Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 09:07 PM EDT

PDB ID	:	5DK2
Title	:	Fc Heterodimer E356K/D399K + K392D/K409D
Authors	:	Atwell, S.; Leaver-Fay, A.; Froning, K.J.; Aldaz, H.; Pustilnik, A.; Lu, F.; Huang, F.; Yuan, R.; Dhanani, S.H.; Chamberlain, A.K.; Fitchett, J.R.; Gutierrez, B.; Hendle, J.; Demarest, S.J.; Kuhlman, B.
Deposited on	:	2015-09-02
Resolution	:	2.60 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:

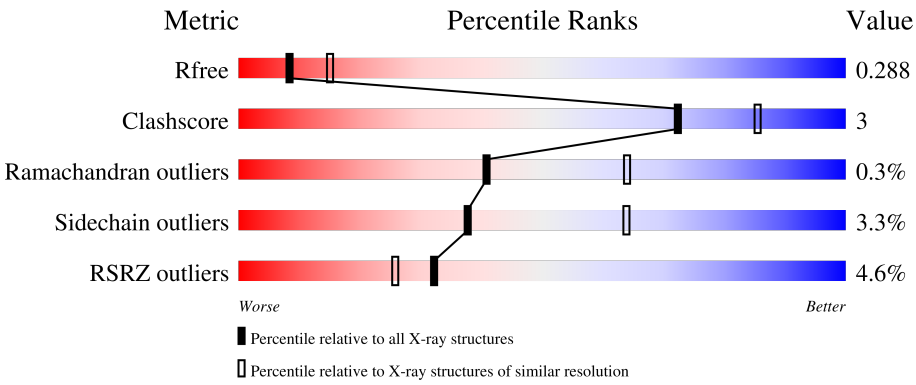
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	227	79% 12% 9%
1	D	227	4% 8% • 91%
2	B	240	80% 7% 13%
2	E	240	8% 59% 7% • 34%
3	C	13	77% 15% 8%

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Mol	Chain	Length	Quality of chain
4	F	8	25% 62% 12%
4	G	8	88% 12%
5	H	7	14% 86%

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
5	MAN	H	7	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5114 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1643	1050	274	312	7	0	1	0
			Total	C	N	O				
1	D	21	138	90	21	27		0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	LYS	ASP	variant	UNP P01857
A	358	MET	LEU	variant	UNP P01857
A	399	LYS	ASP	engineered mutation	UNP P01857
D	356	LYS	ASP	variant	UNP P01857
D	358	MET	LEU	variant	UNP P01857
D	399	LYS	ASP	engineered mutation	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	208	1637	1039	269	323	6	0	0	0
			Total	C	N	O	S			
2	E	159	1206	778	195	228	5	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	208	HIS	-	expression tag	UNP P01857
B	209	HIS	-	expression tag	UNP P01857
B	210	HIS	-	expression tag	UNP P01857
B	211	HIS	-	expression tag	UNP P01857
B	212	HIS	-	expression tag	UNP P01857
B	213	HIS	-	expression tag	UNP P01857

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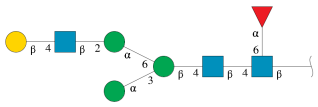
Chain	Residue	Modelled	Actual	Comment	Reference
B	214	HIS	-	expression tag	UNP P01857
B	215	HIS	-	expression tag	UNP P01857
B	216	SER	-	expression tag	UNP P01857
B	217	GLY	-	expression tag	UNP P01857
B	218	SER	-	expression tag	UNP P01857
B	219	GLY	-	expression tag	UNP P01857
B	220	SER	-	expression tag	UNP P01857
B	252	GLU	MET	engineered mutation	UNP P01857
B	253	ALA	ILE	engineered mutation	UNP P01857
B	356	GLU	ASP	variant	UNP P01857
B	358	MET	LEU	variant	UNP P01857
B	392	ASP	LYS	engineered mutation	UNP P01857
B	409	ASP	LYS	engineered mutation	UNP P01857
B	435	ALA	HIS	engineered mutation	UNP P01857
E	208	HIS	-	expression tag	UNP P01857
E	209	HIS	-	expression tag	UNP P01857
E	210	HIS	-	expression tag	UNP P01857
E	211	HIS	-	expression tag	UNP P01857
E	212	HIS	-	expression tag	UNP P01857
E	213	HIS	-	expression tag	UNP P01857
E	214	HIS	-	expression tag	UNP P01857
E	215	HIS	-	expression tag	UNP P01857
E	216	SER	-	expression tag	UNP P01857
E	217	GLY	-	expression tag	UNP P01857
E	218	SER	-	expression tag	UNP P01857
E	219	GLY	-	expression tag	UNP P01857
E	220	SER	-	expression tag	UNP P01857
E	252	GLU	MET	engineered mutation	UNP P01857
E	253	ALA	ILE	engineered mutation	UNP P01857
E	356	GLU	ASP	variant	UNP P01857
E	358	MET	LEU	variant	UNP P01857
E	392	ASP	LYS	engineered mutation	UNP P01857
E	409	ASP	LYS	engineered mutation	UNP P01857
E	435	ALA	HIS	engineered mutation	UNP P01857

- Molecule 3 is a protein called Fc-III peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	13	107	69	17	19	2	0	0	0

