Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 07:50 AM EDT

PDB ID	:	6E3K
Title	:	Interferon gamma signalling complex with IFNGR1 and IFNGR2
Authors	:	Jude, K.M.; Mendoza, J.L.; Garcia, K.C.
Deposited on	:	2018-07-14
Resolution	:	3.25 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 (i) 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 (i)) were used in the production of this report:

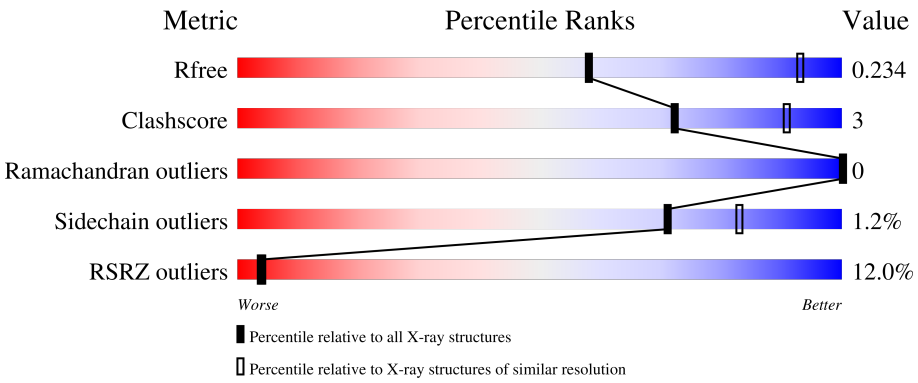
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 <=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	148	.% 75% 9% 16%
1	B	148	3% 78% 7% 15%
2	C	242	2% 77% 8% 14%
2	D	242	11% 73% 11% 16%
3	E	233	39% 82% 9% 9%

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Mol	Chain	Length	Quality of chain
3	I	233	82% 9% 9%
4	F	2	100%
5	G	5	60% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CYS	E	306	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8966 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 Interferon gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	125	1027	653	173	198	3	0	0	0
1	B	126	1020	647	171	199	3	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P01579
A	-2	PRO	-	expression tag	UNP P01579
A	-1	GLY	-	expression tag	UNP P01579
A	0	SER	-	expression tag	UNP P01579
A	134	ALA	-	expression tag	UNP P01579
A	135	ALA	-	expression tag	UNP P01579
A	136	ALA	-	expression tag	UNP P01579
A	137	HIS	-	expression tag	UNP P01579
A	138	HIS	-	expression tag	UNP P01579
A	139	HIS	-	expression tag	UNP P01579
A	140	HIS	-	expression tag	UNP P01579
A	141	HIS	-	expression tag	UNP P01579
A	142	HIS	-	expression tag	UNP P01579
A	143	HIS	-	expression tag	UNP P01579
A	144	HIS	-	expression tag	UNP P01579
B	-3	GLY	-	expression tag	UNP P01579
B	-2	PRO	-	expression tag	UNP P01579
B	-1	GLY	-	expression tag	UNP P01579
B	0	SER	-	expression tag	UNP P01579
B	134	ALA	-	expression tag	UNP P01579
B	135	ALA	-	expression tag	UNP P01579
B	136	ALA	-	expression tag	UNP P01579
B	137	HIS	-	expression tag	UNP P01579
B	138	HIS	-	expression tag	UNP P01579
B	139	HIS	-	expression tag	UNP P01579

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Chain	Residue	Modelled	Actual	Comment	Reference
B	140	HIS	-	expression tag	UNP P01579
B	141	HIS	-	expression tag	UNP P01579
B	142	HIS	-	expression tag	UNP P01579
B	143	HIS	-	expression tag	UNP P01579
B	144	HIS	-	expression tag	UNP P01579

- Molecule 2 is a protein called Interferon gamma receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	207	1649	1049	274	315	11	0	0	0
			Total	C	N	O	S			
2	D	203	1577	999	263	305	10	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P15260
C	0	SER	-	expression tag	UNP P15260
C	149	ILE	THR	engineered mutation	UNP P15260
C	161	LYS	MET	engineered mutation	UNP P15260
C	167	LYS	GLN	engineered mutation	UNP P15260
C	174	ASN	LYS	engineered mutation	UNP P15260
C	182	ARG	GLN	engineered mutation	UNP P15260
C	205	ASN	HIS	engineered mutation	UNP P15260
C	230	ALA	-	expression tag	UNP P15260
C	231	ALA	-	expression tag	UNP P15260
C	232	ALA	-	expression tag	UNP P15260
C	233	HIS	-	expression tag	UNP P15260
C	234	HIS	-	expression tag	UNP P15260
C	235	HIS	-	expression tag	UNP P15260
C	236	HIS	-	expression tag	UNP P15260
C	237	HIS	-	expression tag	UNP P15260
C	238	HIS	-	expression tag	UNP P15260
C	239	HIS	-	expression tag	UNP P15260
C	240	HIS	-	expression tag	UNP P15260
D	-1	GLY	-	expression tag	UNP P15260
D	0	SER	-	expression tag	UNP P15260
D	149	ILE	THR	engineered mutation	UNP P15260
D	161	LYS	MET	engineered mutation	UNP P15260
D	167	LYS	GLN	engineered mutation	UNP P15260
D	174	ASN	LYS	engineered mutation	UNP P15260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	182	ARG	GLN	engineered mutation	UNP P15260
D	205	ASN	HIS	engineered mutation	UNP P15260
D	230	ALA	-	expression tag	UNP P15260
D	231	ALA	-	expression tag	UNP P15260
D	232	ALA	-	expression tag	UNP P15260
D	233	HIS	-	expression tag	UNP P15260
D	234	HIS	-	expression tag	UNP P15260
D	235	HIS	-	expression tag	UNP P15260
D	236	HIS	-	expression tag	UNP P15260
D	237	HIS	-	expression tag	UNP P15260
D	238	HIS	-	expression tag	UNP P15260
D	239	HIS	-	expression tag	UNP P15260
D	240	HIS	-	expression tag	UNP P15260

