Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:02 AM BST

PDB ID	:	5O4E
Title	:	Crystal structure of VEGF in complex with heterodimeric Fcab JanusCT6
Authors	:	Mlynek, G.; Lobner, E.; Kubinger, K.; Humm, A.; Obinger, C.; Djinovic-Carugo, K.
Deposited on	:	2017-05-29
Resolution	:	2.15 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 following versions of software and data (see references ①) were used in the production of this report:

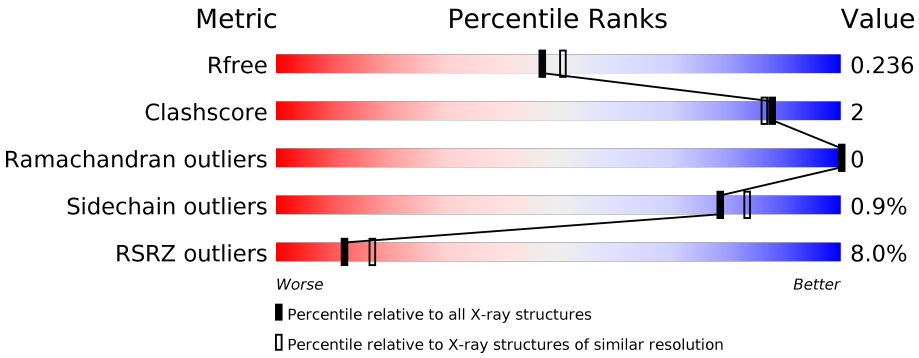
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	223	89% 5% 6%
2	B	228	3% 94% 5%
2	D	228	11% 90% 6%
3	C	222	19% 78% 18%
4	E	96	% 88% 11%
4	F	96	5% 86% 13%

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Mol	Chain	Length	Quality of chain
5	G	8	38% 50% 13%
5	H	8	50% 38% 13%
6	I	2	50% 50%
7	J	6	50% 50%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17198 atoms, of which 8385 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	209	Total	C	H	N	O	S	0	2	0
			3331	1076	1647	282	320	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	VAL	THR	engineered mutation	UNP P0DOX5
A	366	LEU	THR	engineered mutation	UNP P0DOX5
A	392	LEU	LYS	engineered mutation	UNP P0DOX5
A	394	TRP	THR	engineered mutation	UNP P0DOX5

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	216	Total	C	H	N	O	S	0	0	0
			3438	1123	1696	289	323	7			
2	D	214	Total	C	H	N	O	S	0	0	0
			3417	1116	1686	287	321	7			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	350	VAL	THR	engineered mutation	UNP P0DOX5
B	351	TYR	LEU	engineered mutation	UNP P0DOX5
B	359	ARG	THR	engineered mutation	UNP P0DOX5
B	360	PHE	LYS	engineered mutation	UNP P0DOX5
B	361	TYR	ASN	engineered mutation	UNP P0DOX5
B	388	ASP	-	insertion	UNP P0DOX5
B	389	ILE	-	insertion	UNP P0DOX5
B	389A	PHE	-	insertion	UNP P0DOX5
B	389B	PRO	-	insertion	UNP P0DOX5
B	389C	ASN	-	insertion	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	389D	GLY	GLU	engineered mutation	UNP P0DOX5
B	389E	LEU	ASN	engineered mutation	UNP P0DOX5
B	405	ALA	PHE	engineered mutation	UNP P0DOX5
B	407	VAL	TYR	engineered mutation	UNP P0DOX5
B	413	PRO	ASP	engineered mutation	UNP P0DOX5
B	414	TYR	LYS	engineered mutation	UNP P0DOX5
B	415	PRO	SER	engineered mutation	UNP P0DOX5
B	416	SER	ARG	engineered mutation	UNP P0DOX5
B	418	LEU	GLN	engineered mutation	UNP P0DOX5
B	419	MET	GLN	engineered mutation	UNP P0DOX5
B	421	THR	ASN	engineered mutation	UNP P0DOX5
B	422	ARG	VAL	engineered mutation	UNP P0DOX5
B	440	HIS	SER	engineered mutation	UNP P0DOX5
B	442	GLU	SER	engineered mutation	UNP P0DOX5
B	443	TYR	LEU	engineered mutation	UNP P0DOX5
B	444	GLN	SER	engineered mutation	UNP P0DOX5
B	445	TRP	PRO	engineered mutation	UNP P0DOX5
B	446	PRO	GLY	engineered mutation	UNP P0DOX5
B	447	THR	LYS	engineered mutation	UNP P0DOX5
D	350	VAL	THR	engineered mutation	UNP P0DOX5
D	351	TYR	LEU	engineered mutation	UNP P0DOX5
D	359	ARG	THR	engineered mutation	UNP P0DOX5
D	360	PHE	LYS	engineered mutation	UNP P0DOX5
D	361	TYR	ASN	engineered mutation	UNP P0DOX5
D	388	ASP	-	insertion	UNP P0DOX5
D	389	ILE	-	insertion	UNP P0DOX5
D	390	PHE	-	insertion	UNP P0DOX5
D	391	PRO	-	insertion	UNP P0DOX5
D	392	ASN	-	insertion	UNP P0DOX5
D	393	GLY	GLU	engineered mutation	UNP P0DOX5
D	394	LEU	ASN	engineered mutation	UNP P0DOX5
D	410	ALA	PHE	engineered mutation	UNP P0DOX5
D	412	VAL	TYR	engineered mutation	UNP P0DOX5
D	418	PRO	ASP	engineered mutation	UNP P0DOX5
D	419	TYR	LYS	engineered mutation	UNP P0DOX5
D	420	PRO	SER	engineered mutation	UNP P0DOX5
D	421	SER	ARG	engineered mutation	UNP P0DOX5
D	423	LEU	GLN	engineered mutation	UNP P0DOX5
D	424	MET	GLN	engineered mutation	UNP P0DOX5
D	426	THR	ASN	engineered mutation	UNP P0DOX5
D	427	ARG	VAL	engineered mutation	UNP P0DOX5
D	445	HIS	SER	engineered mutation	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	447	GLU	SER	engineered mutation	UNP P0DOX5
D	448	TYR	LEU	engineered mutation	UNP P0DOX5
D	449	GLN	SER	engineered mutation	UNP P0DOX5
D	450	TRP	PRO	engineered mutation	UNP P0DOX5
D	451	PRO	GLY	engineered mutation	UNP P0DOX5
D	452	THR	LYS	engineered mutation	UNP P0DOX5

- Molecule 3 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	181	Total	C	H	N	O	S	0	0	0
			2907	940	1445	244	272	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	350	VAL	THR	engineered mutation	UNP P0DOX5
C	366	LEU	THR	engineered mutation	UNP P0DOX5
C	392	LEU	LYS	engineered mutation	UNP P0DOX5
C	394	TRP	THR	engineered mutation	UNP P0DOX5

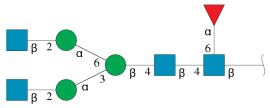
- Molecule 4 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	95	Total	C	H	N	O	S	0	2	0
			1522	489	743	132	144	14			
4	F	95	Total	C	H	N	O	S	0	0	0
			1504	483	735	129	143	14			

There are 2 discrepancies between the modelled and reference sequences:

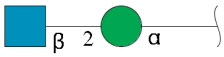
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	MET	GLU	engineered mutation	UNP P15692
F	13	MET	GLU	engineered mutation	UNP P15692

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



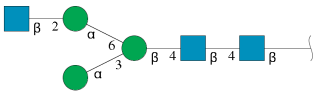
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	8	Total	C	H	N	O	0	0	0
			184	56	85	4	39			
5	H	8	Total	C	H	N	O	0	0	0
			184	56	85	4	39			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose.



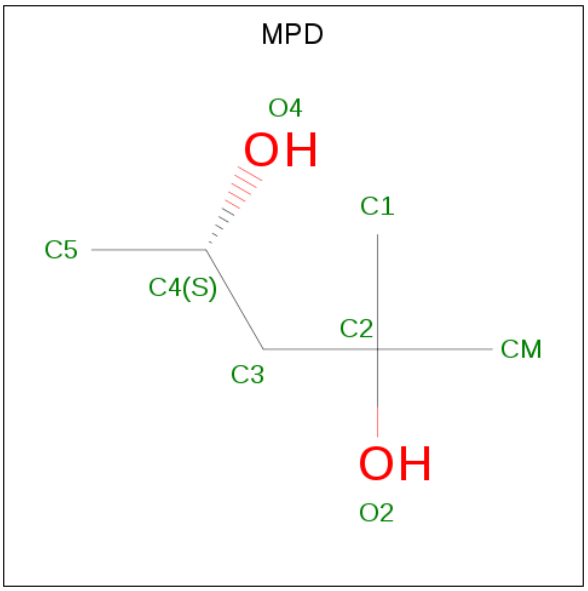
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	2	Total	C	H	N	O	0	0	0
			47	14	22	1	10			

- Molecule 7 is an oligosaccharide called 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.