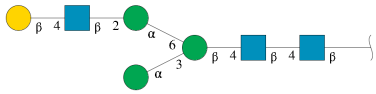
- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	8	96	54	3	39	0	0	0
4	G	8	96	54	3	39	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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	H	7	86	48	3	35	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	46	46	46	0	0
6	B	49	49	49	0	0
6	E	10	10	10	0	0

3 Residue-property plots (i)

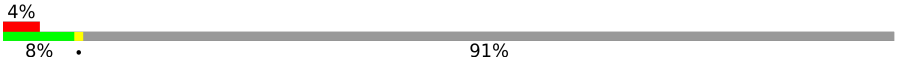
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

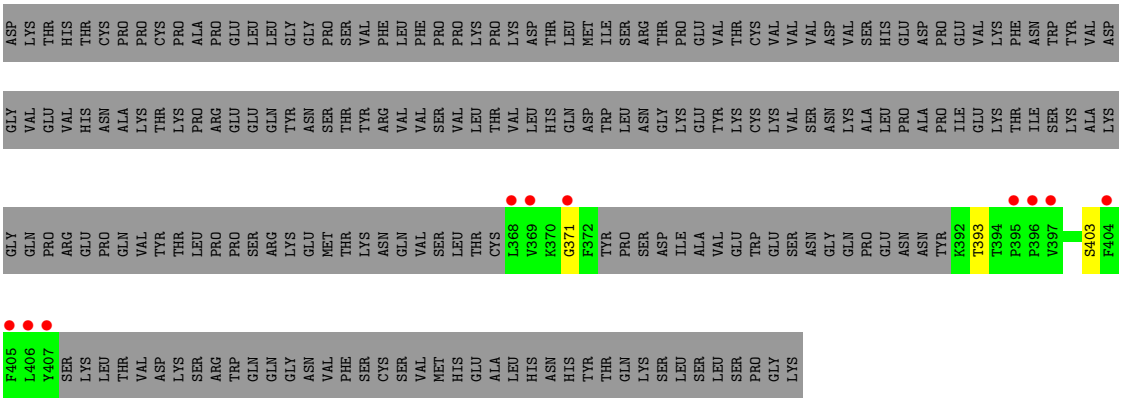
• Molecule 1: Ig gamma-1 chain C region

Chain A:

• Molecule 1: Ig gamma-1 chain C region

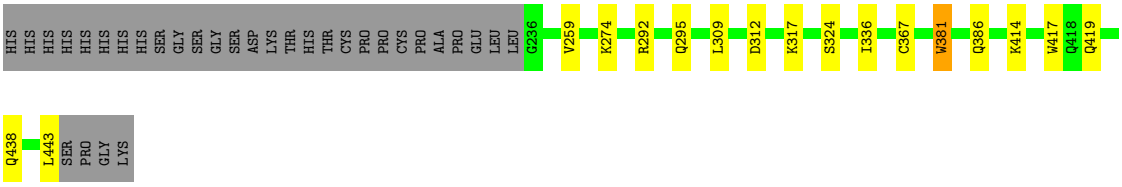
Chain D:





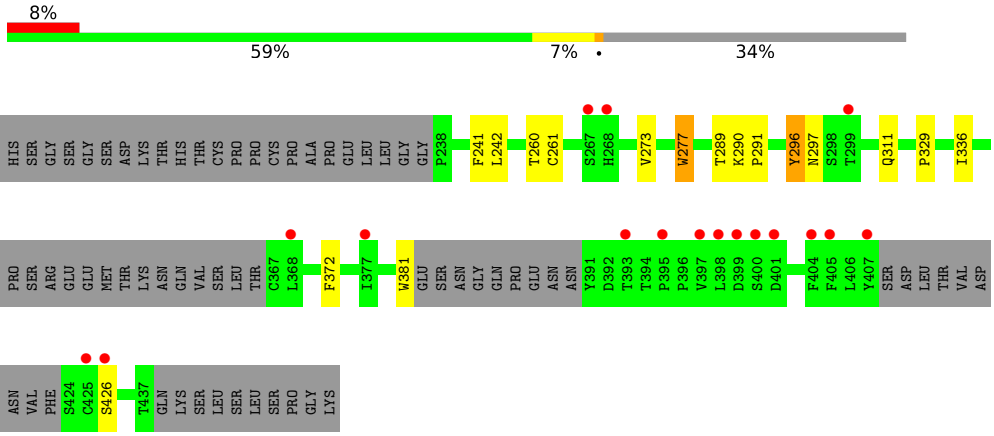
• Molecule 2: Ig gamma-1 chain C region

Chain B:



• Molecule 2: Ig gamma-1 chain C region

Chain E:

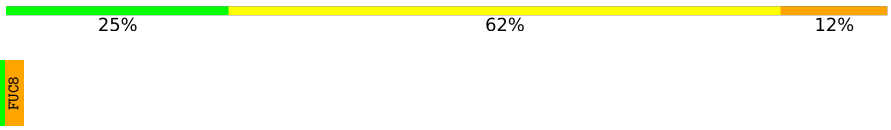


- Molecule 3: Fc-III peptide

Chain C:

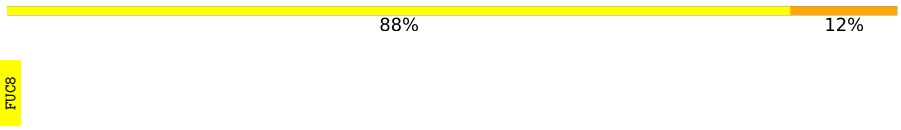
- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