- Molecule 3 is a protein called Interferon gamma receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	213	1692	1087	283	313	9	0	0	0
			Total	C	N	O	S			
3	I	213	1698	1090	286	313	9	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	26	GLY	-	expression tag	UNP P38484
E	27	SER	-	expression tag	UNP P38484
E	248	ALA	-	expression tag	UNP P38484
E	249	ALA	-	expression tag	UNP P38484
E	250	ALA	-	expression tag	UNP P38484
E	251	HIS	-	expression tag	UNP P38484
E	252	HIS	-	expression tag	UNP P38484
E	253	HIS	-	expression tag	UNP P38484
E	254	HIS	-	expression tag	UNP P38484
E	255	HIS	-	expression tag	UNP P38484
E	256	HIS	-	expression tag	UNP P38484
E	257	HIS	-	expression tag	UNP P38484
E	258	HIS	-	expression tag	UNP P38484
I	26	GLY	-	expression tag	UNP P38484
I	27	SER	-	expression tag	UNP P38484
I	248	ALA	-	expression tag	UNP P38484
I	249	ALA	-	expression tag	UNP P38484

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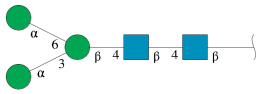
Chain	Residue	Modelled	Actual	Comment	Reference
I	250	ALA	-	expression tag	UNP P38484
I	251	HIS	-	expression tag	UNP P38484
I	252	HIS	-	expression tag	UNP P38484
I	253	HIS	-	expression tag	UNP P38484
I	254	HIS	-	expression tag	UNP P38484
I	255	HIS	-	expression tag	UNP P38484
I	256	HIS	-	expression tag	UNP P38484
I	257	HIS	-	expression tag	UNP P38484
I	258	HIS	-	expression tag	UNP P38484

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

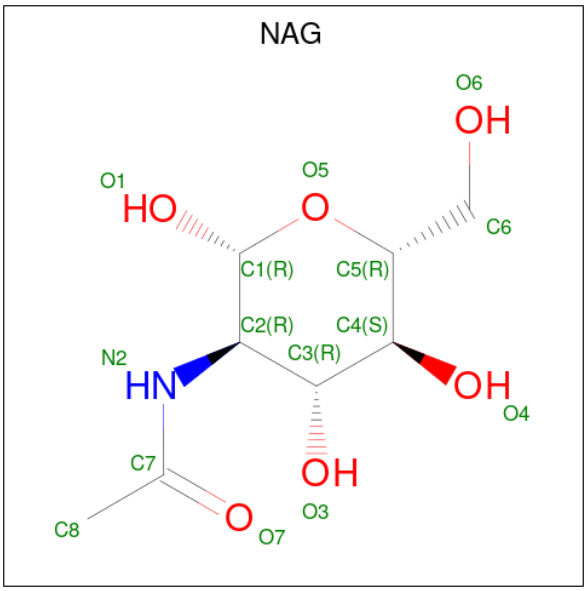
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



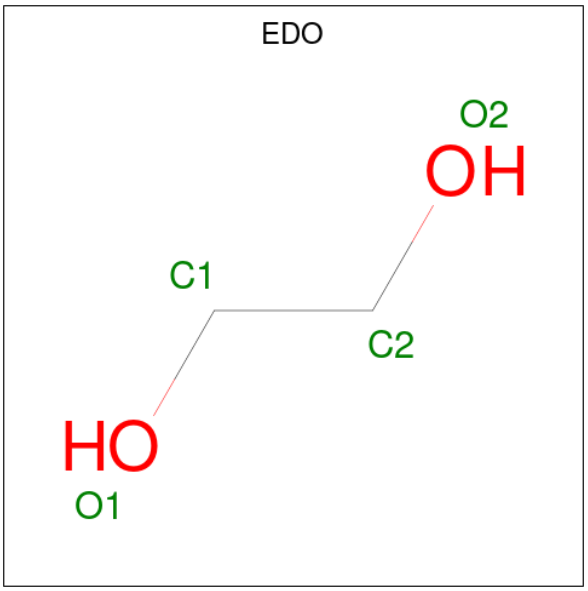
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	G	5	61	34	2	25	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



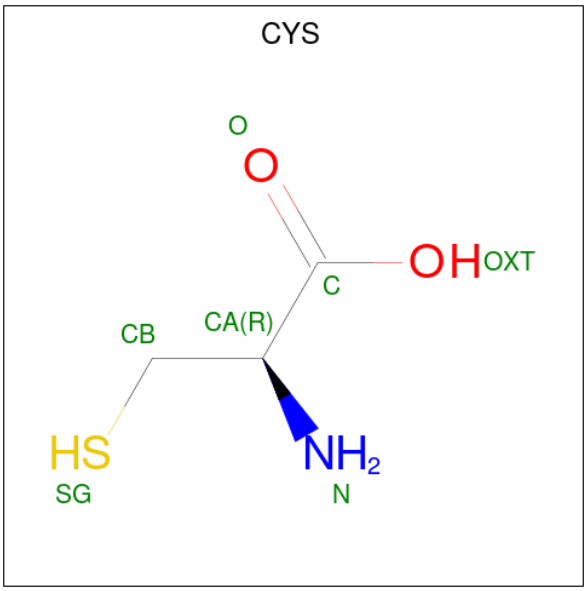
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	C	1	14	8	1	5	0	0
6	C	1	14	8	1	5	0	0
6	D	1	14	8	1	5	0	0
6	D	1	14	8	1	5	0	0
6	E	1	14	8	1	5	0	0
6	E	1	14	8	1	5	0	0
6	E	1	14	8	1	5	0	0
6	I	1	14	8	1	5	0	0
6	I	1	14	8	1	5	0	0
6	I	1	14	8	1	5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	D	1	4	2	2	0	0
7	I	1	4	2	2	0	0
7	I	1	4	2	2	0	0

- Molecule 8 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	E	1	7	3	1	2	1	0	0
			Total	C	N	O	S		
8	I	1	7	3	1	2	1	0	0

- Molecule 9 is water.