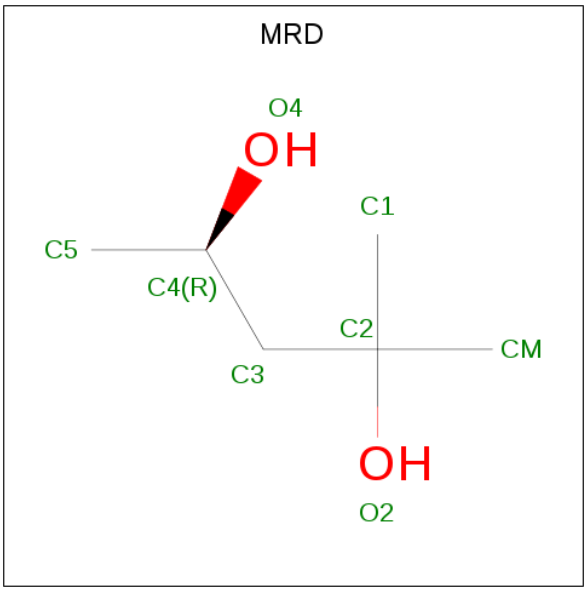
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	6	Total	C	H	N	O	0	0	0
			139	42	64	3	30			

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



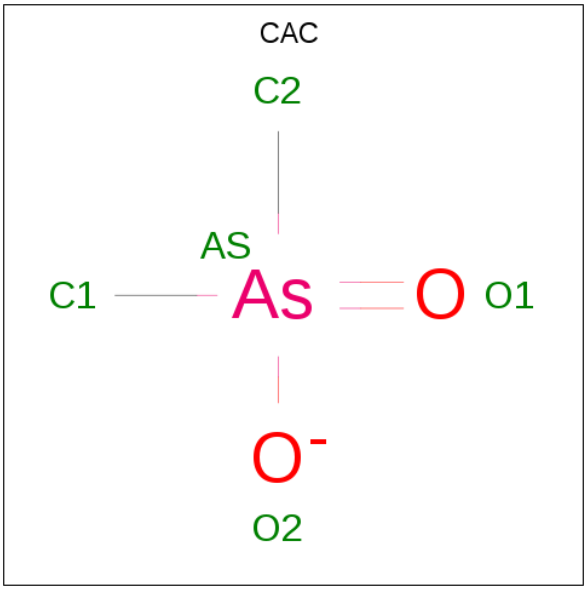
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			22	6	14	2		
8	A	1	Total	C	H	O	0	0
			22	6	14	2		
8	C	1	Total	C	H	O	0	0
			22	6	14	2		
8	D	1	Total	C	H	O	0	0
			22	6	14	2		
8	D	1	Total	C	H	O	0	0
			22	6	14	2		
8	E	1	Total	C	H	O	0	0
			22	6	14	2		
8	E	1	Total	C	H	O	0	0
			22	6	14	2		
8	E	1	Total	C	H	O	0	0
			22	6	14	2		
8	F	1	Total	C	H	O	0	0
			22	6	14	2		
8	F	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 9 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
9	A	1	22	6	14	2	0	0

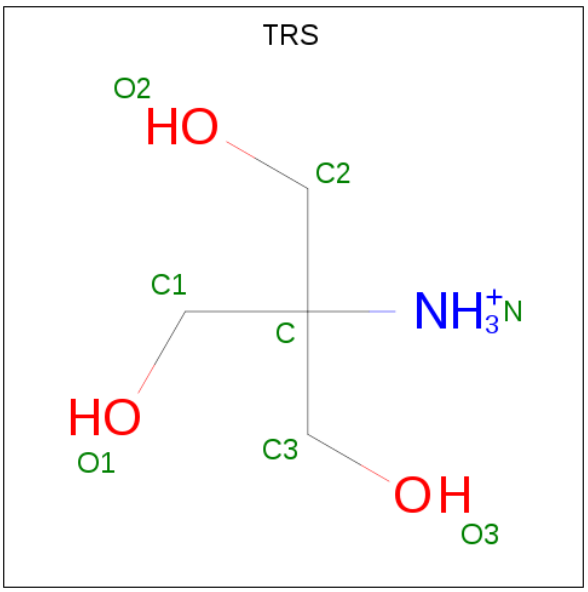
- Molecule 10 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	As	C	H	O		
10	A	1	11	1	2	6	2	0	0
			Total	As	C	H	O		
10	E	1	11	1	2	6	2	0	0

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	H	N	O	0	0
			19	4	11	1	3		

- Molecule 12 is water.

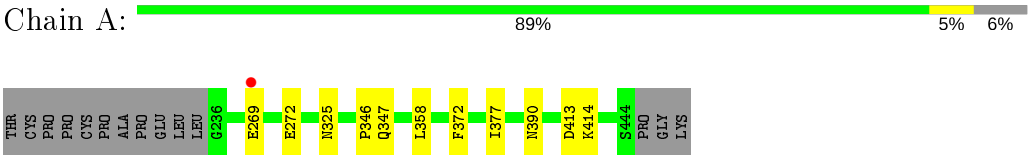
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	59	Total	O	0	0
			59	59		
12	B	52	Total	O	0	0
			52	52		
12	C	40	Total	O	0	0
			40	40		
12	D	65	Total	O	0	0
			65	65		
12	E	15	Total	O	0	0
			15	15		
12	F	11	Total	O	0	0
			11	11		

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.

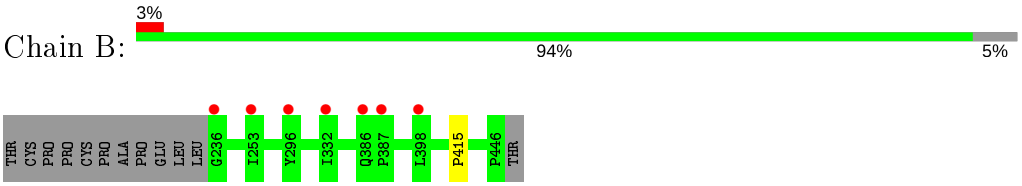
- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain A:



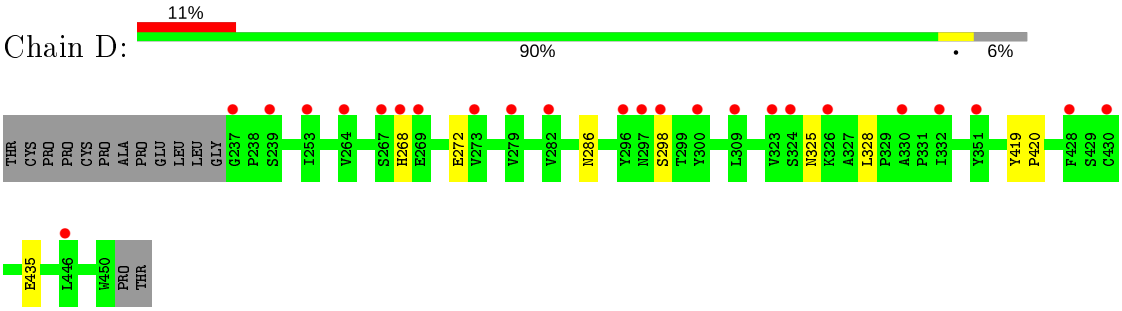
- Molecule 2: Immunoglobulin gamma-1 heavy chain

Chain B:



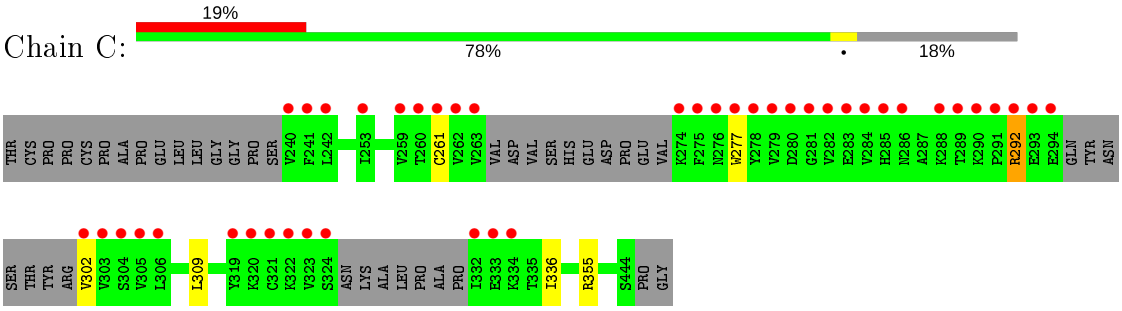
- Molecule 2: Immunoglobulin gamma-1 heavy chain