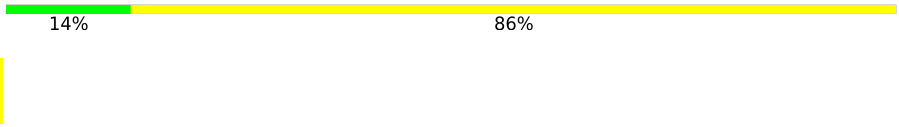
- Molecule 4: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.86Å 60.56Å 159.45Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 64.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.60) 97.1 (64.26-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0017	Depositor
R, R_{free}	0.225 , 0.289 0.225 , 0.288	Depositor DCC
R_{free} test set	1848 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5114	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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, BMA, FUC, GAL, 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	0.58	4/1693 (0.2%)	0.61	0/2309
1	D	0.41	0/140	0.56	0/192
2	B	0.54	2/1682 (0.1%)	0.62	0/2298
2	E	0.53	2/1242 (0.2%)	0.57	1/1707 (0.1%)
3	C	0.93	0/111	0.60	0/151
All	All	0.56	8/4868 (0.2%)	0.60	1/6657 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	TRP	CD2-CE2	5.92	1.48	1.41
1	A	417	TRP	CD2-CE2	5.53	1.48	1.41
2	E	381	TRP	CD2-CE2	5.51	1.48	1.41
1	A	381	TRP	CD2-CE2	5.38	1.47	1.41
1	A	313	TRP	CD2-CE2	5.15	1.47	1.41
2	B	381	TRP	CD2-CE2	5.09	1.47	1.41
2	E	277	TRP	CD2-CE2	5.05	1.47	1.41
2	B	417	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	296	TYR	N-CA-C	5.69	126.36	111.00

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	1643	0	1591	11	0
1	D	138	0	113	1	0
2	B	1637	0	1559	9	0
2	E	1206	0	1090	12	0
3	C	107	0	93	2	0
4	F	96	0	82	1	0
4	G	96	0	82	1	0
5	H	86	0	73	1	0
6	A	46	0	0	3	0
6	B	49	0	0	1	0
6	E	10	0	0	0	0
All	All	5114	0	4683	33	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 (33) 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:E:296:TYR:H	2:E:297:ASN:HB2	1.41	0.86
2:E:346:PRO:HB3	2:E:372:PHE:HB3	1.68	0.76
2:E:296:TYR:N	2:E:297:ASN:HB2	2.08	0.67
2:B:419:GLN:NE2	2:E:273:VAL:O	2.33	0.61
6:A:632:HOH:O	4:F:8:FUC:H2	1.98	0.61
1:A:353:PRO:HD3	1:A:365:LEU:CD2	2.31	0.61
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.89	0.55
2:B:274:LYS:HB3	2:B:324:SER:HB2	1.91	0.52
1:A:293:GLU:HG3	1:A:295:GLN:NE2	2.26	0.51
1:D:371:GLY:HA2	1:D:403:SER:HB2	1.93	0.50
2:B:367:CYS:HB2	2:B:381:TRP:CZ2	2.47	0.50
2:E:296:TYR:H	2:E:297:ASN:CB	2.19	0.50
2:B:295:GLN:OE1	4:G:1:NAG:H62	2.12	0.48
2:E:242:LEU:HG	2:E:336:ILE:HG12	1.96	0.48
1:A:296:TYR:C	1:A:298:SER:H	2.17	0.47
3:C:1:ASP:O	3:C:12:CYS:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASN:OD1	3:C:13:THR:HG23	2.15	0.46
2:B:386:GLN:HB2	6:B:607:HOH:O	2.15	0.46
2:B:259:VAL:HG13	2:B:336:ILE:HD11	1.97	0.45
2:E:242:LEU:HD12	2:E:260:THR:O	2.16	0.45
2:B:312:ASP:CG	2:B:317:LYS:HD2	2.36	0.45
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.52	0.45
1:A:316:GLY:HA2	6:A:619:HOH:O	2.17	0.45
2:B:419:GLN:HG3	2:E:289:THR:HG21	1.99	0.45
1:A:276:ASN:HA	6:A:605:HOH:O	2.16	0.44
1:A:269:GLU:O	1:A:271:PRO:HD3	2.18	0.44
1:A:406:LEU:C	1:A:406:LEU:HD12	2.38	0.44
2:E:261:CYS:HB2	2:E:277:TRP:CZ2	2.55	0.42
2:E:290:LYS:HA	2:E:291:PRO:HD2	1.91	0.41
1:A:353:PRO:HD3	1:A:365:LEU:HD23	2.02	0.41
2:B:414:LYS:HB3	2:B:414:LYS:HE2	1.92	0.40
2:E:241:PHE:CE2	5:H:2:NAG:H4	2.57	0.40
2:E:296:TYR:N	2:E:297:ASN:CB	2.79	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	206/227 (91%)	199 (97%)	7 (3%)	0	100	100
1	D	17/227 (8%)	13 (76%)	4 (24%)	0	100	100
2	B	206/240 (86%)	202 (98%)	3 (2%)	1 (0%)	29	52
2	E	151/240 (63%)	145 (96%)	5 (3%)	1 (1%)	22	43
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
All	All	591/947 (62%)	569 (96%)	20 (3%)	2 (0%)	41	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	329	PRO
2	B	292	ARG