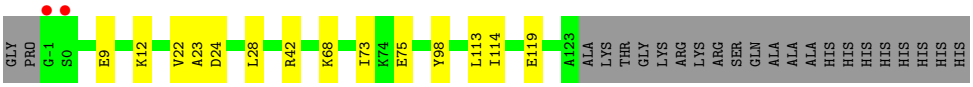
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	B	1	1	1	0	0
			Total	O		
9	C	1	1	1	0	0
			Total	O		
9	I	6	6	6	0	0

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.

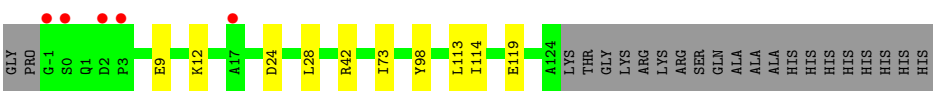
- Molecule 1: Interferon gamma

Chain A:



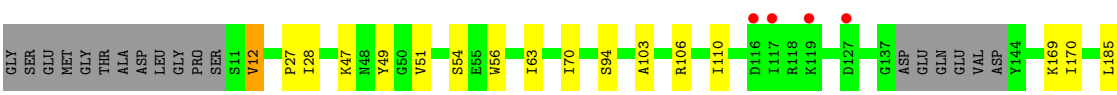
- Molecule 1: Interferon gamma

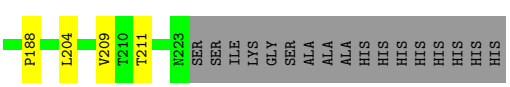
Chain B:



- Molecule 2: Interferon gamma receptor 1

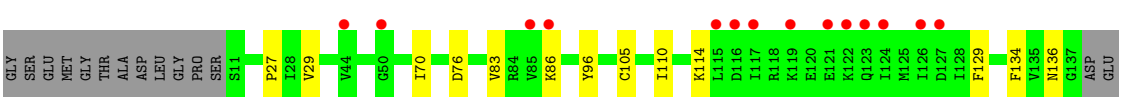
Chain C:

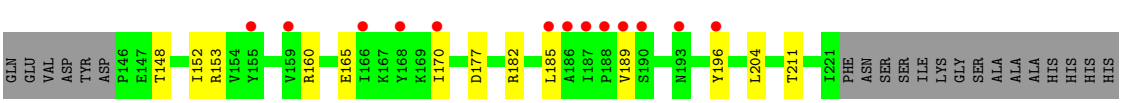




- Molecule 2: Interferon gamma receptor 1

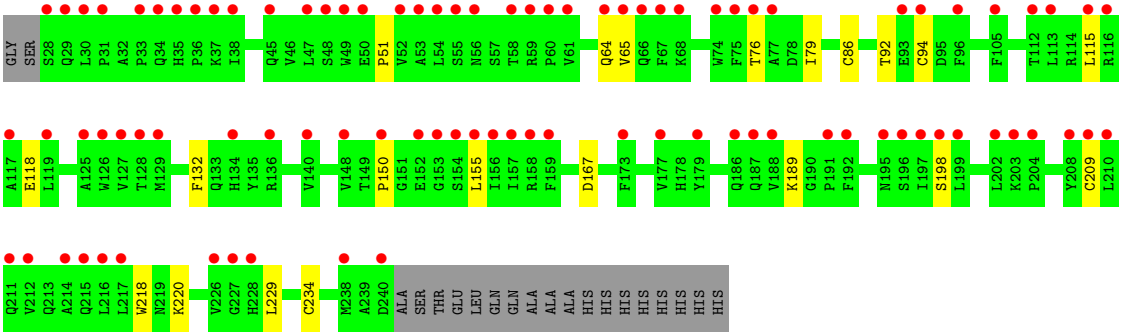
Chain D:





• Molecule 3: Interferon gamma receptor 2

Chain E:

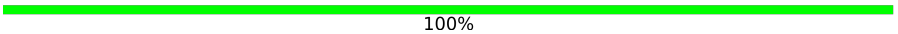


• Molecule 3: Interferon gamma receptor 2

Chain I:

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

Chain F:



• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.28Å 151.46Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 3.25 49.49 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.19-3.25) 89.0 (49.49-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.190 , 0.232 0.191 , 0.234	Depositor DCC
R_{free} test set	1783 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å^2)	111.2	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 119.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8966	wwPDB-VP
Average B, all atoms (Å^2)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, EDO, BMA, MAN

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	0.29	0/1045	0.40	0/1399
1	B	0.27	0/1038	0.39	0/1394
2	C	0.29	0/1687	0.48	0/2296
2	D	0.27	0/1613	0.47	0/2201
3	E	0.25	0/1743	0.46	0/2381
3	I	0.31	0/1749	0.52	0/2388
All	All	0.28	0/8875	0.47	0/12059

