG1	2:E:34:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:CG2	1:A:156:VAL:HG13	2.40	0.52
2:E:34:THR:HA	2:E:106:PHE:O	2.09	0.52
1:A:30:THR:HG22	1:A:90:VAL:HG22	1.93	0.51
2:F:50:LEU:HD23	2:F:127:LEU:HD12	1.91	0.51
1:B:107:LYS:HG2	1:B:112:GLU:HG3	1.92	0.50
2:G:2:ASP:OD1	2:G:89:SER:HB2	2.10	0.50
2:G:68:ARG:O	2:G:71:THR:HB	2.11	0.50
1:A:86:THR:OG1	2:E:34:THR:CG2	2.60	0.50
1:A:106:MET:HE3	1:A:113:VAL:CG2	2.42	0.50
2:F:49:TYR:HD1	2:F:50:LEU:HD13	1.77	0.50
2:G:50:LEU:HD21	2:G:123:GLU:HB3	1.94	0.49
2:G:94:ASP:HB3	2:G:140:ASN:ND2	2.27	0.49
2:E:109:THR:HG22	2:E:112:GLN:H	1.77	0.49
2:E:17:GLN:HB3	2:E:21:ARG:NH2	2.28	0.49
2:G:58:GLN:NE2	5:G:329:HOH:O	2.46	0.48
1:A:31:LEU:HD22	1:A:117:GLU:HG2	1.94	0.48
1:A:52:GLY:O	1:A:54:GLY:HA2	2.13	0.48
1:A:37:ARG:HD2	2:E:66:ARG:NE	2.29	0.48
1:D:53:PRO:HA	1:D:54:GLY:HA2	1.58	0.48
1:D:156:VAL:HB	1:D:187:VAL:HG23	1.96	0.48
1:D:29:VAL:HG13	1:D:91:VAL:HG13	1.96	0.47
2:F:109:THR:HB	2:F:112:GLN:OE1	2.13	0.47
1:D:32:THR:HG22	1:D:88:PHE:CD1	2.49	0.47
2:E:56:LEU:HD11	2:E:103:VAL:CG2	2.45	0.47
1:D:136:PHE:CG	1:D:137:PRO:HA	2.51	0.46
2:F:109:THR:HG23	5:F:325:HOH:O	2.14	0.46
1:B:105:ARG:HG2	1:B:114:THR:HG22	1.98	0.46
1:A:38:VAL:HG21	2:E:33:ILE:HD12	1.99	0.45
1:D:20:ALA:CB	1:D:21:VAL:CA	2.60	0.45
2:F:19:LEU:HD13	2:F:80:LEU:HD21	1.99	0.45
1:A:136:PHE:CG	1:A:137:PRO:HA	2.52	0.45
2:G:94:ASP:HB3	2:G:140:ASN:HD21	1.80	0.45
2:F:64:THR:HB	2:F:113:LEU:HD11	1.99	0.44
2:E:68:ARG:O	2:E:71:THR:HB	2.18	0.44
1:D:95:ASN:HB2	5:D:425:HOH:O	2.18	0.44
2:F:124:THR:O	2:F:128:LEU:HB2	2.17	0.44
2:G:64:THR:HB	2:G:113:LEU:HD11	2.00	0.43
1:A:79:ASP:CG	1:A:80:ILE:N	2.76	0.43
1:D:63:MET:HA	1:D:67:VAL:O	2.19	0.43
1:D:143:THR:HA	1:D:189:LEU:O	2.17	0.43
2:G:56:LEU:HD22	2:G:60:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:CG1	1:D:91:VAL:HG13	2.49	0.43
1:D:50:LYS:HB2	1:D:60:ILE:HD11	2.00	0.43
1:B:36:ARG:HH22	2:F:59:ASP:HB3	1.82	0.43
1:D:38:VAL:HG21	2:G:33:ILE:HD12	2.00	0.43
2:G:109:THR:HG22	2:G:111:LEU:N	2.33	0.42
1:A:43:GLU:O	1:A:64:HIS:HE1	2.02	0.42
2:E:45:ASP:HA	2:E:46:PRO:HD3	1.93	0.42
2:F:16:LEU:HD11	2:F:125:LYS:HD3	2.01	0.42
1:A:154:PRO:HG3	1:A:183:LEU:HB2	2.02	0.42
2:G:42:GLN:HE21	2:G:146:CYS:HB3	1.83	0.42