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	187/210 (89%)	177 (95%)	10 (5%)	22	45
1	D	12/210 (6%)	11 (92%)	1 (8%)	11	22
2	B	186/219 (85%)	183 (98%)	3 (2%)	62	82
2	E	126/219 (58%)	124 (98%)	2 (2%)	62	82
3	C	11/11 (100%)	10 (91%)	1 (9%)	9	18
All	All	522/869 (60%)	505 (97%)	17 (3%)	38	64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	292	ARG
1	A	298	SER
1	A	328	LEU
1	A	340	LYS
1	A	362	GLN
1	A	376	ASP
1	A	383	SER
1	A	415	SER
1	A	426	SER
2	B	309	LEU
2	B	438	GLN
2	B	443	LEU
3	C	1	ASP
1	D	393	THR
2	E	311	GLN
2	E	426	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	386	GLN
2	B	347	GLN
2	B	361	ASN
2	B	418	GLN
2	B	421	ASN
2	B	434	ASN
2	B	438	GLN

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)

23 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	4,1	14,14,15	0.38	0	17,19,21	1.52	3 (17%)
4	NAG	F	2	4	14,14,15	0.57	0	17,19,21	0.87	0
4	BMA	F	3	4	11,11,12	0.40	0	15,15,17	1.33	1 (6%)
4	MAN	F	4	4	11,11,12	0.58	0	15,15,17	1.51	2 (13%)
4	NAG	F	5	4	14,14,15	0.59	0	17,19,21	1.35	3 (17%)
4	GAL	F	6	4	11,11,12	0.60	0	15,15,17	2.82	3 (20%)
4	MAN	F	7	4	11,11,12	0.57	0	15,15,17	0.89	0
4	FUC	F	8	4	10,10,11	0.76	0	14,14,16	1.26	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	1	2,4	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
4	NAG	G	2	4	14,14,15	0.41	0	17,19,21	1.10	1 (5%)
4	BMA	G	3	4	11,11,12	0.61	0	15,15,17	1.34	2 (13%)
4	MAN	G	4	4	11,11,12	0.64	0	15,15,17	1.26	3 (20%)
4	NAG	G	5	4	14,14,15	0.68	0	17,19,21	1.11	2 (11%)
4	GAL	G	6	4	11,11,12	0.56	0	15,15,17	0.98	1 (6%)
4	MAN	G	7	4	11,11,12	0.52	0	15,15,17	2.17	6 (40%)
4	FUC	G	8	4	10,10,11	0.69	0	14,14,16	1.01	1 (7%)
5	NAG	H	1	2,5	14,14,15	0.46	0	17,19,21	2.04	1 (5%)
5	NAG	H	2	5	14,14,15	0.54	0	17,19,21	0.92	0
5	BMA	H	3	5	11,11,12	0.60	0	15,15,17	1.55	3 (20%)
5	MAN	H	4	5	11,11,12	0.56	0	15,15,17	1.05	1 (6%)
5	NAG	H	5	5	14,14,15	0.61	0	17,19,21	1.29	2 (11%)
5	GAL	H	6	5	11,11,12	0.62	0	15,15,17	0.92	0
5	MAN	H	7	5	11,11,12	0.59	0	15,15,17	1.19	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
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	NAG	F	5	4	-	0/6/23/26	0/1/1/1
4	GAL	F	6	4	-	2/2/19/22	0/1/1/1
4	MAN	F	7	4	-	2/2/19/22	0/1/1/1
4	FUC	F	8	4	-	-	0/1/1/1
4	NAG	G	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	NAG	G	5	4	-	0/6/23/26	0/1/1/1
4	GAL	G	6	4	-	0/2/19/22	0/1/1/1
4	MAN	G	7	4	-	1/2/19/22	0/1/1/1
4	FUC	G	8	4	-	-	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	1/6/23/26	0/1/1/1
5	GAL	H	6	5	-	2/2/19/22	0/1/1/1
5	MAN	H	7	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6	GAL	C1-O5-C5	9.89	125.59	112.19
5	H	1	NAG	C1-O5-C5	7.06	121.75	112.19
4	G	7	MAN	C1-O5-C5	5.77	120.01	112.19
4	F	3	BMA	C1-O5-C5	4.30	118.01	112.19
5	H	3	BMA	C1-C2-C3	3.99	114.58	109.67
5	H	5	NAG	C4-C3-C2	3.99	116.86	111.02
4	F	4	MAN	C1-O5-C5	3.98	117.59	112.19
4	G	4	MAN	C1-O5-C5	3.65	117.14	112.19
4	F	1	NAG	C6-C5-C4	-3.56	104.66	113.00
4	F	1	NAG	O5-C5-C6	3.47	112.65	107.20
4	F	6	GAL	O5-C1-C2	3.27	115.82	110.77
4	G	8	FUC	O5-C1-C2	-3.23	105.79	110.77
4	F	8	FUC	C3-C4-C5	3.17	114.71	109.77
4	G	7	MAN	O5-C5-C6	3.10	112.06	107.20
5	H	7	MAN	C1-O5-C5	3.06	116.33	112.19
5	H	4	MAN	C1-O5-C5	2.71	115.86	112.19
4	G	7	MAN	O5-C1-C2	2.70	114.93	110.77
4	F	4	MAN	O2-C2-C3	-2.68	104.78	110.14
4	G	2	NAG	C1-O5-C5	2.66	115.80	112.19
4	G	7	MAN	C3-C4-C5	2.64	114.95	110.24
4	G	1	NAG	C1-O5-C5	2.60	115.71	112.19
4	F	1	NAG	C1-O5-C5	2.59	115.70	112.19
5	H	3	BMA	C3-C4-C5	2.56	114.81	110.24
4	F	5	NAG	C1-C2-N2	-2.52	106.18	110.49
4	G	7	MAN	C1-C2-C3	2.46	112.69	109.67
4	G	3	BMA	O5-C5-C6	2.37	110.92	107.20
4	F	5	NAG	O4-C4-C5	2.29	114.97	109.30
4	F	8	FUC	O5-C5-C6	2.21	112.09	107.33
4	G	3	BMA	C1-C2-C3	2.20	112.37	109.67
5	H	5	NAG	C3-C4-C5	2.19	114.15	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3	BMA	C1-O5-C5	2.12	115.06	112.19
4	G	4	MAN	O3-C3-C2	-2.08	106.01	109.99
4	G	5	NAG	C1-O5-C5	2.08	115.01	112.19
4	F	5	NAG	O5-C1-C2	-2.07	108.02	111.29
4	G	5	NAG	C3-C4-C5	2.05	113.89	110.24
4	G	7	MAN	C2-C3-C4	2.03	114.41	110.89
4	G	6	GAL	C1-C2-C3	2.02	112.15	109.67
4	F	6	GAL	O5-C5-C4	2.01	115.72	110.83
4	G	4	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O5-C5-C6-O6
5	H	6	GAL	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	F	7	MAN	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	H	6	GAL	C4-C5-C6-O6
4	F	6	GAL	C4-C5-C6-O6
5	H	7	MAN	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	7	MAN	O5-C5-C6-O6
5	H	7	MAN	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	6	GAL	O5-C5-C6-O6
4	G	7	MAN	O5-C5-C6-O6
5	H	5	NAG	C4-C5-C6-O6