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1027	0	1021	12	0
1	B	1020	0	993	8	0
2	C	1649	0	1596	14	0
2	D	1577	0	1489	13	0
3	E	1692	0	1624	11	0
3	I	1698	0	1633	14	0
4	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	61	0	52	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	28	0	26	1	0
6	D	28	0	26	0	0
6	E	42	0	39	1	0
6	I	42	0	39	0	0
7	B	4	0	6	0	0
7	C	8	0	12	0	0
7	D	4	0	6	0	0
7	I	8	0	12	1	0
8	E	7	0	3	0	0
8	I	7	0	3	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	I	6	0	0	1	0
All	All	8966	0	8631	59	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 (59) 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:C:12:VAL:HG22	2:C:94:SER:HB3	1.68	0.75
3:I:158:ARG:NH1	9:I:401:HOH:O	2.23	0.72
1:A:75:GLU:OE1	3:I:70:THR:HG22	2.03	0.59
2:C:110:ILE:HB	2:C:211:THR:HG22	1.86	0.58
3:E:189:LYS:NZ	3:E:198:SER:O	2.37	0.57
3:I:86:CYS:HA	3:I:89:ILE:HD13	1.88	0.56
3:E:150:PRO:HA	3:E:155:LEU:HD23	1.88	0.55
3:E:132:PHE:HB3	6:E:302:NAG:H82	1.90	0.53
1:A:119:GLU:HB3	1:B:42:ARG:HH12	1.73	0.53
1:B:9:GLU:HA	1:B:12:LYS:HB2	1.90	0.53
2:C:28:ILE:HD11	6:C:301:NAG:H82	1.91	0.52
2:D:110:ILE:HD12	2:D:204:LEU:HD11	1.91	0.52
3:I:118:GLU:HA	3:I:123:HIS:HA	1.93	0.50
2:D:27:PRO:HG2	2:D:70:ILE:HG13	1.93	0.50
1:A:42:ARG:HH12	1:B:119:GLU:HB3	1.77	0.49
1:A:113:LEU:HD21	1:B:73:ILE:HD13	1.94	0.49
3:E:51:PRO:HB3	3:E:92:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:PRO:HG2	2:C:70:ILE:HG13	1.94	0.49
2:D:29:VAL:HG21	2:D:83:VAL:HG11	1.95	0.48
1:A:9:GLU:HG2	1:A:12:LYS:HD3	1.95	0.48
2:C:51:VAL:O	2:C:54:SER:OG	2.30	0.47
2:C:204:LEU:HD22	2:C:209:VAL:HB	1.96	0.47
2:D:134:PHE:CE2	2:D:152:ILE:HD11	2.49	0.47
1:A:73:ILE:HD13	1:B:113:LEU:HD21	1.96	0.47
1:A:28:LEU:HB3	1:B:98:TYR:CE2	2.50	0.47
2:D:105:CYS:SG	2:D:204:LEU:HD23	2.55	0.47
2:C:169:LYS:NZ	3:I:164:ASP:OD1	2.33	0.46
2:D:170:ILE:HD11	2:D:185:LEU:HD13	1.97	0.46
1:A:98:TYR:CE2	1:B:28:LEU:HB3	2.50	0.46
3:E:79:ILE:HD12	3:E:79:ILE:H	1.80	0.46
3:I:118:GLU:HB3	3:I:123:HIS:HB3	1.97	0.46
2:C:188:PRO:HB2	3:I:156:ILE:HD12	1.98	0.46
1:A:68:LYS:HE3	3:I:81:SER:O	2.16	0.46
3:I:56:ASN:ND2	7:I:310:EDO:O2	2.49	0.45
2:D:76:ASP:OD1	2:D:148:THR:OG1	2.31	0.45
1:A:114:ILE:H	1:A:114:ILE:HD12	1.82	0.45
2:D:114:LYS:HB2	2:D:129:PHE:HB2	1.99	0.45
1:A:22:VAL:HG12	2:C:49:TYR:HE2	1.82	0.44
3:I:72:SER:OG	3:I:73:LYS:N	2.50	0.44
2:D:110:ILE:HB	2:D:211:THR:HG22	1.99	0.44
3:E:86:CYS:SG	3:E:94:CYS:HB2	2.56	0.44
2:D:86:LYS:HD3	2:D:96:TYR:CZ	2.53	0.44
3:E:64:GLN:NE2	3:E:118:GLU:OE2	2.51	0.43
3:E:65:VAL:HG22	3:E:115:LEU:HD13	2.01	0.43
2:D:153:ARG:NH2	3:E:167:ASP:HA	2.34	0.43
2:D:160:ARG:HA	2:D:165:GLU:HA	1.99	0.43
1:B:114:ILE:H	1:B:114:ILE:HD12	1.84	0.42
2:D:189:VAL:HG12	2:D:196:TYR:CZ	2.54	0.42
2:C:170:ILE:HD11	2:C:185:LEU:HD13	2.02	0.42
3:I:150:PRO:HA	3:I:155:LEU:HD23	2.02	0.42
3:E:218:TRP:CZ2	3:E:220:LYS:HD2	2.54	0.42
3:E:209:CYS:HA	3:E:234:CYS:HA	2.01	0.41
2:C:103:ALA:HB3	2:C:106:ARG:HB3	2.02	0.41
3:I:149:THR:HA	3:I:150:PRO:HD3	1.95	0.40
2:C:63:ILE:HD12	2:C:63:ILE:HA	1.94	0.40
1:A:23:ALA:HA	2:C:49:TYR:CD2	2.57	0.40
3:I:28:SER:OG	3:I:29:GLN:N	2.55	0.40
3:I:213:GLN:HB2	3:I:229:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47:LYS:HB2	2:C:56:TRP:CE3	2.56	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	123/148 (83%)	121 (98%)	2 (2%)	0	100	100
1	B	124/148 (84%)	123 (99%)	1 (1%)	0	100	100
2	C	203/242 (84%)	197 (97%)	6 (3%)	0	100	100
2	D	199/242 (82%)	194 (98%)	5 (2%)	0	100	100
3	E	211/233 (91%)	203 (96%)	8 (4%)	0	100	100
3	I	211/233 (91%)	205 (97%)	6 (3%)	0	100	100
All	All	1071/1246 (86%)	1043 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/132 (87%)	114 (99%)	1 (1%)	78	87
1	B	112/132 (85%)	111 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	188/218 (86%)	187 (100%)	1 (0%)	88	93
2	D	175/218 (80%)	172 (98%)	3 (2%)	60	78
3	E	187/203 (92%)	185 (99%)	2 (1%)	73	84
3	I	188/203 (93%)	184 (98%)	4 (2%)	53	75
All	All	965/1106 (87%)	953 (99%)	12 (1%)	71	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	B	24	ASP
2	C	12	VAL
2	D	136	ASN
2	D	177	ASP
2	D	182	ARG
3	E	76	THR
3	E	229	LEU
3	I	55	SER
3	I	76	THR
3	I	217	LEU
3	I	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

7 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	4,3	14,14,15	0.54	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.35	0
5	NAG	G	1	5,3	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.20	0	17,19,21	0.43	0
5	BMA	G	3	5	11,11,12	0.61	0	15,15,17	0.90	0
5	MAN	G	4	5	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
5	MAN	G	5	5	11,11,12	0.91	0	15,15,17	1.10	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
5	NAG	G	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	4	MAN	C1-O5-C5	2.62	115.74	112.19
5	G	5	MAN	C1-O5-C5	2.26	115.25	112.19
5	G	5	MAN	O2-C2-C3	-2.16	105.82	110.14
5	G	4	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