2:F:87:LEU:O	2:F:88:LYS:C	2.60	0.41
1:D:95:ASN:OD1	1:D:95:ASN:C	2.63	0.41
1:D:197:LEU:HD13	1:D:216:SER:HA	2.02	0.41
1:D:160:MET:HA	1:D:161:PRO:HD2	1.94	0.41
1:B:153:HIS:H	1:B:205:ASN:ND2	2.17	0.41
1:D:148:VAL:HG23	1:D:156:VAL:HG13	2.03	0.41
2:E:11:ILE:HG12	2:E:83:LEU:HD21	2.03	0.41
2:F:36:GLU:HG2	2:F:103:VAL:CG1	2.51	0.41
1:B:70:ILE:O	1:B:75:ARG:NH1	2.51	0.40
1:B:160:MET:O	1:B:161:PRO:C	2.64	0.40
1:A:70:ILE:HB	1:A:75:ARG:HD2	2.04	0.40
2:F:114:LEU:HD12	2:F:114:LEU:HA	1.95	0.40
1:D:86:THR:OG1	2:G:34:THR:CG2	2.66	0.40
1:A:44:ILE:CD1	1:A:44:ILE:N	2.85	0.40
2:G:23:ILE:HG12	2:G:114:LEU:HB3	2.04	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	184/203 (91%)	178 (97%)	5 (3%)	1 (0%)	24 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	185/203 (91%)	177 (96%)	7 (4%)	1 (0%)	24	27
1	D	184/203 (91%)	176 (96%)	6 (3%)	2 (1%)	11	10
2	E	143/147 (97%)	138 (96%)	5 (4%)	0	100	100
2	F	144/147 (98%)	140 (97%)	4 (3%)	0	100	100
2	G	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
All	All	985/1050 (94%)	948 (96%)	33 (3%)	4 (0%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41	GLY
1	A	41	GLY
1	B	41	GLY
1	D	109	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	167/177 (94%)	159 (95%)	8 (5%)	23	30
1	B	168/177 (95%)	161 (96%)	7 (4%)	26	36
1	D	167/177 (94%)	156 (93%)	11 (7%)	15	18
2	E	138/140 (99%)	118 (86%)	20 (14%)	3	2
2	F	139/140 (99%)	123 (88%)	16 (12%)	5	5
2	G	139/140 (99%)	121 (87%)	18 (13%)	4	4
All	All	918/951 (96%)	838 (91%)	80 (9%)	9	10

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	38	VAL

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Mol	Chain	Res	Type
1	A	44	ILE
1	A	91	VAL
1	A	111	THR
1	A	129	VAL
1	A	144	VAL
1	A	156	VAL
1	B	21	VAL
1	B	30	THR
1	B	38	VAL
1	B	57	GLN
1	B	91	VAL
1	B	113	VAL
1	B	156	VAL
1	D	21	VAL
1	D	30	THR
1	D	37	ARG
1	D	38	VAL
1	D	47	SER
1	D	91	VAL
1	D	113	VAL
1	D	114	THR
1	D	143	THR
1	D	156	VAL
1	D	187	VAL
2	E	9	HIS
2	E	10	MET
2	E	17	GLN
2	E	19	LEU
2	E	34	THR
2	E	38	VAL
2	E	43	LEU
2	E	50	LEU
2	E	54	PHE
2	E	60	ILE
2	E	71	THR
2	E	80	LEU
2	E	87	LEU
2	E	92	THR
2	E	93	LYS
2	E	103	VAL
2	E	109	THR
2	E	113	LEU

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Mol	Chain	Res	Type