Chain D:



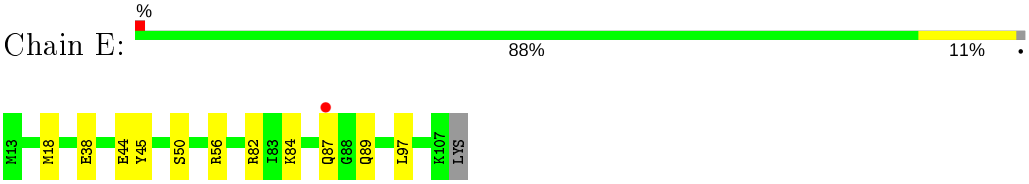
- Molecule 3: Immunoglobulin gamma-1 heavy chain

Chain C:



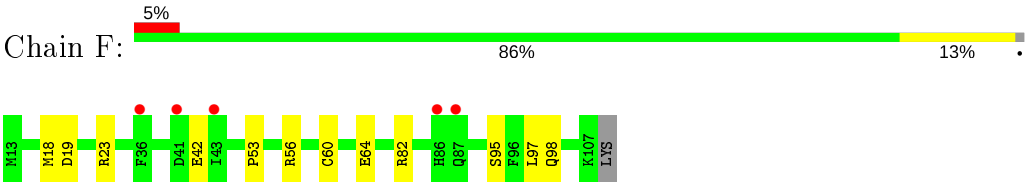
- Molecule 4: Vascular endothelial growth factor A

Chain E:



• Molecule 4: Vascular endothelial growth factor A

Chain F:



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

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose

Chain I:

• Molecule 7: 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 J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.50Å 130.34Å 139.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.75 – 2.15 44.75 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.75-2.15) 97.8 (44.75-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.16Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.200 , 0.236 0.200 , 0.236	Depositor DCC
R_{free} test set	2004 reflections (2.30%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.0	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	0.96	EDS
Total number of atoms	17198	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, CAC, FUC, MRD, TRS, 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	0.24	0/1738	0.42	0/2369
2	B	0.24	0/1799	0.41	0/2458
2	D	0.24	0/1787	0.41	0/2441
3	C	0.24	0/1500	0.42	0/2037
4	E	0.25	0/806	0.44	0/1086
4	F	0.25	0/787	0.43	0/1060
All	All	0.24	0/8417	0.42	0/11451

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

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	1684	1647	1641	6	0
2	B	1742	1696	1696	1	0
2	D	1731	1686	1686	6	0
3	C	1462	1445	1443	3	0
4	E	779	743	731	8	0
4	F	769	735	735	9	0
5	G	99	85	85	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	99	85	85	1	0
6	I	25	22	22	0	0
7	J	75	64	64	0	0
8	A	16	28	28	1	0
8	C	8	14	14	0	0
8	D	16	28	28	0	0
8	E	24	42	42	2	0
8	F	16	28	28	3	0
9	A	8	14	14	1	0
10	A	5	6	0	0	0
10	E	5	6	0	0	0
11	D	8	11	12	0	0
12	A	59	0	0	0	0
12	B	52	0	0	0	0
12	C	40	0	0	0	0
12	D	65	0	0	2	0
12	E	15	0	0	1	0
12	F	11	0	0	2	0
All	All	8813	8385	8354	34	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 2.

All (34) 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)
5:G:4:MAN:HO4	5:H:4:MAN:HO4	1.12	0.87
8:F:201:MPD:H52	8:F:201:MPD:H11	1.64	0.79
8:F:202:MPD:H52	8:F:202:MPD:HM1	1.67	0.75
4:E:50:SER:OG	4:F:60:CYS:SG	2.52	0.68
1:A:358:LEU:O	1:A:414:LYS:NZ	2.22	0.67
4:E:56:ARG:NH1	4:E:97:LEU:O	2.27	0.67
2:D:435:GLU:OE1	12:D:601:HOH:O	2.13	0.66
2:D:286:ASN:OD1	12:D:602:HOH:O	2.14	0.63
2:D:268:HIS:NE2	2:D:298:SER:O	2.30	0.63
2:D:272:GLU:O	2:D:325:ASN:ND2	2.38	0.56
8:E:202:MPD:H11	4:F:23:ARG:HH11	1.73	0.54
1:A:377:ILE:O	9:A:510:MRD:H5C2	2.08	0.54
1:A:269:GLU:N	1:A:269:GLU:OE1	2.41	0.54
4:F:53:PRO:O	8:F:201:MPD:HM1	2.08	0.53
2:B:415:PRO:HB2	4:F:18:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:64:GLU:N	4:F:64:GLU:OE1	2.40	0.51
3:C:261:CYS:HB2	3:C:277:TRP:CH2	2.46	0.51
4:F:98:GLN:OE1	12:F:301:HOH:O	2.19	0.51
2:D:420:PRO:HG2	4:E:18:MET:HE1	1.94	0.49
3:C:309:LEU:HD23	3:C:309:LEU:H	1.78	0.49
4:E:84:LYS:NZ	4:E:87:GLN:OE1	2.46	0.47
3:C:292:ARG:HG2	3:C:302:VAL:HG22	1.98	0.46
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.97	0.46
4:E:18:MET:HA	4:E:18:MET:HE2	1.98	0.46
4:F:19:ASP:OD2	12:F:302:HOH:O	2.21	0.45
4:F:56:ARG:NH2	4:F:97:LEU:O	2.45	0.44
1:A:272:GLU:O	1:A:325:ASN:ND2	2.45	0.43
4:E:89:GLN:OE1	4:E:89:GLN:N	2.52	0.43
4:F:42:GLU:OE1	4:F:82:ARG:NH1	2.42	0.43
8:E:201:MPD:O4	8:E:201:MPD:H12	2.19	0.42
4:E:38:GLU:OE1	12:E:301:HOH:O	2.22	0.41
1:A:390:ASN:ND2	8:A:512:MPD:H53	2.36	0.41
2:D:419:TYR:N	2:D:420:PRO:HD2	2.36	0.41
4:E:45:TYR:CD2	4:E:82:ARG:HG2	2.56	0.41

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	209/223 (94%)	208 (100%)	1 (0%)	0	100	100
2	B	214/228 (94%)	212 (99%)	2 (1%)	0	100	100
2	D	212/228 (93%)	209 (99%)	3 (1%)	0	100	100
3	C	173/222 (78%)	170 (98%)	3 (2%)	0	100	100
4	E	95/96 (99%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	F	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
All	All	996/1093 (91%)	978 (98%)	18 (2%)	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	196/206 (95%)	194 (99%)	2 (1%)	76 81
2	B	199/210 (95%)	199 (100%)	0	100 100
2	D	198/210 (94%)	197 (100%)	1 (0%)	88 92
3	C	170/205 (83%)	167 (98%)	3 (2%)	59 63
4	E	92/91 (101%)	91 (99%)	1 (1%)	73 78
4	F	90/91 (99%)	89 (99%)	1 (1%)	73 78
All	All	945/1013 (93%)	937 (99%)	8 (1%)	78 86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	413	ASP
3	C	292	ARG
3	C	336	ILE
3	C	355	ARG
2	D	328	LEU
4	E	44	GLU
4	F	95	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	438	HIS

