Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 07:39 am GMT

PDB ID	:	5K64
Title	:	Crystal structure of VEGF binding IgG1-Fc (Fcab 448)
Authors	:	Humm, A.; Lobner, E.; Kitzmuller, M.; Mlynek, G.; Obinger, C.; Djinovic-Carugo, K.
Deposited on	:	2016-05-24
Resolution	:	2.44 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:

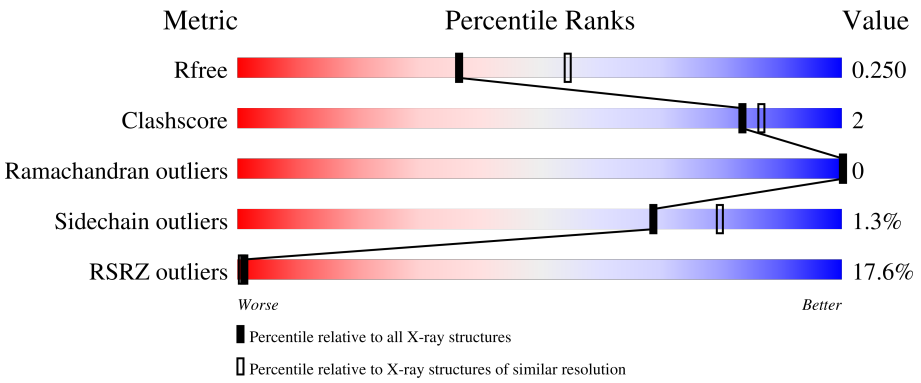
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	228	26% 84% 9% 7%
1	B	228	7% 91% • 7%
2	C	5	60% 40%
3	D	6	50% 50%

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	MES	A	507	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7159 atoms, of which 3526 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	H	N	O	S			
1	A	213	3396	1104	1682	283	320	7	0	1	0
1	B	213	3388	1100	1680	282	319	7	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ARG	THR	engineered mutation	UNP P01857
A	360	PHE	LYS	engineered mutation	UNP P01857
A	361	TYR	ASN	engineered mutation	UNP P01857
A	388	ASP	GLU	engineered mutation	UNP P01857
A	389	ILE	ASN	engineered mutation	UNP P01857
A	389A	PHE	-	insertion	UNP P01857
A	389B	PRO	-	insertion	UNP P01857
A	389C	ASN	-	insertion	UNP P01857
A	389D	GLY	-	insertion	UNP P01857
A	389E	LEU	-	insertion	UNP P01857
A	413	PRO	ASP	engineered mutation	UNP P01857
A	414	TYR	LYS	engineered mutation	UNP P01857
A	415	PRO	SER	engineered mutation	UNP P01857
A	416	SER	ARG	engineered mutation	UNP P01857
A	418	LEU	GLN	engineered mutation	UNP P01857
A	419	MET	GLN	engineered mutation	UNP P01857
A	421	THR	ASN	engineered mutation	UNP P01857
A	422	ARG	VAL	engineered mutation	UNP P01857
B	359	ARG	THR	engineered mutation	UNP P01857
B	360	PHE	LYS	engineered mutation	UNP P01857
B	361	TYR	ASN	engineered mutation	UNP P01857
B	388	ASP	GLU	engineered mutation	UNP P01857
B	389	ILE	ASN	engineered mutation	UNP P01857
B	389A	PHE	-	insertion	UNP P01857
B	389B	PRO	-	insertion	UNP P01857

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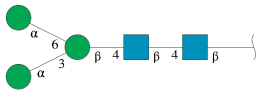
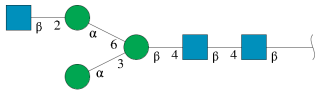
Chain	Residue	Modelled	Actual	Comment	Reference
B	389C	ASN	-	insertion	UNP P01857
B	389D	GLY	-	insertion	UNP P01857
B	389E	LEU	-	insertion	UNP P01857
B	413	PRO	ASP	engineered mutation	UNP P01857
B	414	TYR	LYS	engineered mutation	UNP P01857
B	415	PRO	SER	engineered mutation	UNP P01857
B	416	SER	ARG	engineered mutation	UNP P01857
B	418	LEU	GLN	engineered mutation	UNP P01857
B	419	MET	GLN	engineered mutation	UNP P01857
B	421	THR	ASN	engineered mutation	UNP P01857
B	422	ARG	VAL	engineered mutation	UNP P01857

- Molecule 2 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.