2	E	114	LEU
2	E	123	GLU
2	F	5	GLU
2	F	19	LEU
2	F	38	VAL
2	F	50	LEU
2	F	57	VAL
2	F	60	ILE
2	F	71	THR
2	F	80	LEU
2	F	87	LEU
2	F	89	SER
2	F	93	LYS
2	F	104	ARG
2	F	109	THR
2	F	113	LEU
2	F	114	LEU
2	F	128	LEU
2	G	19	LEU
2	G	34	THR
2	G	38	VAL
2	G	40	GLN
2	G	43	LEU
2	G	44	LYS
2	G	50	LEU
2	G	56	LEU
2	G	60	ILE
2	G	71	THR
2	G	80	LEU
2	G	87	LEU
2	G	93	LYS
2	G	109	THR
2	G	113	LEU
2	G	114	LEU
2	G	128	LEU
2	G	147	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	65	HIS

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Mol	Chain	Res	Type
1	A	118	HIS
1	A	155	HIS
1	A	205	ASN
1	B	65	HIS
1	B	101	ASN
1	B	157	GLN
1	B	205	ASN
1	D	64	HIS
1	D	157	GLN
1	D	196	HIS
2	E	9	HIS
2	E	42	GLN
2	E	81	GLN
2	E	119	ASN
2	E	126	ASN
2	E	141	ASN
2	F	42	GLN
2	F	141	ASN
2	G	42	GLN
2	G	58	GLN
2	G	98	HIS
2	G	119	ASN
2	G	140	ASN
2	G	141	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](#)

9 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
3	NAG	C	1	1,3	14,14,15	0.62	0	17,19,21	1.09	2 (11%)
3	NAG	C	2	3	14,14,15	0.68	0	17,19,21	0.97	0
3	BMA	C	3	3	11,11,12	0.38	0	15,15,17	1.40	3 (20%)
3	NAG	H	1	1,3	14,14,15	0.76	0	17,19,21	1.25	2 (11%)
3	NAG	H	2	3	14,14,15	0.72	0	17,19,21	1.09	2 (11%)
3	BMA	H	3	3	11,11,12	0.63	0	15,15,17	1.80	3 (20%)
3	NAG	I	1	1,3	14,14,15	0.78	0	17,19,21	1.41	2 (11%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	1.22	2 (11%)
3	BMA	I	3	3	11,11,12	0.32	0	15,15,17	0.84	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	5.14	119.07	112.19
3	I	1	NAG	O5-C1-C2	-3.74	105.50	111.29
3	I	1	NAG	C2-N2-C7	-3.72	117.92	122.90
3	H	1	NAG	C1-O5-C5	3.12	116.37	112.19
3	H	3	BMA	C1-C2-C3	3.10	114.16	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	O5-C5-C6	3.06	113.62	107.66
3	C	3	BMA	C1-C2-C3	2.69	113.56	109.64
3	I	2	NAG	C2-N2-C7	2.67	126.48	122.90
3	C	1	NAG	C2-N2-C7	-2.51	119.53	122.90
3	H	1	NAG	O5-C1-C2	-2.48	107.45	111.29
3	H	2	NAG	C3-C4-C5	-2.42	105.85	110.23
3	H	3	BMA	C6-C5-C4	-2.38	107.18	113.02
3	C	3	BMA	C1-O5-C5	-2.33	109.06	112.19
3	C	1	NAG	C1-O5-C5	2.33	115.31	112.19
3	I	2	NAG	C8-C7-N2	2.21	119.78	116.12
3	H	2	NAG	C1-O5-C5	-2.16	109.29	112.19
3	I	3	BMA	O5-C5-C6	2.07	111.70	107.66

There are no chirality outliers.