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)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	G	1	1,5	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.41	0
5	BMA	G	3	5	11,11,12	0.57	0	15,15,17	1.08	1 (6%)
5	MAN	G	4	5	11,11,12	0.54	0	15,15,17	1.02	1 (6%)
5	NAG	G	5	5	14,14,15	0.27	0	17,19,21	0.64	1 (5%)
5	MAN	G	6	5	11,11,12	0.60	0	15,15,17	0.92	2 (13%)
5	NAG	G	7	5	14,14,15	0.18	0	17,19,21	0.47	0
5	FUC	G	8	5	10,10,11	0.66	0	14,14,16	1.16	1 (7%)
5	NAG	H	1	2,5	14,14,15	0.20	0	17,19,21	0.38	0
5	NAG	H	2	5	14,14,15	0.21	0	17,19,21	0.40	0
5	BMA	H	3	5	11,11,12	0.90	0	15,15,17	1.10	1 (6%)
5	MAN	H	4	5	11,11,12	1.00	1 (9%)	15,15,17	1.62	3 (20%)
5	NAG	H	5	5	14,14,15	0.48	0	17,19,21	0.38	0
5	MAN	H	6	5	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
5	NAG	H	7	5	14,14,15	0.23	0	17,19,21	0.42	0
5	FUC	H	8	5	10,10,11	0.82	0	14,14,16	1.10	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	I	1	6	11,11,12	0.91	0	15,15,17	1.17	1 (6%)
6	NAG	I	2	6	14,14,15	0.25	0	17,19,21	0.39	0
7	NAG	J	1	2,7	14,14,15	0.29	0	17,19,21	0.55	0
7	NAG	J	2	7	14,14,15	0.23	0	17,19,21	0.43	0
7	BMA	J	3	7	11,11,12	0.99	1 (9%)	15,15,17	1.10	1 (6%)
7	MAN	J	4	7	11,11,12	0.68	0	15,15,17	1.11	2 (13%)
7	NAG	J	5	7	14,14,15	0.19	0	17,19,21	0.41	0
7	MAN	J	6	7	11,11,12	0.77	0	15,15,17	0.96	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
5	NAG	G	1	1,5	-	2/6/23/26	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	-	2/2/19/22	0/1/1/1
5	NAG	G	5	5	-	2/6/23/26	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
5	NAG	G	7	5	-	2/6/23/26	0/1/1/1
5	FUC	G	8	5	-	-	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	NAG	H	5	5	-	4/6/23/26	0/1/1/1
5	MAN	H	6	5	-	1/2/19/22	0/1/1/1
5	NAG	H	7	5	-	0/6/23/26	0/1/1/1
5	FUC	H	8	5	-	-	0/1/1/1
6	MAN	I	1	6	-	0/2/19/22	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
7	NAG	J	5	7	-	2/6/23/26	0/1/1/1
7	MAN	J	6	7	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	3	BMA	C1-C2	2.61	1.58	1.52
5	H	4	MAN	O5-C1	-2.03	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	4	MAN	O2-C2-C3	-4.07	101.98	110.14
5	H	4	MAN	C1-O5-C5	3.01	116.28	112.19
5	G	4	MAN	C1-O5-C5	2.88	116.10	112.19
5	H	3	BMA	C1-C2-C3	2.57	112.82	109.67
5	G	8	FUC	C1-O5-C5	2.53	118.51	112.78
5	H	4	MAN	O2-C2-C1	2.53	114.32	109.15
7	J	4	MAN	O2-C2-C3	-2.52	105.09	110.14
7	J	6	MAN	O2-C2-C3	-2.39	105.36	110.14
7	J	3	BMA	O3-C3-C2	2.37	114.54	109.99
5	H	6	MAN	O2-C2-C3	-2.37	105.39	110.14
5	H	6	MAN	C1-O5-C5	2.34	115.36	112.19
7	J	4	MAN	C1-O5-C5	2.31	115.32	112.19
6	I	1	MAN	O5-C1-C2	2.23	114.22	110.77
5	H	8	FUC	C1-C2-C3	2.23	112.41	109.67
5	G	5	NAG	C1-O5-C5	2.22	115.20	112.19
5	G	3	BMA	C1-O5-C5	2.18	115.14	112.19
5	G	6	MAN	C1-O5-C5	2.14	115.10	112.19
5	G	6	MAN	O2-C2-C3	-2.09	105.96	110.14
5	H	8	FUC	C1-O5-C5	2.00	117.31	112.78

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	H	1	NAG	C4-C5-C6-O6
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
7	J	2	NAG	C4-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
5	G	4	MAN	C4-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
5	G	5	NAG	C4-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
5	G	5	NAG	O5-C5-C6-O6
5	H	5	NAG	C3-C2-N2-C7
5	H	5	NAG	C1-C2-N2-C7

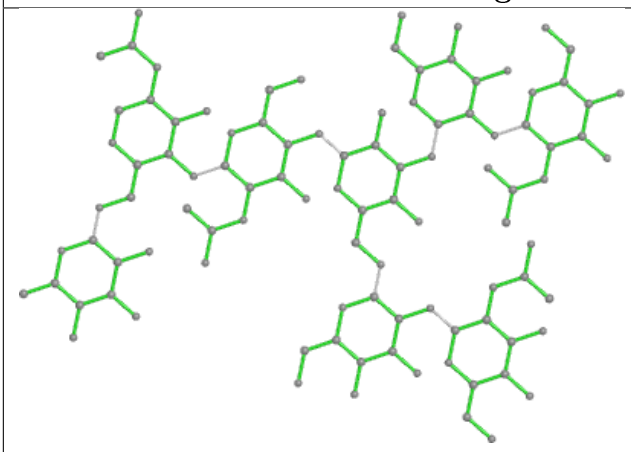
There are no ring outliers.

2 monomers are involved in 1 short contact:

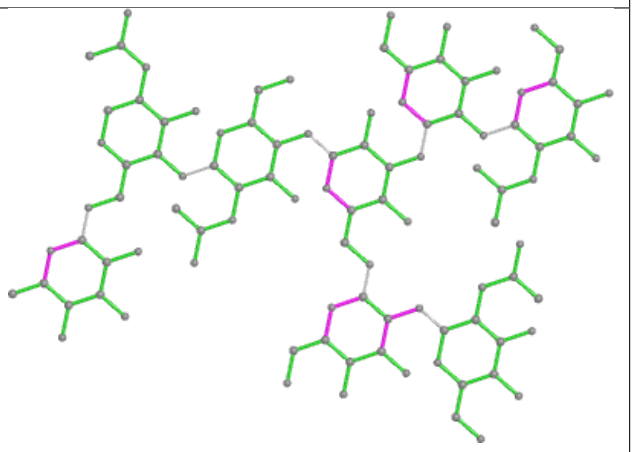
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	4	MAN	1	0
5	H	4	MAN	1	0