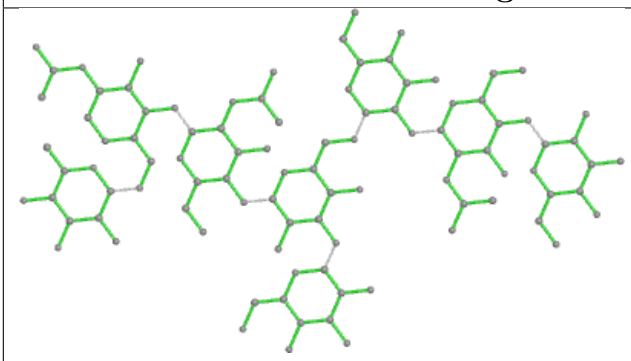
There are no ring outliers.

3 monomers are involved in 3 short contacts:

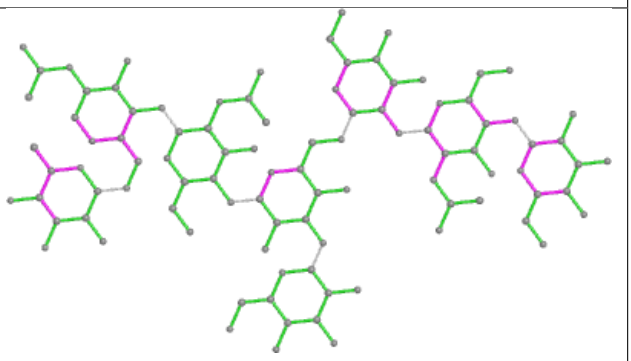
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
4	G	1	NAG	1	0
4	F	8	FUC	1	0