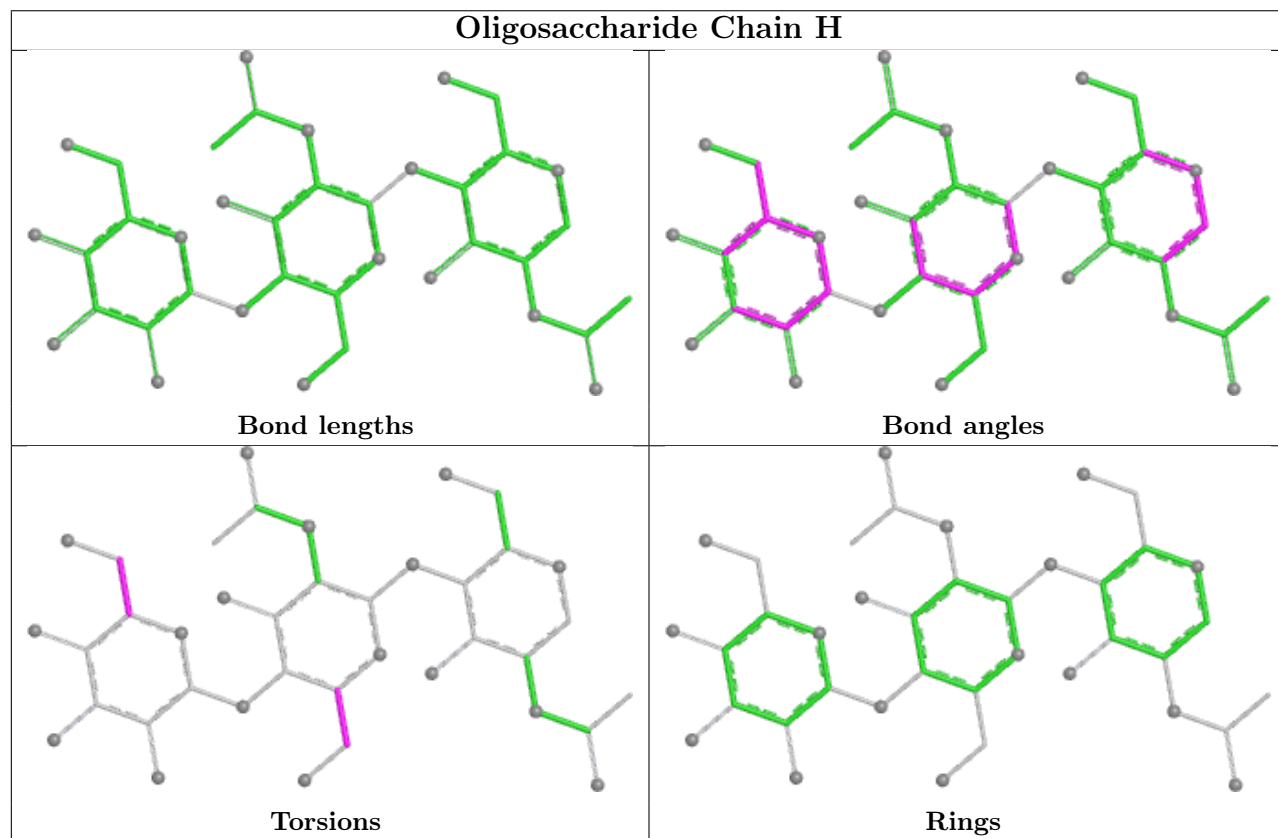
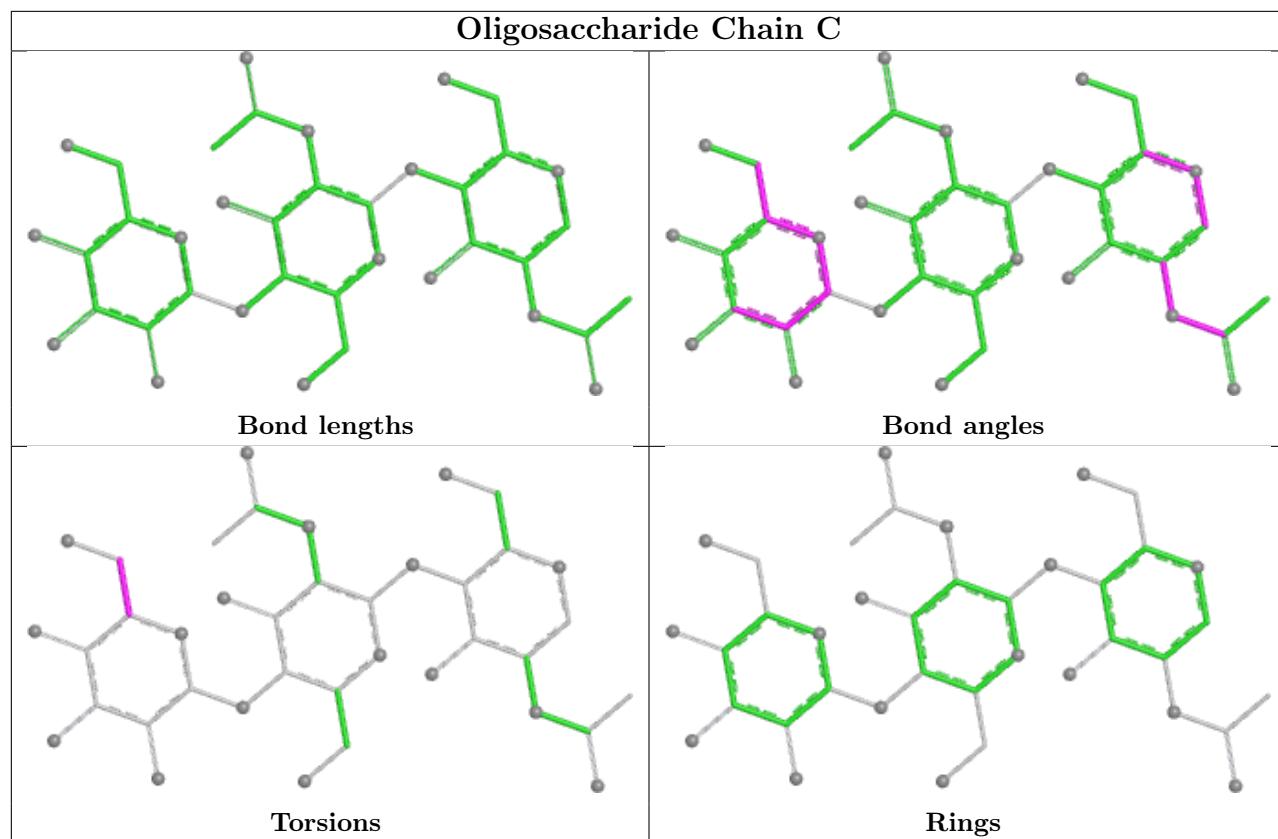
All (8) torsion outliers are listed below:

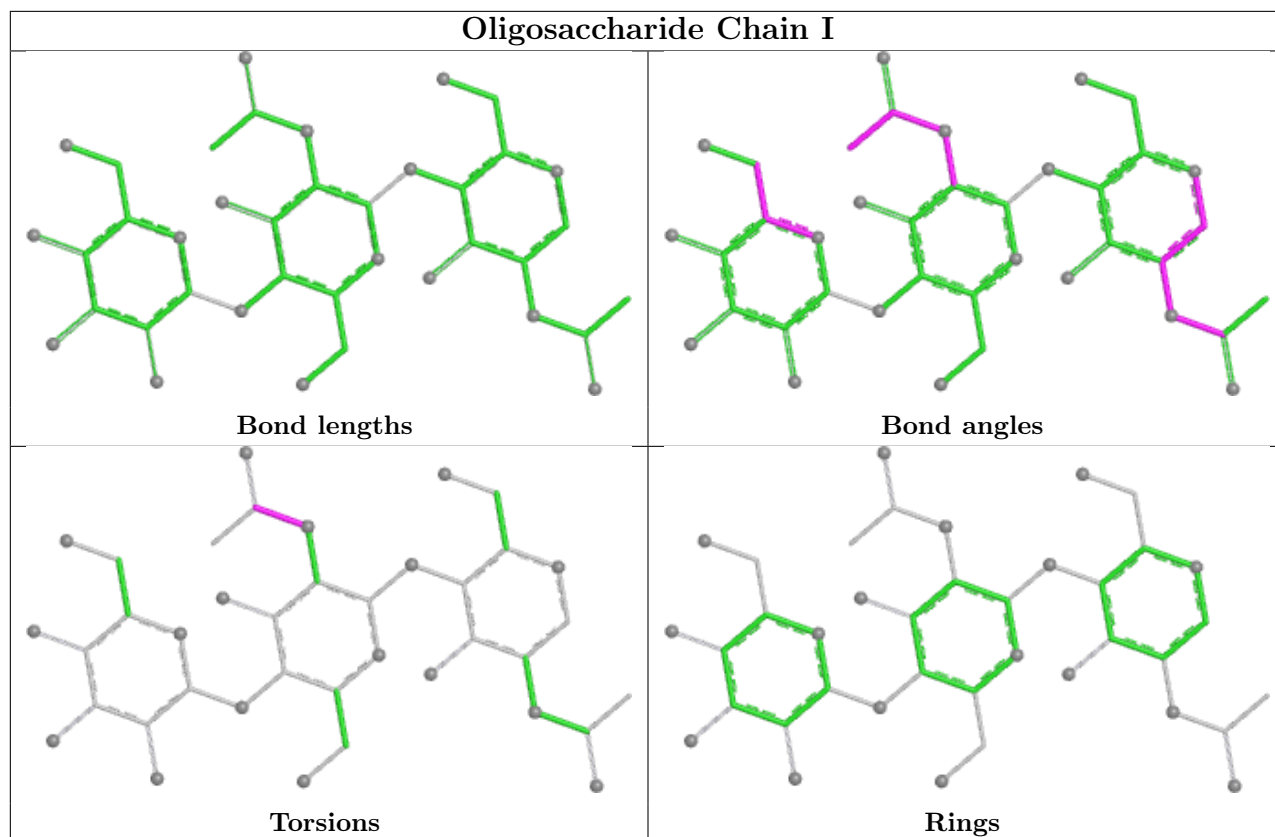
Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

3 ligands 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	F	201	2	14,14,15	0.44	0	17,19,21	0.80	1 (5%)
4	NAG	E	201	2	14,14,15	0.65	0	17,19,21	1.15	1 (5%)
4	NAG	G	201	2	14,14,15	0.51	0	17,19,21	0.77	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1
4	NAG	E	201	2	-	0/6/23/26	0/1/1/1
4	NAG	G	201	2	-	2/6/23/26	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(°)
4	E	201	NAG	C4-C3-C2	2.97	115.36	111.02