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

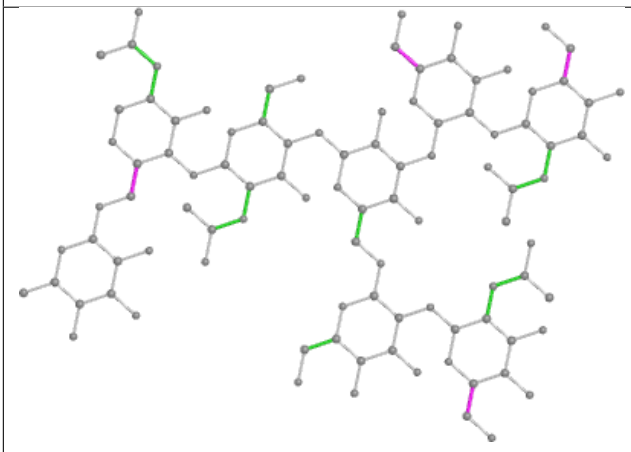
Oligosaccharide Chain G



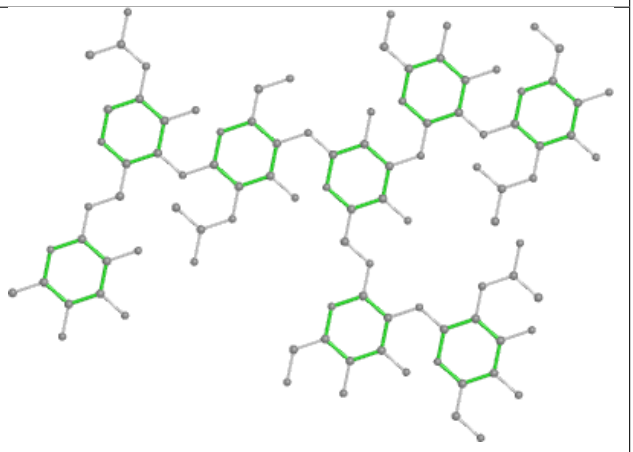
Bond lengths



Bond angles

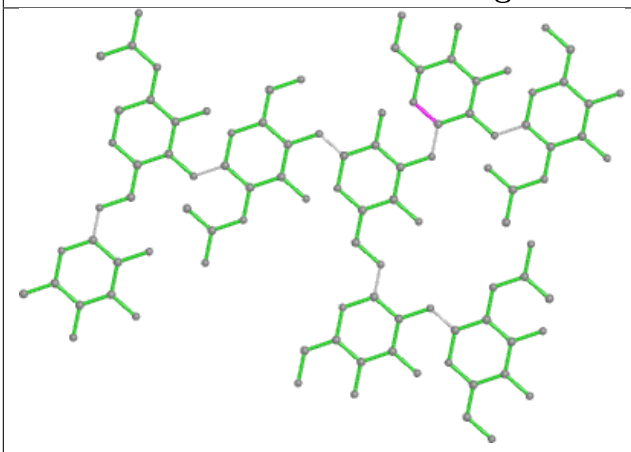


Torsions

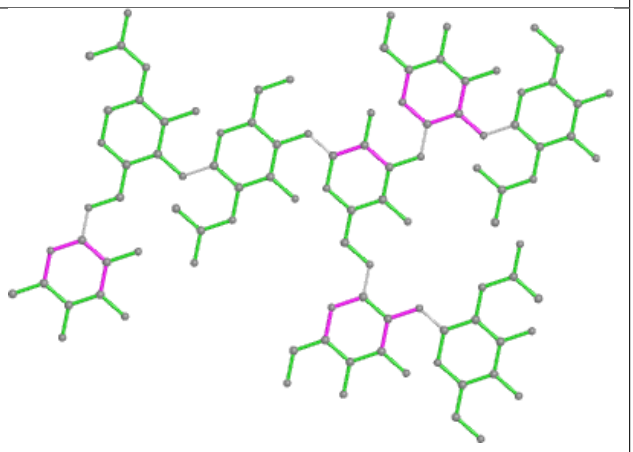


Rings

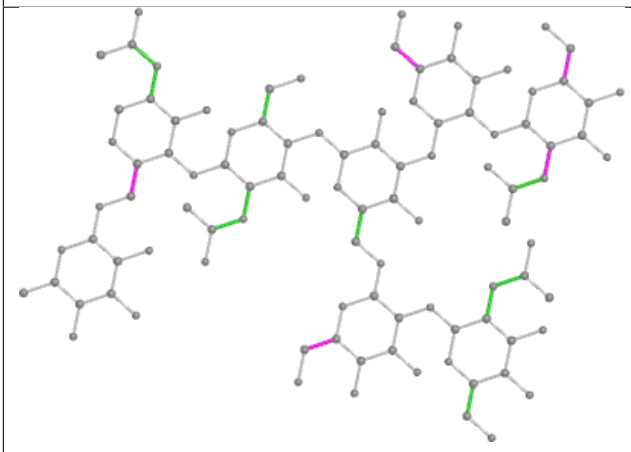
Oligosaccharide Chain H



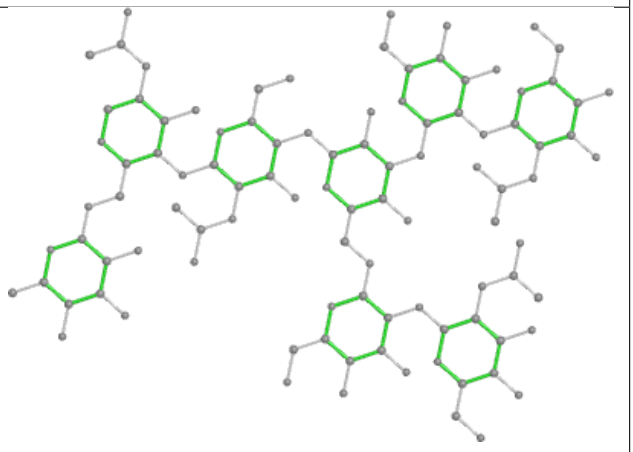
Bond lengths



Bond angles

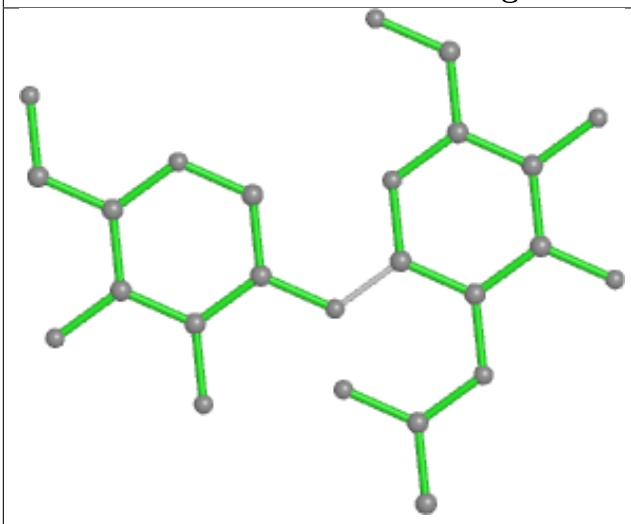


Torsions

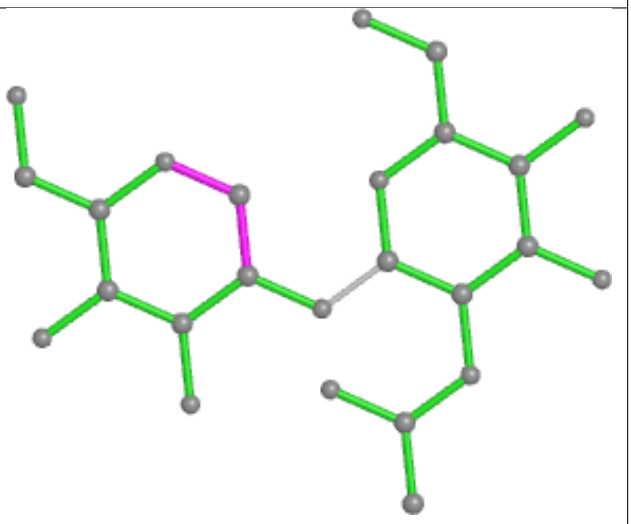


Rings

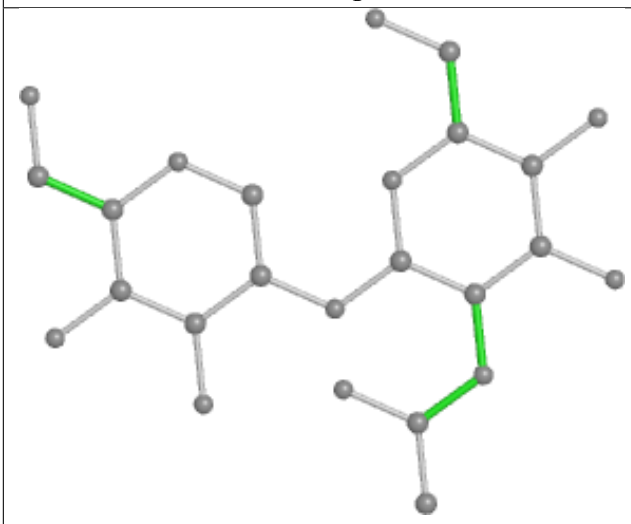
Oligosaccharide Chain I



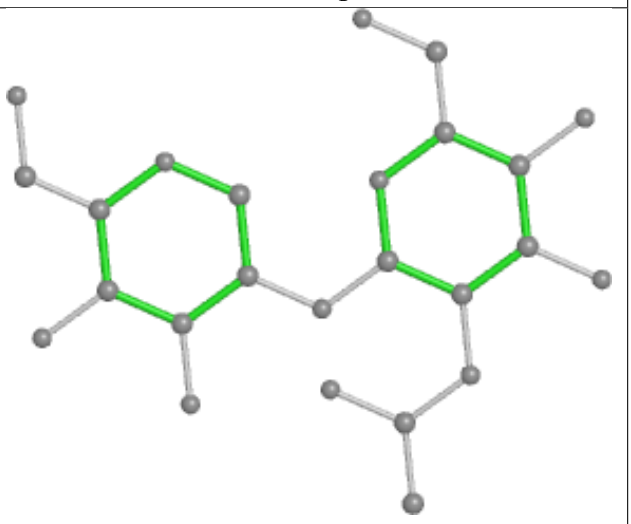
Bond lengths



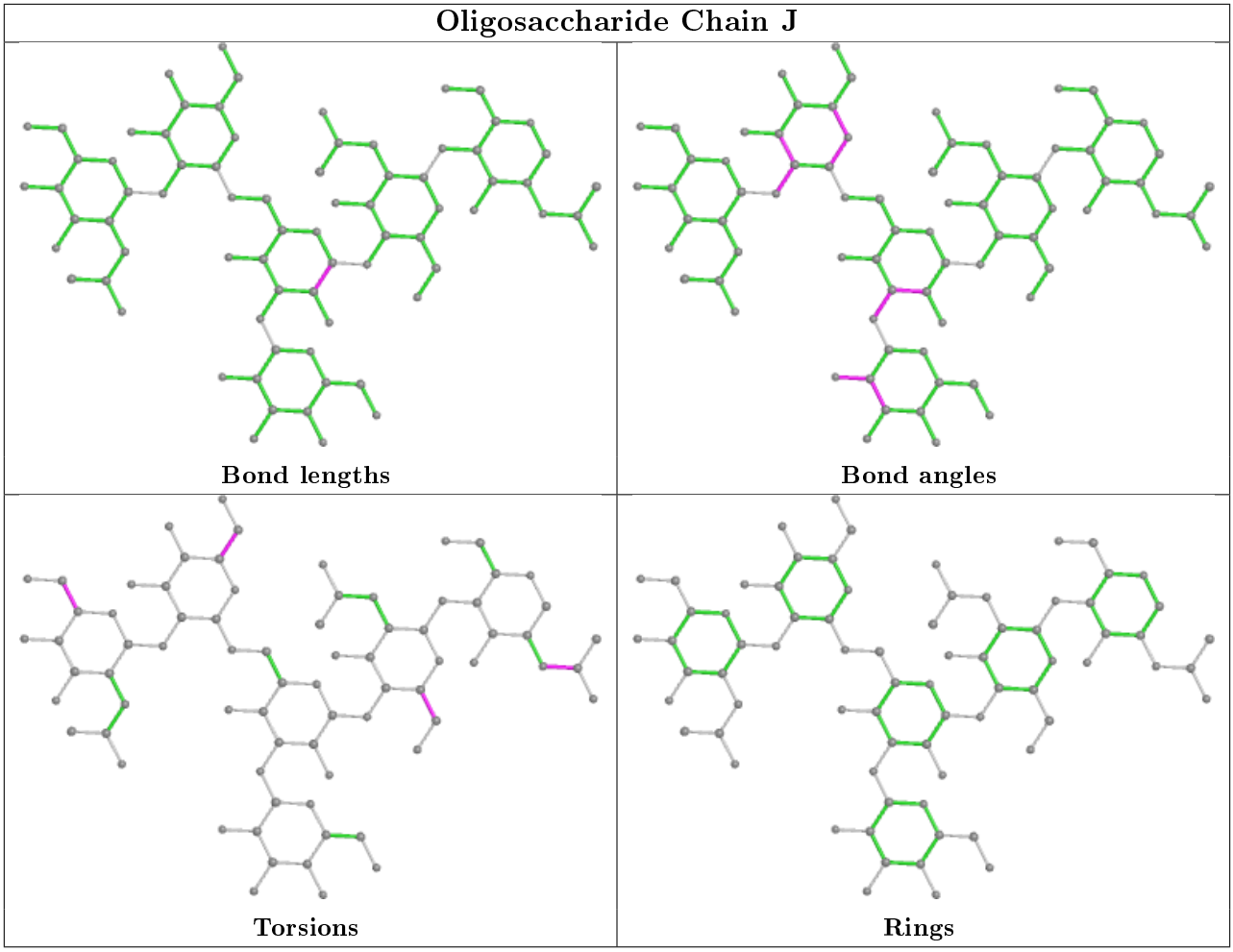
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
9	MRD	A	510	-	7,7,7	0.32	0	9,10,10	0.39	0
8	MPD	F	201	-	7,7,7	0.49	0	9,10,10	0.64	0
8	MPD	F	202	-	7,7,7	0.39	0	9,10,10	0.64	0
10	CAC	A	511	-	0,4,4	0.00	-	0,6,6	0.00	-
8	MPD	E	202	-	7,7,7	0.34	0	9,10,10	0.29	0
8	MPD	D	508	-	7,7,7	0.38	0	9,10,10	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	MPD	E	204	-	7,7,7	0.51	0	9,10,10	0.55	0
8	MPD	E	201	-	7,7,7	0.35	0	9,10,10	0.27	0
8	MPD	C	503	-	7,7,7	0.45	0	9,10,10	0.50	0
10	CAC	E	203	-	0,4,4	0.00	-	0,6,6	0.00	-
11	TRS	D	509	-	7,7,7	0.54	0	9,9,9	0.53	0
8	MPD	A	509	-	7,7,7	0.37	0	9,10,10	0.40	0