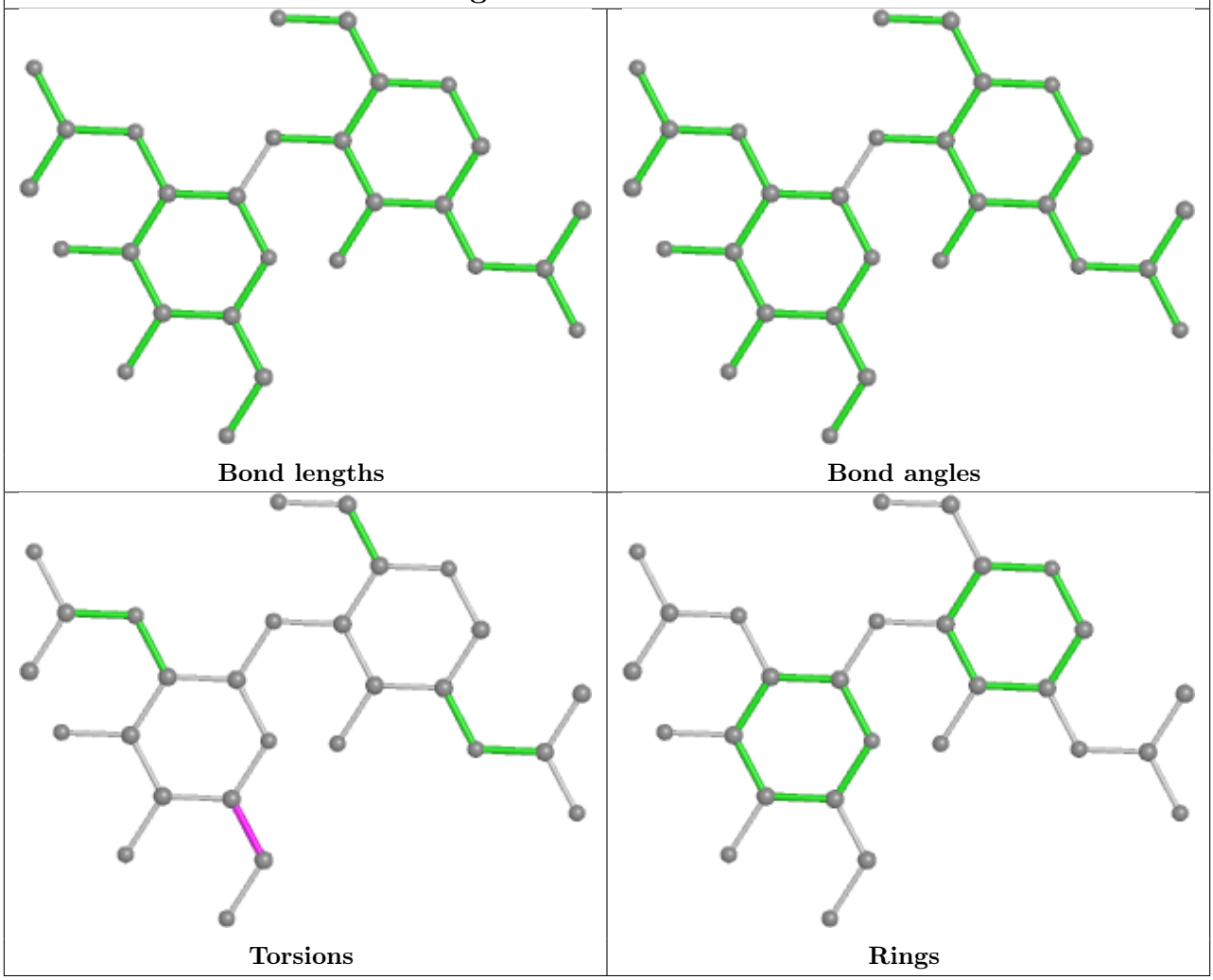
Mol	Chain	Res	Type	Atoms
5	G	5	MAN	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