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

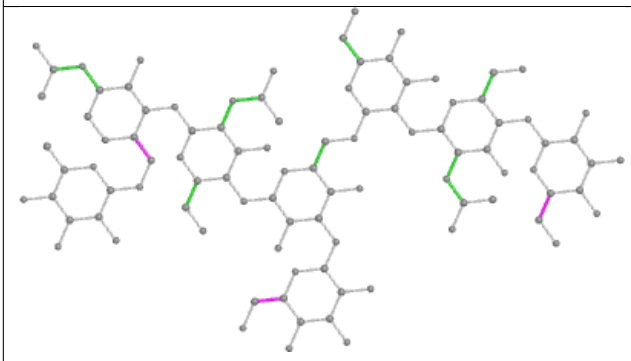
Oligosaccharide Chain F



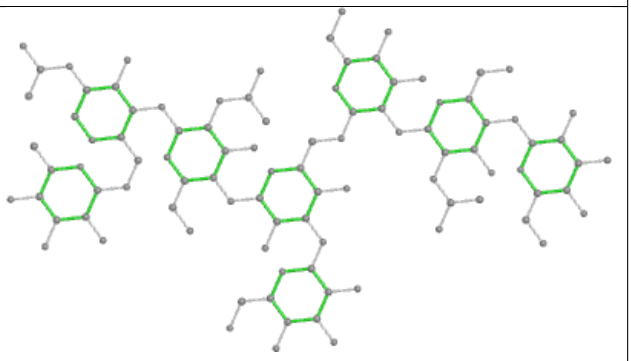
Bond lengths



Bond angles

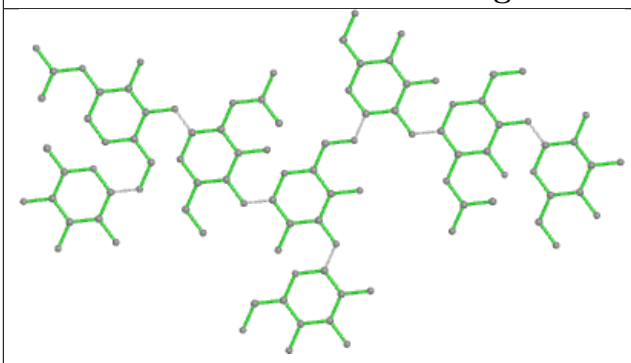


Torsions

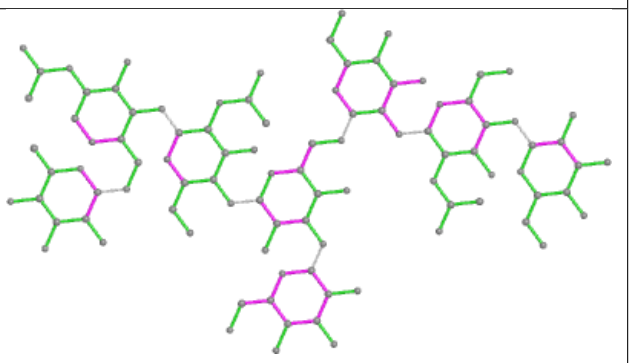


Rings

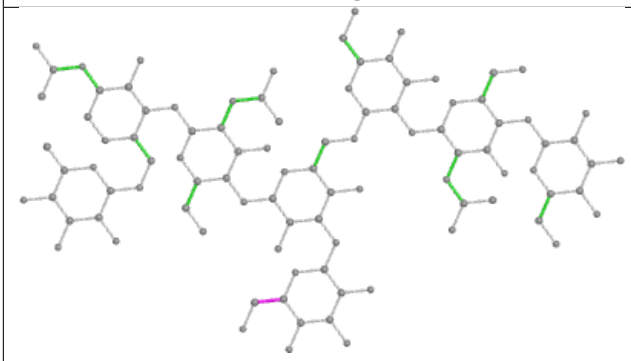
Oligosaccharide Chain G



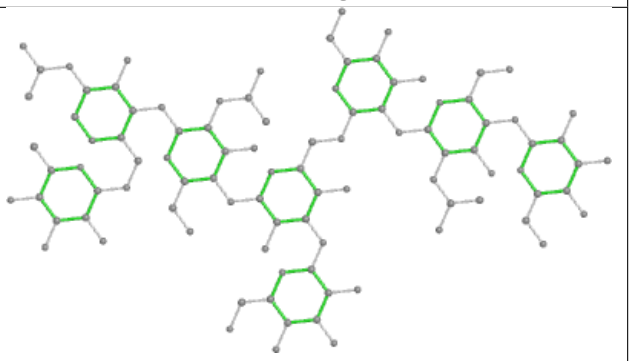
Bond lengths



Bond angles

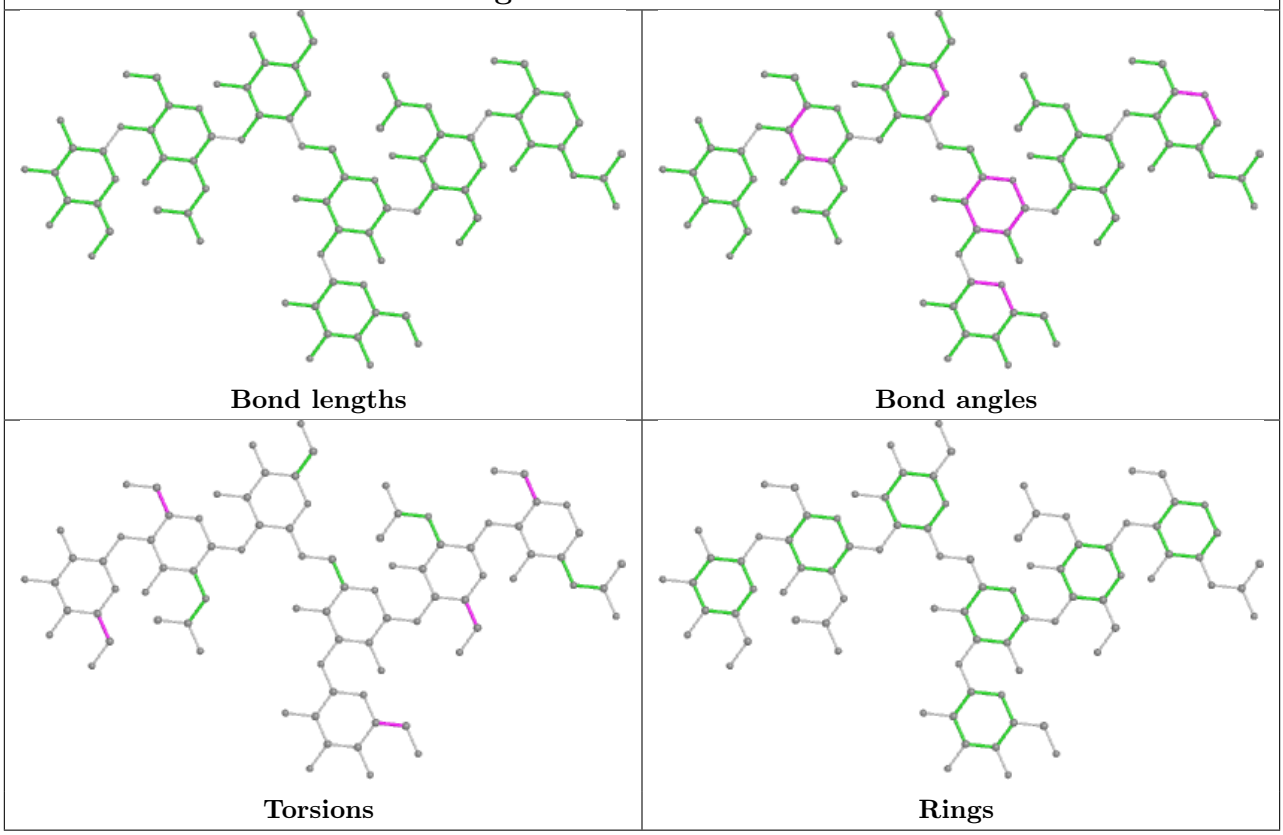


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	207/227 (91%)	-0.22	0 100 100	21, 40, 64, 89	0
1	D	21/227 (9%)	2.26	10 (47%) 0 0	91, 102, 117, 123	0
2	B	208/240 (86%)	-0.15	0 100 100	23, 44, 64, 90	0
2	E	159/240 (66%)	0.50	18 (11%) 5 3	38, 71, 105, 134	0
3	C	13/13 (100%)	-0.00	0 100 100	33, 47, 65, 65	0
All	All	608/947 (64%)	0.08	28 (4%) 32 26	21, 47, 96, 134	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	369	VAL	6.6
1	D	368	LEU	4.9
1	D	406	LEU	4.8
2	E	400	SER	4.7
2	E	398	LEU	4.3
1	D	405	PHE	4.1
1	D	396	PRO	3.9
2	E	368	LEU	3.9
2	E	348	VAL	3.6
2	E	407	TYR	3.3
2	E	401	ASP	3.2
2	E	299	THR	3.1
1	D	395	PRO	3.1
2	E	405	PHE	3.0