8	MPD	A	512	-	7,7,7	0.51	0	9,10,10	0.81	0
8	MPD	D	507	-	7,7,7	0.35	0	9,10,10	0.28	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
9	MRD	A	510	-	-	1/5/5/5	-
8	MPD	F	201	-	-	4/5/5/5	-
8	MPD	F	202	-	-	2/5/5/5	-
8	MPD	E	202	-	-	1/5/5/5	-
8	MPD	D	508	-	-	1/5/5/5	-
8	MPD	E	204	-	-	4/5/5/5	-
8	MPD	E	201	-	-	2/5/5/5	-
8	MPD	C	503	-	-	3/5/5/5	-
11	TRS	D	509	-	-	3/9/9/9	-
8	MPD	A	509	-	-	0/5/5/5	-
8	MPD	A	512	-	-	3/5/5/5	-
8	MPD	D	507	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	201	MPD	C1-C2-C3-C4
8	F	202	MPD	C2-C3-C4-O4
8	F	202	MPD	C2-C3-C4-C5
8	E	202	MPD	C2-C3-C4-C5
8	E	201	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
11	D	509	TRS	C2-C-C1-O1
8	A	512	MPD	O2-C2-C3-C4
11	D	509	TRS	C3-C-C1-O1
8	F	201	MPD	O2-C2-C3-C4
8	D	508	MPD	O2-C2-C3-C4
8	E	204	MPD	O2-C2-C3-C4
11	D	509	TRS	N-C-C1-O1
8	E	201	MPD	C2-C3-C4-C5
8	C	503	MPD	C2-C3-C4-C5
8	C	503	MPD	C2-C3-C4-O4
8	F	201	MPD	CM-C2-C3-C4
8	E	204	MPD	C1-C2-C3-C4
8	E	204	MPD	CM-C2-C3-C4
8	A	512	MPD	C1-C2-C3-C4
8	A	512	MPD	CM-C2-C3-C4
8	C	503	MPD	O2-C2-C3-C4
8	F	201	MPD	C2-C3-C4-C5
9	A	510	MRD	C2-C3-C4-O4
8	E	204	MPD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	510	MRD	1	0
8	F	201	MPD	2	0
8	F	202	MPD	1	0
8	E	202	MPD	1	0
8	E	201	MPD	1	0
8	A	512	MPD	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