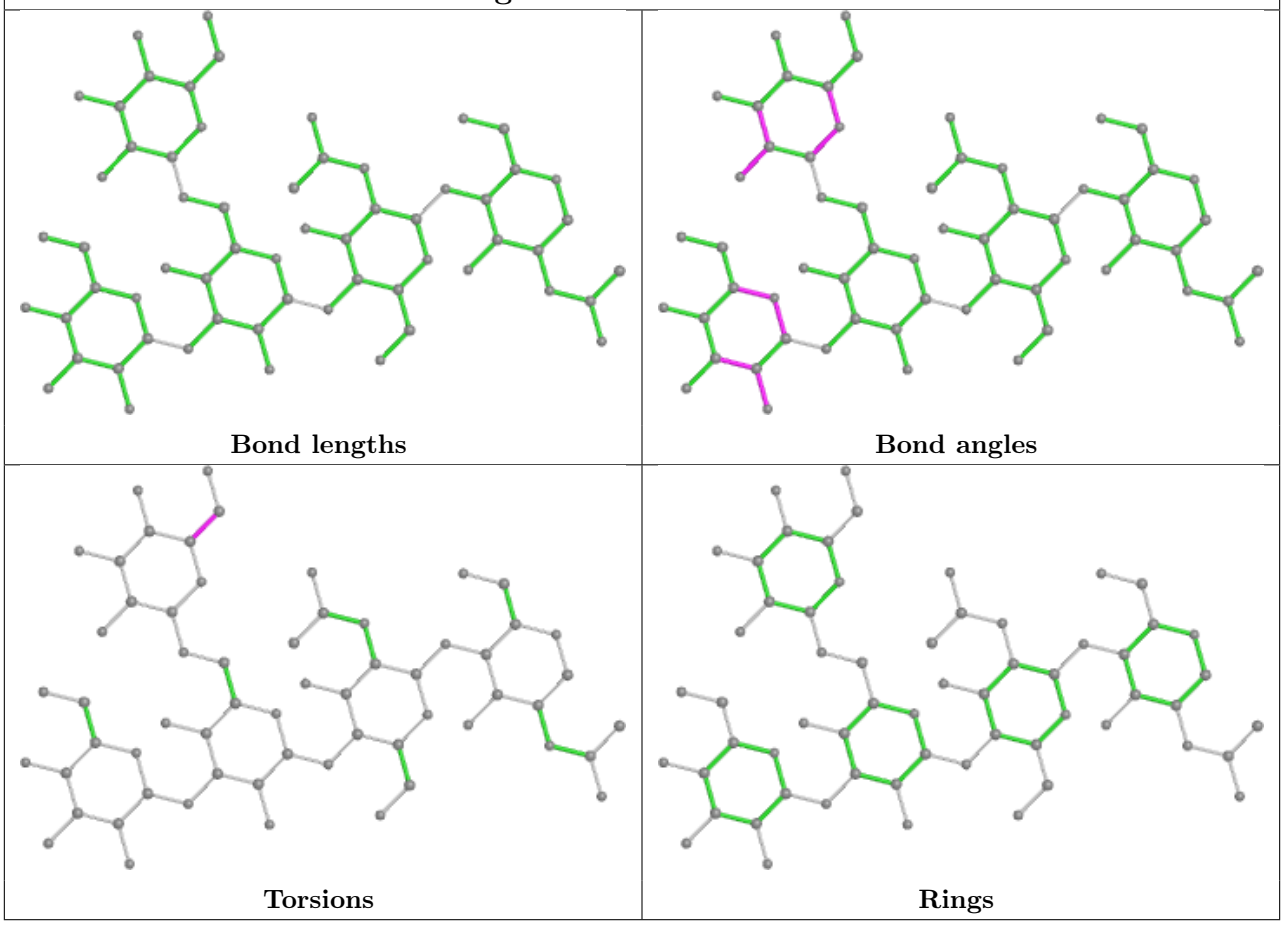
No monomer is involved in short contacts.

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

Oligosaccharide Chain F



Oligosaccharide Chain G



5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
7	EDO	C	303	-	3,3,3	0.46	0	2,2,2	0.43	0
8	CYS	I	309	3	5,6,6	1.04	1 (20%)	5,7,7	1.64	2 (40%)
6	NAG	I	308	3	14,14,15	0.31	0	17,19,21	0.49	0
6	NAG	I	301	3	14,14,15	0.27	0	17,19,21	0.48	0
8	CYS	E	306	3	5,6,6	1.20	1 (20%)	5,7,7	1.73	2 (40%)
7	EDO	C	304	-	3,3,3	0.52	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	301	1	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	C	301	2	14,14,15	0.39	0	17,19,21	0.48	0
6	NAG	I	307	3	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	E	302	3	14,14,15	0.21	0	17,19,21	0.38	0
7	EDO	I	311	-	3,3,3	0.49	0	2,2,2	0.25	0
6	NAG	D	301	2	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	E	301	3	14,14,15	0.19	0	17,19,21	0.49	0
7	EDO	B	302	-	3,3,3	0.46	0	2,2,2	0.35	0
6	NAG	D	302	2	14,14,15	0.30	0	17,19,21	0.51	0
6	NAG	C	302	2	14,14,15	0.23	0	17,19,21	0.42	0
7	EDO	D	303	-	3,3,3	0.47	0	2,2,2	0.38	0
7	EDO	I	310	-	3,3,3	0.49	0	2,2,2	0.24	0
6	NAG	B	301	1	14,14,15	0.22	0	17,19,21	0.46	0
6	NAG	E	305	3	14,14,15	0.25	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	303	-	-	0/1/1/1	-
8	CYS	I	309	3	-	1/6/6/6	-
6	NAG	I	308	3	-	1/6/23/26	0/1/1/1
6	NAG	I	301	3	-	2/6/23/26	0/1/1/1
8	CYS	E	306	3	-	1/6/6/6	-
7	EDO	C	304	-	-	0/1/1/1	-
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	301	2	-	2/6/23/26	0/1/1/1
6	NAG	I	307	3	-	2/6/23/26	0/1/1/1
6	NAG	E	302	3	-	2/6/23/26	0/1/1/1
7	EDO	I	311	-	-	1/1/1/1	-
6	NAG	D	301	2	-	2/6/23/26	0/1/1/1
6	NAG	E	301	3	-	2/6/23/26	0/1/1/1
7	EDO	B	302	-	-	1/1/1/1	-
6	NAG	D	302	2	-	1/6/23/26	0/1/1/1
6	NAG	C	302	2	-	2/6/23/26	0/1/1/1
7	EDO	D	303	-	-	0/1/1/1	-
7	EDO	I	310	-	-	0/1/1/1	-
6	NAG	B	301	1	-	1/6/23/26	0/1/1/1
6	NAG	E	305	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	306	CYS	OXT-C	-2.11	1.23	1.30
8	I	309	CYS	OXT-C	-2.01	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	306	CYS	OXT-C-O	-3.01	117.25	124.09
8	I	309	CYS	OXT-C-O	-2.76	117.83	124.09
8	I	309	CYS	OXT-C-CA	2.31	121.27	113.38
8	E	306	CYS	OXT-C-CA	2.27	121.12	113.38

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	309	CYS	C-CA-CB-SG
6	C	301	NAG	O5-C5-C6-O6
6	E	301	NAG	O5-C5-C6-O6
6	I	301	NAG	O5-C5-C6-O6
6	E	305	NAG	C4-C5-C6-O6
6	C	301	NAG	C4-C5-C6-O6
6	I	301	NAG	C4-C5-C6-O6
6	E	305	NAG	O5-C5-C6-O6
6	E	301	NAG	C4-C5-C6-O6
6	I	307	NAG	C4-C5-C6-O6
6	D	301	NAG	O5-C5-C6-O6
6	C	302	NAG	O5-C5-C6-O6
6	I	307	NAG	O5-C5-C6-O6
6	D	301	NAG	C4-C5-C6-O6
6	C	302	NAG	C4-C5-C6-O6
6	A	301	NAG	O5-C5-C6-O6
6	E	302	NAG	C4-C5-C6-O6
6	E	302	NAG	O5-C5-C6-O6
6	B	301	NAG	O5-C5-C6-O6
6	I	308	NAG	O5-C5-C6-O6
7	B	302	EDO	O1-C1-C2-O2
7	I	311	EDO	O1-C1-C2-O2
6	D	302	NAG	O5-C5-C6-O6
8	E	306	CYS	C-CA-CB-SG
6	A	301	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	301	NAG	1	0
6	E	302	NAG	1	0
7	I	310	EDO	1	0