2	E	397	VAL	2.9
1	D	407	TYR	2.9
2	E	268	HIS	2.7
2	E	404	PHE	2.6
1	D	397	VAL	2.6
2	E	393	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	267	SER	2.5
2	E	425	CYS	2.4
1	D	404	PHE	2.4
2	E	395	PRO	2.3
2	E	426	SER	2.2
1	D	371	GLY	2.2
2	E	377	ILE	2.1
2	E	399	ASP	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	H	7	11/12	0.70	0.41	126,132,144,146	0
5	GAL	H	6	11/12	0.85	0.29	51,90,108,113	0
4	MAN	G	7	11/12	0.87	0.16	62,85,98,107	0
5	NAG	H	5	14/15	0.89	0.22	74,100,112,119	0
5	NAG	H	1	14/15	0.90	0.29	74,90,105,108	0
5	BMA	H	3	11/12	0.91	0.18	66,90,104,111	0
4	GAL	F	6	11/12	0.91	0.24	40,56,65,69	0
5	MAN	H	4	11/12	0.93	0.17	70,87,103,103	0
4	MAN	F	7	11/12	0.93	0.14	58,70,83,84	0
5	NAG	H	2	14/15	0.94	0.23	70,81,92,97	0
4	FUC	F	8	10/11	0.94	0.17	57,75,93,93	0
4	NAG	G	5	14/15	0.95	0.13	38,50,62,70	0
4	GAL	G	6	11/12	0.96	0.19	55,60,70,71	0
4	BMA	G	3	11/12	0.96	0.12	39,44,52,63	0
4	BMA	F	3	11/12	0.96	0.12	40,48,52,54	0
4	NAG	G	1	14/15	0.97	0.16	23,34,52,59	0
4	NAG	F	5	14/15	0.97	0.14	35,44,49,52	0
4	MAN	G	4	11/12	0.97	0.13	42,51,57,57	0
4	NAG	F	2	14/15	0.97	0.16	27,39,53,58	0
4	NAG	F	1	14/15	0.97	0.16	43,49,56,57	0