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, 95^{th} 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	209/223 (93%)	0.19	1 (0%) 91 93	43, 59, 105, 136	0
2	B	216/228 (94%)	0.33	7 (3%) 47 56	43, 66, 98, 157	0
2	D	214/228 (93%)	0.91	24 (11%) 5 7	37, 65, 123, 151	0
3	C	181/222 (81%)	1.20	43 (23%) 0 0	42, 73, 142, 156	0
4	E	95/96 (98%)	0.25	1 (1%) 80 85	45, 60, 113, 126	0
4	F	95/96 (98%)	0.37	5 (5%) 26 35	50, 66, 112, 129	0
All	All	1010/1093 (92%)	0.58	81 (8%) 12 17	37, 65, 123, 157	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	323	VAL	9.3
3	C	240	VAL	8.7
3	C	263	VAL	7.9
3	C	241	PHE	7.0
2	D	296	TYR	6.8
3	C	275	PHE	6.6
3	C	302	VAL	6.6
3	C	291	PRO	6.2
3	C	277	TRP	6.2
3	C	261	CYS	5.8
3	C	332	ILE	5.6
3	C	323	VAL	5.6
3	C	303	VAL	5.4
3	C	278	TYR	5.3
3	C	276	ASN	5.2
3	C	324	SER	5.1
3	C	282	VAL	5.1
3	C	321	CYS	5.0
3	C	284	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	289	THR	4.8
3	C	274	LYS	4.6
3	C	262	VAL	4.5
2	D	267	SER	4.4
2	D	300	TYR	4.3
2	D	297	ASN	4.2
3	C	286	ASN	4.1
3	C	322	LYS	4.1
2	D	282	VAL	4.0
2	B	386	GLN	3.6
2	D	264	VAL	3.6
3	C	306	LEU	3.6
2	B	253	ILE	3.5
2	D	237	GLY	3.5
3	C	333	GLU	3.5
3	C	294	GLU	3.4
3	C	285	HIS	3.2
2	B	387	PRO	3.2
3	C	288	LYS	3.2
3	C	320	LYS	3.1
3	C	279	VAL	3.1
2	D	332	ILE	3.1
2	D	269	GLU	3.1
3	C	292	ARG	3.0
4	E	87	GLN	2.9
4	F	86	HIS	2.9
3	C	242	LEU	2.9
3	C	304	SER	2.9
3	C	290	LYS	2.8
4	F	43	ILE	2.8
2	D	446	LEU	2.7
3	C	280	ASP	2.7
4	F	36	PHE	2.7
3	C	293	GLU	2.7
2	D	298	SER	2.6
2	D	268	HIS	2.6
3	C	283	GLU	2.5
2	B	236	GLY	2.5
3	C	305	VAL	2.5
4	F	41	ASP	2.5
3	C	334	LYS	2.5
2	B	296	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	279	VAL	2.4
2	D	351	TYR	2.4
1	A	269	GLU	2.3
2	D	330	ALA	2.3
4	F	87	GLN	2.3
3	C	259	VAL	2.3
3	C	253	ILE	2.3
2	D	253	ILE	2.2
3	C	281	GLY	2.2
2	D	324	SER	2.2
2	D	239	SER	2.2
2	B	398	LEU	2.2
2	D	430	CYS	2.1
2	D	273	VAL	2.1
3	C	260	THR	2.1
2	D	428	PHE	2.1
2	D	326	LYS	2.1
3	C	319	TYR	2.0
2	B	332	ILE	2.0
2	D	309	LEU	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, 95^{th} 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
7	NAG	J	1	14/15	0.56	0.31	106,131,158,168	0
7	MAN	J	6	11/12	0.78	0.16	119,143,170,174	0
6	NAG	I	2	14/15	0.82	0.26	107,132,158,165	0
6	MAN	I	1	11/12	0.85	0.16	119,138,166,166	0
5	NAG	G	5	14/15	0.85	0.15	100,133,162,168	0
7	NAG	J	2	14/15	0.85	0.35	100,129,151,160	0
7	BMA	J	3	11/12	0.85	0.21	93,114,153,158	0
5	NAG	H	5	14/15	0.89	0.16	102,133,159,166	0

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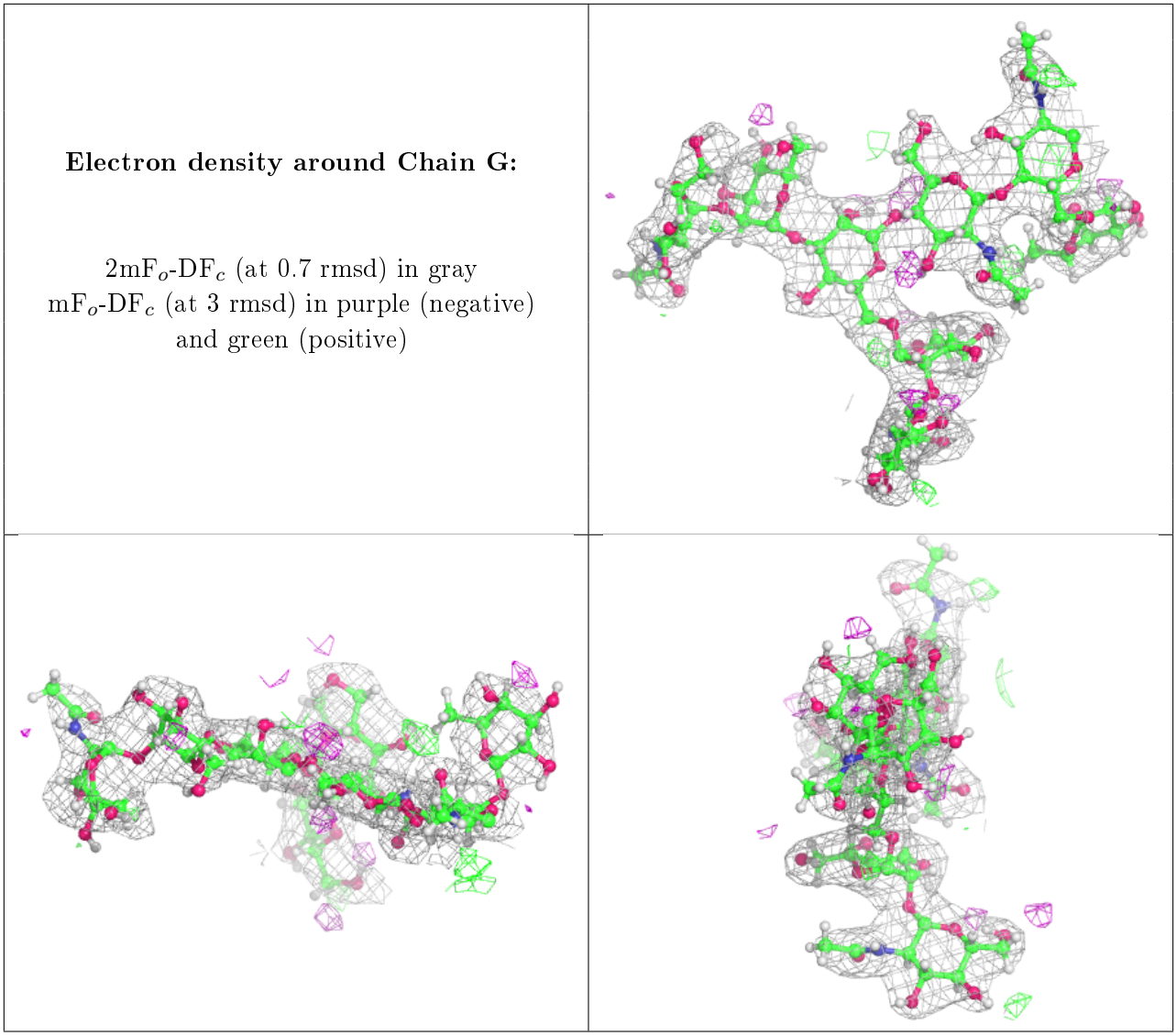
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	H	4	11/12	0.91	0.10	78,110,134,141	0
7	MAN	J	4	11/12	0.91	0.14	105,126,143,168	0
5	NAG	G	7	14/15	0.93	0.14	55,79,95,110	0
5	FUC	H	8	10/11	0.93	0.15	96,118,142,146	0
5	MAN	G	4	11/12	0.94	0.10	85,108,140,141	0
5	MAN	H	6	11/12	0.94	0.12	87,112,149,161	0
5	NAG	G	2	14/15	0.94	0.12	52,79,111,111	0
5	BMA	G	3	11/12	0.94	0.11	52,71,98,118	0
5	BMA	H	3	11/12	0.94	0.08	56,72,98,98	0
5	NAG	G	1	14/15	0.94	0.14	72,95,122,126	0
5	NAG	H	7	14/15	0.95	0.10	63,93,112,117	0
5	NAG	H	2	14/15	0.95	0.10	64,84,112,124	0
7	NAG	J	5	14/15	0.95	0.16	84,112,143,154	0
5	FUC	G	8	10/11	0.95	0.12	88,113,139,161	0
5	NAG	H	1	14/15	0.97	0.10	66,84,98,101	0
5	MAN	G	6	11/12	0.97	0.19	49,80,96,99	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.