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	125/148 (84%)	0.35	2 (1%)	72	69	95, 125, 166, 216	0
1	B	126/148 (85%)	0.39	5 (3%)	38	35	97, 143, 187, 246	0
2	C	207/242 (85%)	0.23	4 (1%)	66	64	102, 140, 197, 265	0
2	D	203/242 (83%)	0.68	27 (13%)	3	3	105, 172, 245, 284	0
3	E	213/233 (91%)	2.02	91 (42%)	0	0	179, 244, 297, 339	0
3	I	213/233 (91%)	0.10	1 (0%)	91	90	81, 114, 182, 241	0
All	All	1087/1246 (87%)	0.67	130 (11%)	4	4	81, 149, 270, 339	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	197	ILE	9.8
3	E	157	ILE	8.9
3	E	53	ALA	8.1
1	B	-1	GLY	7.5
2	D	189	VAL	7.1
3	E	155	LEU	6.6
3	E	54	LEU	6.6
3	E	33	PRO	6.5
3	E	28	SER	6.5
1	A	-1	GLY	6.3
2	D	168	TYR	6.3
3	E	60	PRO	6.3
3	E	198	SER	6.0
3	E	113	LEU	5.6
2	D	119	LYS	5.5
3	E	36	PRO	5.0
3	E	47	LEU	5.0
3	E	156	ILE	4.9
3	E	210	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
3	E	34	GLN	4.8
3	E	112	THR	4.8
2	D	126	ILE	4.7
3	E	129	MET	4.7
3	E	66	GLN	4.6
3	E	127	VAL	4.5
3	E	128	THR	4.5
3	E	96	PHE	4.5
3	E	58	THR	4.4
3	E	199	LEU	4.4
3	E	215	GLN	4.4
3	E	35	HIS	4.3
3	E	29	GLN	4.3
3	E	203	LYS	4.2
1	B	0	SER	4.2
3	E	61	VAL	4.1
3	E	38	ILE	4.1
3	E	65	VAL	4.0
3	E	30	LEU	4.0
2	D	124	ILE	4.0
2	D	121	GLU	4.0
3	E	152	GLU	4.0
3	E	211	GLN	3.9
2	D	196	TYR	3.9
3	E	159	PHE	3.8
2	D	188	PRO	3.8
2	D	190	SER	3.8
2	D	122	LYS	3.7
3	E	105	PHE	3.7
3	E	45	GLN	3.6
3	E	125	ALA	3.6
3	E	94	CYS	3.6
3	E	67	PHE	3.6
3	E	126	TRP	3.6
3	E	196	SER	3.6
3	E	240	ASP	3.5
2	C	117	ILE	3.5
2	D	187	ILE	3.5
3	E	153	GLY	3.5
3	E	115	LEU	3.4
3	E	192	PHE	3.3
3	E	212	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	E	238	MET	3.3
3	E	55	SER	3.3
3	E	37	LYS	3.3
2	D	123	GLN	3.3
3	E	202	LEU	3.3
3	E	52	VAL	3.3
3	E	75	PHE	3.3
2	D	170	ILE	3.3
2	D	155	TYR	3.2
2	D	50	GLY	3.2
3	E	148	VAL	3.2
3	E	140	VAL	3.2
2	C	127	ASP	3.2
3	E	59	ARG	3.1
3	E	226	VAL	3.1
3	E	77	ALA	3.0
3	E	74	TRP	3.0
3	E	158	ARG	3.0
3	E	214	ALA	3.0
3	E	179	TYR	2.8
2	D	86	LYS	2.8
3	E	177	VAL	2.8
3	I	54	LEU	2.8
3	E	49	TRP	2.8
1	B	2	ASP	2.8
3	E	150	PRO	2.7
2	D	186	ALA	2.7
3	E	209	CYS	2.7
3	E	217	LEU	2.7
2	D	127	ASP	2.6
3	E	76	THR	2.6
3	E	227	GLY	2.6
3	E	134	HIS	2.6
1	B	3	PRO	2.6
3	E	195	ASN	2.6
3	E	48	SER	2.6
3	E	154	SER	2.6
3	E	50	GLU	2.5
3	E	116	ARG	2.4
2	D	85	VAL	2.4
2	D	115	LEU	2.4
1	A	0	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	31	PRO	2.4
2	D	193	ASN	2.3
3	E	228	HIS	2.3
3	E	187	GLN	2.3
1	B	17	ALA	2.3
2	D	117	ILE	2.3
2	D	166	ILE	2.3
2	D	116	ASP	2.3
3	E	68	LYS	2.2
3	E	188	VAL	2.2
2	D	159	VAL	2.2
3	E	204	PRO	2.2
3	E	216	LEU	2.2
2	C	116	ASP	2.2
3	E	64	GLN	2.1
3	E	208	TYR	2.1
3	E	186	GLN	2.1
3	E	117	ALA	2.1
3	E	56	ASN	2.1
3	E	173	PHE	2.1
2	D	44	VAL	2.1
3	E	136	ARG	2.1
3	E	93	GLU	2.1
2	D	185	LEU	2.1
3	E	191	PRO	2.1
3	E	119	LEU	2.0
2	C	119	LYS	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MAN	G	5	11/12	0.74	0.35	251,268,292,296	0