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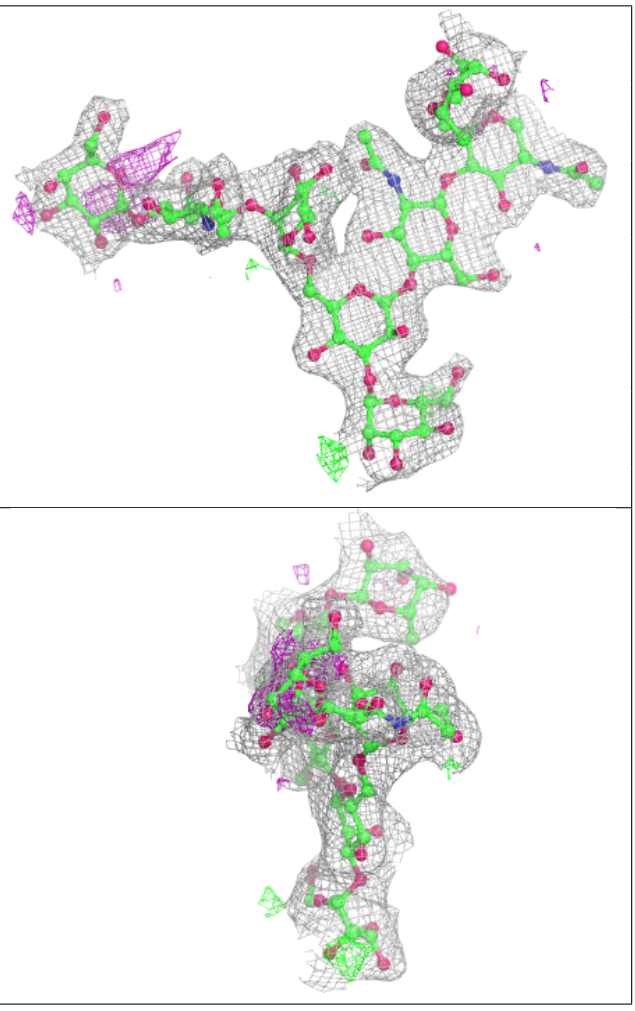
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	F	4	11/12	0.97	0.11	39,43,49,52	0
4	FUC	G	8	10/11	0.97	0.16	45,50,54,59	0
4	NAG	G	2	14/15	0.98	0.13	26,32,44,49	0

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.

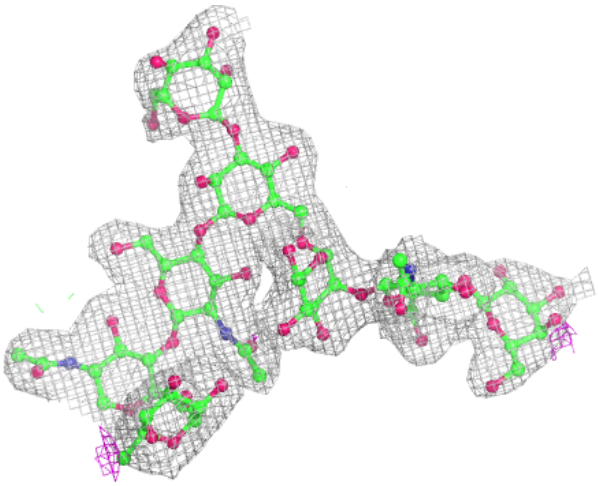
Electron density around Chain F:

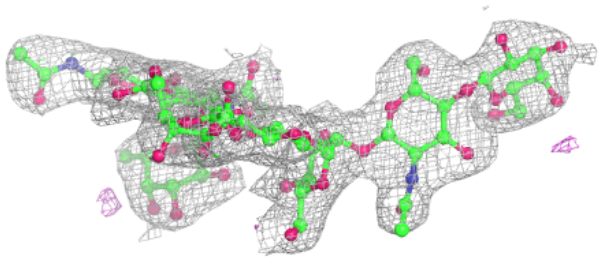
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

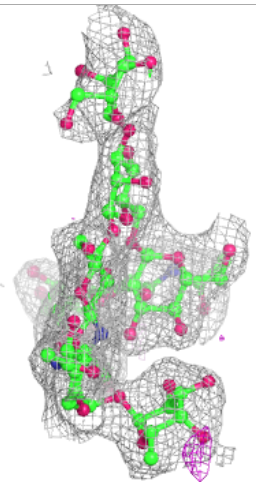


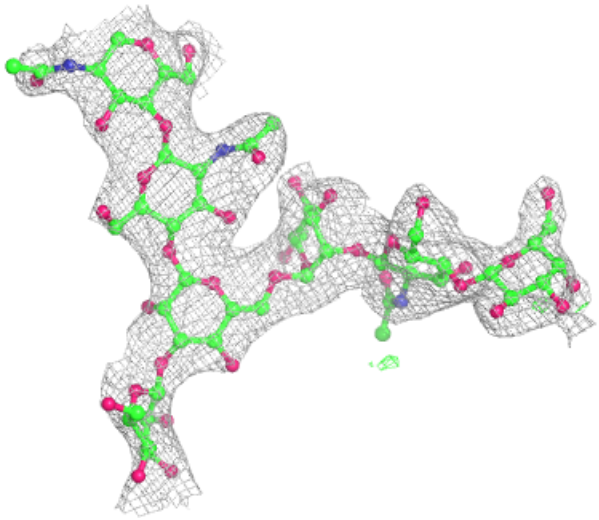
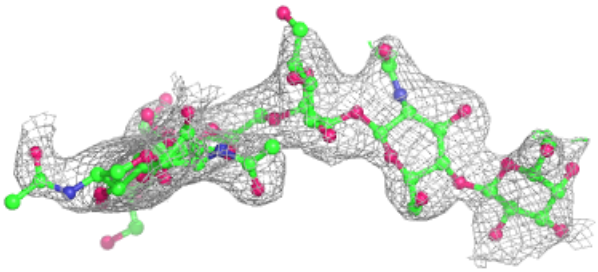
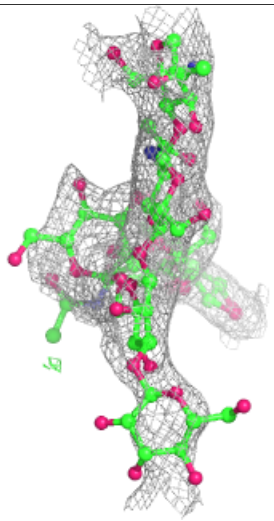
Electron density around Chain G:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.