4	F	201	NAG	O5-C5-C6	2.22	111.97	107.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	201	NAG	C4-C5-C6-O6
4	G	201	NAG	O5-C5-C6-O6

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	188/203 (92%)	-0.05	8 (4%) 40 36	21, 33, 57, 71	0
1	B	189/203 (93%)	-0.03	7 (3%) 45 42	26, 34, 57, 85	0
1	D	188/203 (92%)	0.14	9 (4%) 35 32	24, 42, 69, 85	0
2	E	145/147 (98%)	1.10	26 (17%) 3 3	34, 65, 104, 117	0
2	F	146/147 (99%)	0.26	5 (3%) 48 45	24, 37, 74, 95	0
2	G	147/147 (100%)	0.22	5 (3%) 48 45	28, 40, 71, 97	0
All	All	1003/1050 (95%)	0.24	60 (5%) 27 24	21, 39, 82, 117	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	148	SER	8.6
2	E	95	TYR	5.6
1	A	53	PRO	4.0
1	A	55	GLU	3.8
1	D	53	PRO	3.7
2	E	6	TYR	3.6
2	E	54	PHE	3.4
1	A	176	MET	3.3
2	E	89	SER	3.3
1	D	161	PRO	3.2
2	E	9	HIS	3.2
1	B	55	GLU	3.1
1	A	56	GLU	3.0
2	F	54	PHE	2.9
2	E	68	ARG	2.9
1	D	20	ALA	2.9
1	D	174	GLY	2.8
2	E	86	ARG	2.8
1	D	176	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	55	GLU	2.6
2	F	95	TYR	2.6
1	B	20	ALA	2.6
2	G	93	LYS	2.5
2	E	77	ILE	2.5
2	E	90	CYS	2.5
1	B	53	PRO	2.5
2	F	42	GLN	2.5
1	B	174	GLY	2.5
1	B	161	PRO	2.4
1	D	196	HIS	2.4
2	G	42	GLN	2.4
2	E	5	GLU	2.4
2	E	136	SER	2.3
2	E	98	HIS	2.3
1	D	54	GLY	2.3
2	E	17	GLN	2.3
2	F	122	ASN	2.2
2	E	11	ILE	2.2
2	E	2	ASP	2.2
1	B	176	MET	2.2
1	A	161	PRO	2.2
2	E	75	ILE	2.2
2	E	85	LEU	2.2
2	G	146	CYS	2.2