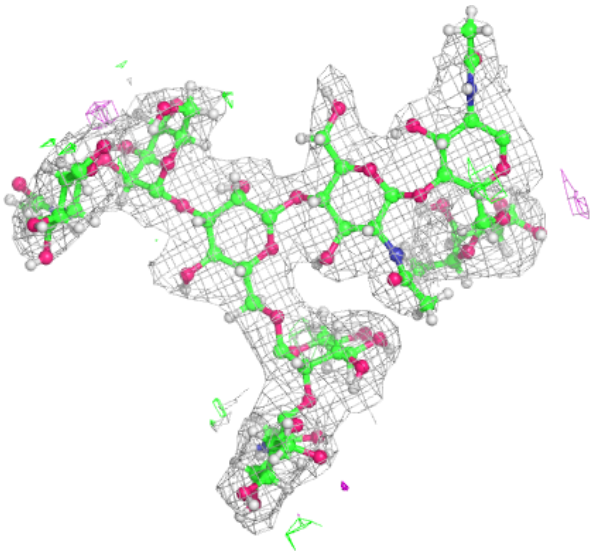
Electron density around Chain G:

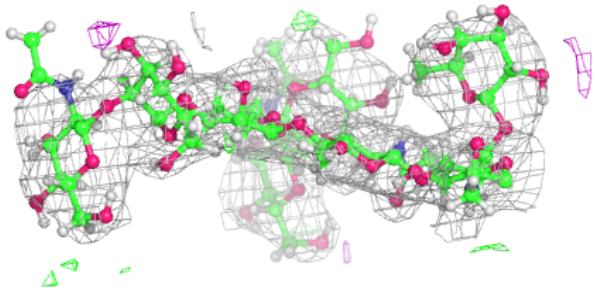
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

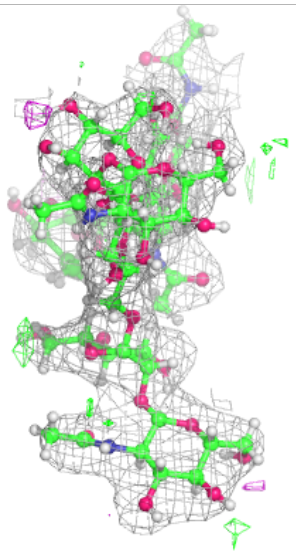


Electron density around Chain H:

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

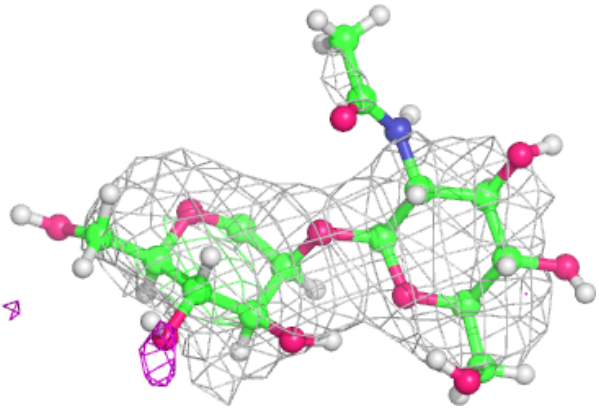


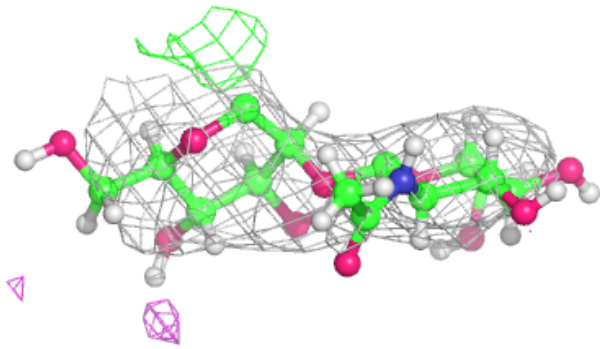


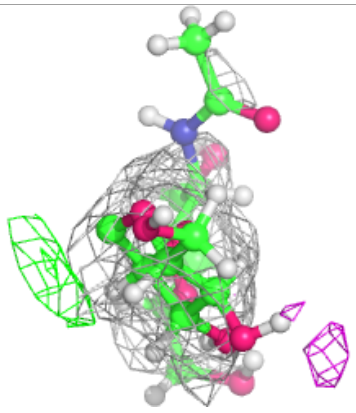


Electron density around Chain I:

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

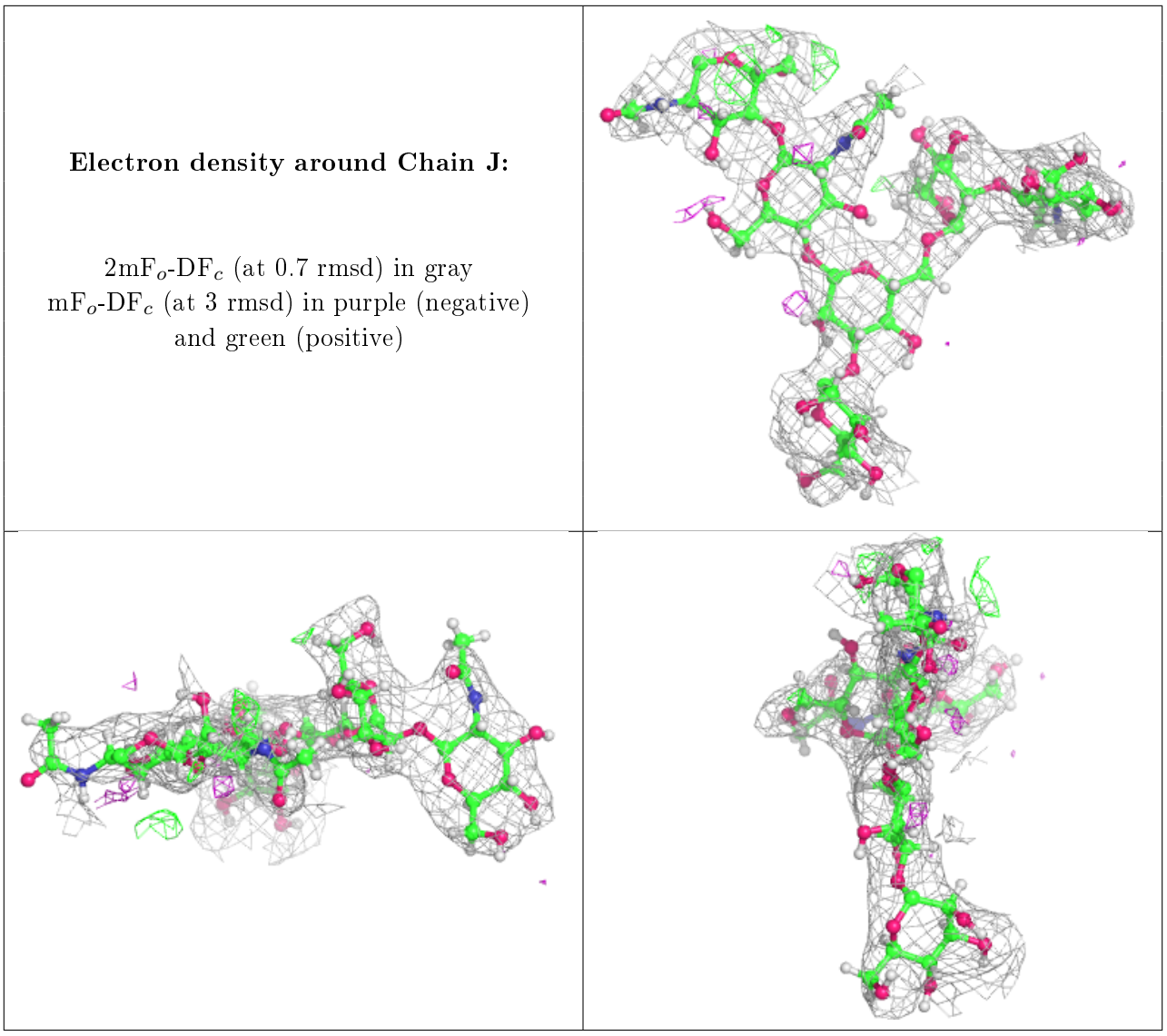






Electron density around Chain J:

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



6.4 Ligands

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, 95^{th} 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
9	MRD	A	510	8/8	0.79	0.22	57,91,108,129	0
8	MPD	A	509	8/8	0.80	0.32	70,102,122,129	0
11	TRS	D	509	8/8	0.82	0.14	68,97,128,128	0
8	MPD	C	503	8/8	0.86	0.21	73,92,112,112	0
8	MPD	D	508	8/8	0.88	0.15	61,92,120,154	0
8	MPD	A	512	8/8	0.88	0.23	72,88,111,111	0
8	MPD	F	202	8/8	0.89	0.24	70,90,102,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MPD	E	204	8/8	0.90	0.26	77,95,110,117	0
8	MPD	E	202	8/8	0.92	0.30	52,88,125,125	0
8	MPD	D	507	8/8	0.92	0.18	67,92,111,111	0
8	MPD	E	201	8/8	0.93	0.23	71,91,111,111	0
8	MPD	F	201	8/8	0.93	0.19	48,85,102,102	0
10	CAC	A	511	5/5	0.94	0.16	42,51,64,93	11
10	CAC	E	203	5/5	0.96	0.35	58,67,81,81	11

6.5 Other polymers

There are no such residues in this entry.