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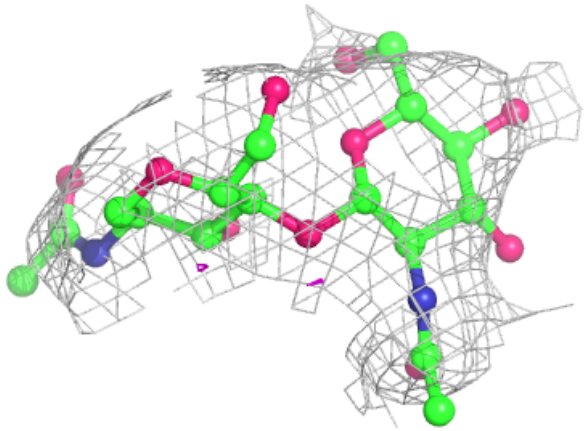
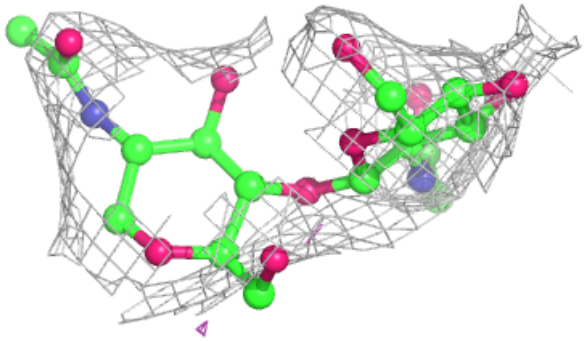
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	G	4	11/12	0.79	0.28	206,244,270,271	0
4	NAG	F	2	14/15	0.80	0.33	190,240,263,276	0
5	BMA	G	3	11/12	0.81	0.18	242,252,272,284	0
4	NAG	F	1	14/15	0.86	0.26	173,226,263,275	0
5	NAG	G	2	14/15	0.93	0.24	144,168,223,244	0
5	NAG	G	1	14/15	0.97	0.22	105,124,150,150	0

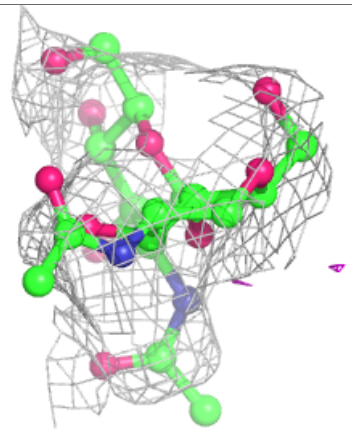
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

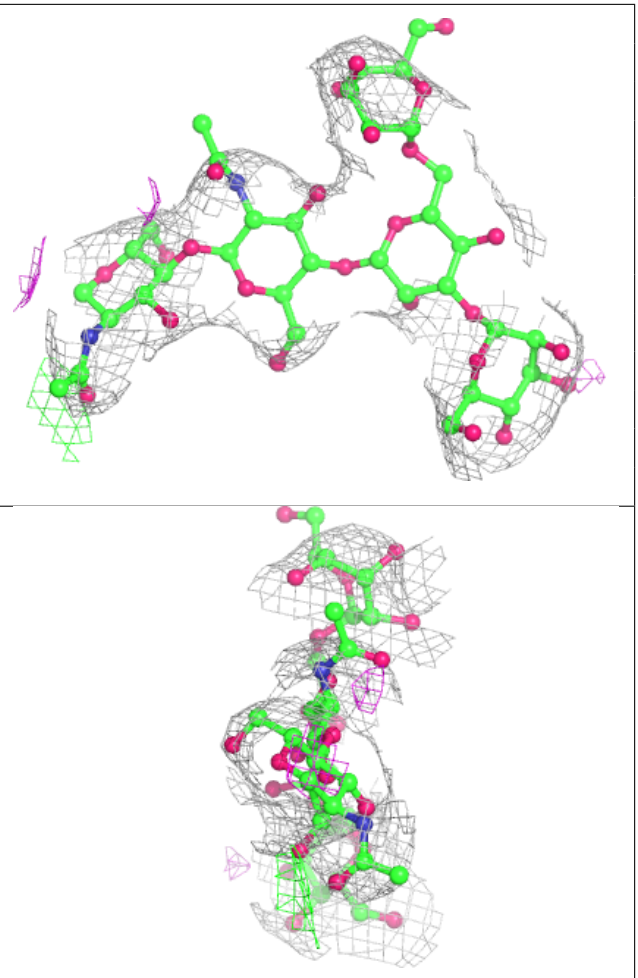






Electron density around Chain G:

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



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
8	CYS	E	306	7/7	0.21	0.46	208,217,245,247	0
7	EDO	C	304	4/4	0.31	0.29	158,158,169,172	0
7	EDO	I	311	4/4	0.61	0.26	144,154,164,171	0
7	EDO	I	310	4/4	0.65	0.28	119,133,158,168	0
8	CYS	I	309	7/7	0.65	0.32	154,180,201,214	0
6	NAG	E	305	14/15	0.67	0.31	208,257,290,291	0
7	EDO	C	303	4/4	0.79	0.20	157,159,174,175	0
6	NAG	E	301	14/15	0.82	0.20	201,238,244,250	0
7	EDO	B	302	4/4	0.82	0.48	148,151,164,166	0
6	NAG	I	307	14/15	0.87	0.28	180,217,239,252	0
6	NAG	B	301	14/15	0.88	0.33	176,210,231,233	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	301	14/15	0.89	0.21	181,225,237,239	0
6	NAG	C	301	14/15	0.89	0.22	115,152,200,215	0
6	NAG	D	301	14/15	0.89	0.17	159,192,217,231	0
7	EDO	D	303	4/4	0.89	0.12	184,184,184,186	0
6	NAG	E	302	14/15	0.90	0.22	185,211,222,224	0
6	NAG	D	302	14/15	0.91	0.27	131,165,219,234	0
6	NAG	I	301	14/15	0.94	0.21	106,140,171,178	0
6	NAG	C	302	14/15	0.94	0.24	149,197,222,231	0
6	NAG	I	308	14/15	0.95	0.27	116,158,235,267	0

6.5 Other polymers (i)

There are no such residues in this entry.