2	E	3	PRO	2.1
2	F	31	CYS	2.1
2	E	99	ASP	2.1
2	E	132	TRP	2.1
2	E	19	LEU	2.1
1	A	52	GLY	2.1
1	A	20	ALA	2.1
2	E	93	LYS	2.1
1	D	110	GLU	2.1
2	E	97	GLU	2.1
1	A	219	LEU	2.1
2	G	31	CYS	2.0
2	E	72	PRO	2.0
1	B	56	GLU	2.0
2	E	92	THR	2.0
2	E	122	ASN	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](#)

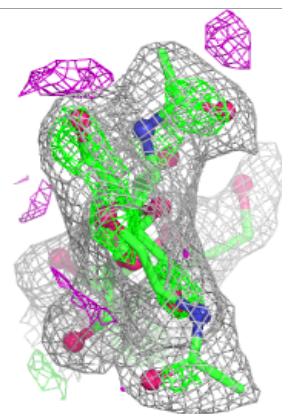
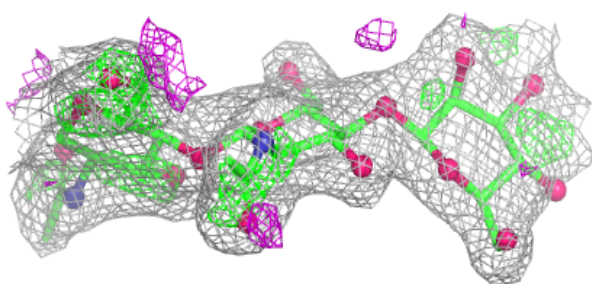
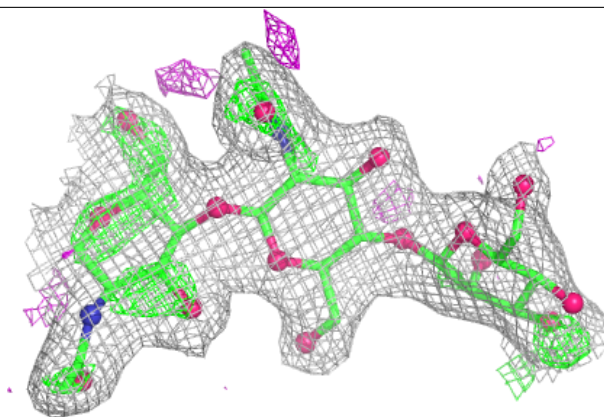
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	59,70,92,99	0
3	NAG	C	2	14/15	-	-	59,71,82,89	0
3	BMA	C	3	11/12	-	-	88,109,121,126	0
3	BMA	H	3	11/12	0.58	0.36	113,131,153,158	0
3	BMA	I	3	11/12	0.62	0.22	88,96,111,117	0
3	NAG	H	2	14/15	0.85	0.27	75,88,101,102	0
3	NAG	I	2	14/15	0.90	0.17	57,70,74,83	0
3	NAG	H	1	14/15	0.92	0.21	69,72,97,103	0
3	NAG	I	1	14/15	0.93	0.15	56,63,83,83	0

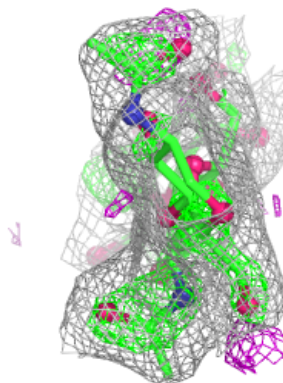
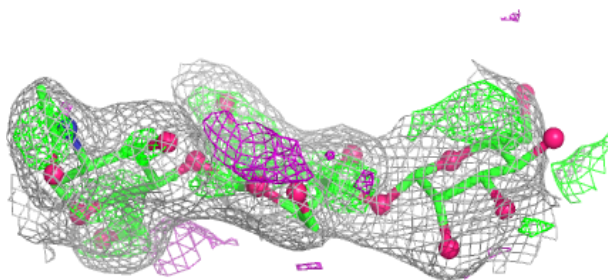
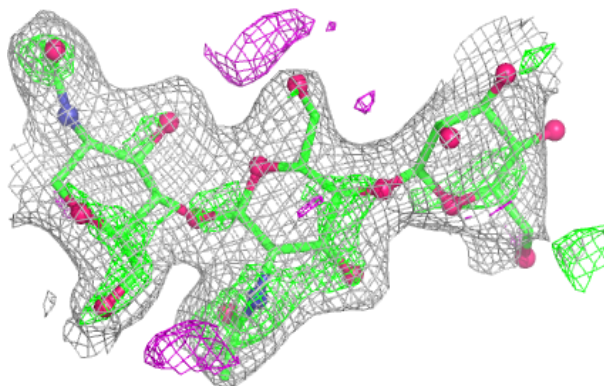
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

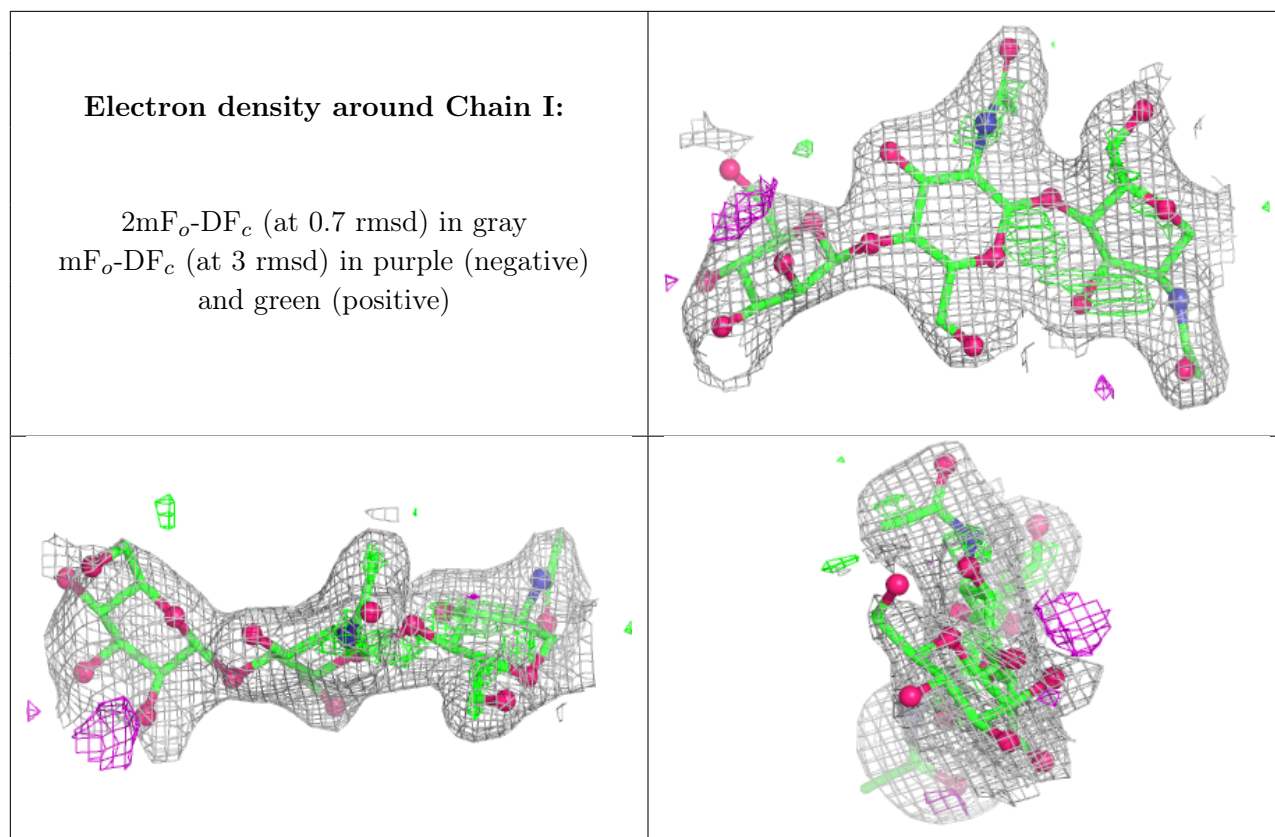
Electron density around Chain C:

$2mF_o-DF_c$ (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
4	NAG	G	201	14/15	0.45	0.20	82,90,100,101	0
4	NAG	E	201	14/15	0.54	0.19	91,98,104,106	0
4	NAG	F	201	14/15	0.68	0.17	51,67,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.