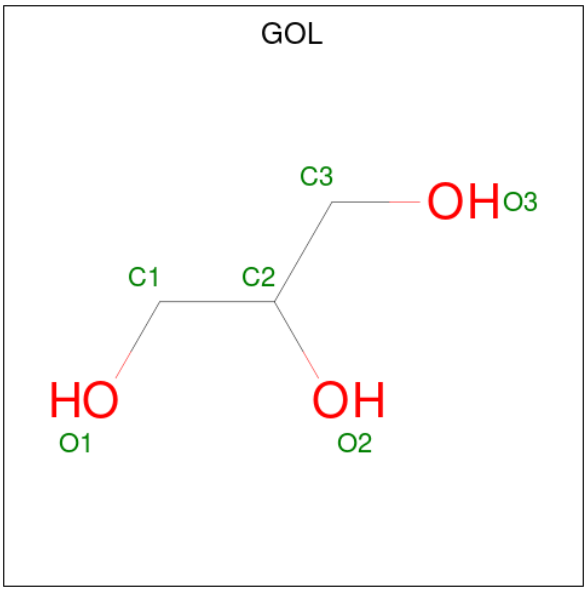
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	5	119	34	58	2	25	0	0	0

- Molecule 3 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.



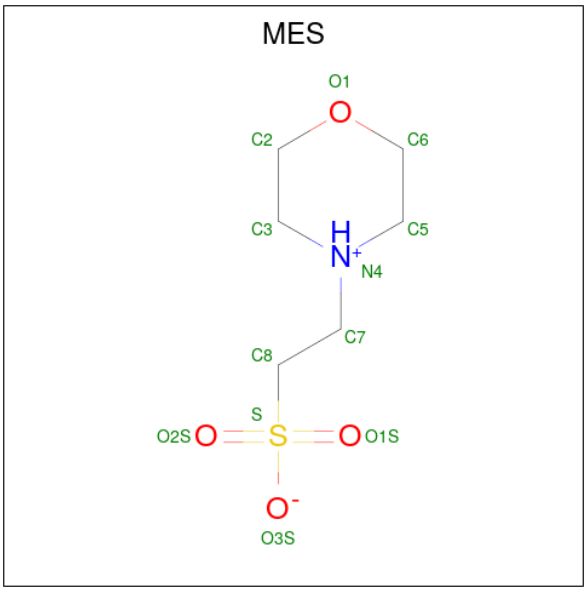
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	D	6	144	42	69	3	30	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
			Total	C	H	O		
4	B	1	14	3	8	3	0	0
			Total	C	H	O		
4	B	1	14	3	8	3	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
5	A	1	25	6	13	1	4	1	0	0

- Molecule 6 is water.

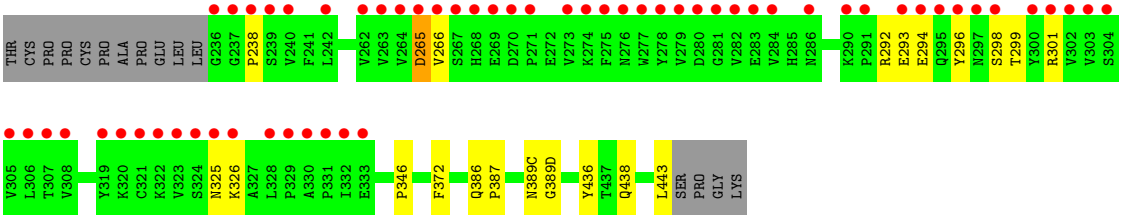
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	18	18	18	0	0
			Total	O		
6	B	27	27	27	0	0

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.

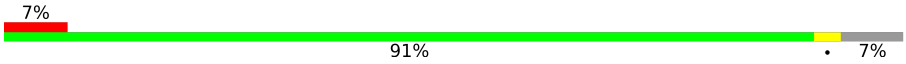
• Molecule 1: Ig gamma-1 chain C region

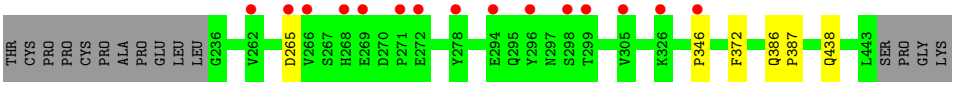
Chain A:



• Molecule 1: Ig gamma-1 chain C region

Chain B:



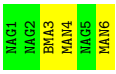


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 3: 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 D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.72Å 38.86Å 97.20Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	46.23 – 2.44 46.23 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.23-2.44) 99.8 (46.23-2.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.10-2247, BUSTER v.20150616	Depositor
R, R_{free}	0.215 , 0.249 0.215 , 0.250	Depositor DCC
R_{free} test set	1997 reflections (7.61%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 84.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7159	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.46% 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: GOL, NAG, MAN, BMA, MES

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	0.28	0/1770	0.45	0/2415
1	B	0.29	0/1761	0.44	0/2403
All	All	0.28	0/3531	0.44	0/4818

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	1714	1682	1682	11	0
1	B	1708	1680	1674	3	0
2	C	61	58	52	4	0
3	D	75	69	64	0	0
4	A	6	8	8	0	0
4	B	12	16	16	0	0
5	A	12	13	13	0	0
6	A	18	0	0	1	0
6	B	27	0	0	1	0
All	All	3633	3526	3509	17	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 (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TYR:OH	1:A:438:GLN:OE1	2.04	0.73
1:A:294:GLU:OE2	1:A:298:SER:HA	1.89	0.72
2:C:1:NAG:O3	2:C:2:NAG:O5	2.05	0.68
1:B:438:GLN:NE2	6:B:601:HOH:O	2.29	0.63
1:A:389(C):ASN:OD1	1:A:389(D):GLY:N	2.43	0.51
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.92	0.51
2:C:2:NAG:HO3	2:C:3:BMA:C5	2.24	0.50
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.97	0.46
2:C:1:NAG:HO3	2:C:2:NAG:C1	2.21	0.46
1:A:386:GLN:NE2	6:A:602:HOH:O	2.41	0.45
1:B:386:GLN:HB3	1:B:387:PRO:HD2	1.99	0.45
1:A:293:GLU:OE1	1:A:301:ARG:NH1	2.52	0.42
1:B:346:PRO:HB3	1:B:372:PHE:HB3	2.00	0.42
1:A:265:ASP:HA	2:C:1:NAG:H83	2.02	0.41
1:A:386:GLN:HB3	1:A:387:PRO:HD2	2.03	0.41
1:A:325:ASN:OD1	1:A:326:LYS:N	2.54	0.40
1:A:266:VAL:O	1:A:299:THR:HG23	2.22	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	212/228 (93%)	210 (99%)	2 (1%)	0	100	100
1	B	211/228 (92%)	205 (97%)	6 (3%)	0	100	100
All	All	423/456 (93%)	415 (98%)	8 (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	198/210 (94%)	194 (98%)	4 (2%)	55 67
1	B	197/210 (94%)	196 (100%)	1 (0%)	88 93
All	All	395/420 (94%)	390 (99%)	5 (1%)	69 80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	A	292	ARG
1	A	296	TYR
1	A	443	LEU
1	B	265	ASP

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)

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.33	0	17,19,21	0.83	1 (5%)
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.66	0
2	BMA	C	3	2	11,11,12	0.61	0	15,15,17	0.98	1 (6%)
2	MAN	C	4	2	11,11,12	0.71	0	15,15,17	0.94	1 (6%)
2	MAN	C	5	2	11,11,12	0.99	1 (9%)	15,15,17	1.19	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.24	0	17,19,21	0.55	0
3	NAG	D	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	BMA	D	3	3	11,11,12	0.79	0	15,15,17	0.92	1 (6%)
3	MAN	D	4	3	11,11,12	0.69	0	15,15,17	1.14	2 (13%)
3	NAG	D	5	3	14,14,15	0.24	0	17,19,21	0.42	0
3	MAN	D	6	3	11,11,12	0.90	0	15,15,17	0.83	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	MAN	C1-C2	2.93	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	MAN	C1-O5-C5	3.10	116.40	112.19
2	C	1	NAG	C1-O5-C5	2.83	116.03	112.19
3	D	4	MAN	C1-O5-C5	2.57	115.67	112.19
3	D	4	MAN	O2-C2-C3	-2.50	105.12	110.14
2	C	4	MAN	C1-O5-C5	2.47	115.54	112.19
2	C	3	BMA	C1-O5-C5	2.25	115.24	112.19
2	C	5	MAN	O2-C2-C3	-2.19	105.75	110.14
3	D	3	BMA	O2-C2-C3	-2.18	105.77	110.14
3	D	6	MAN	O2-C2-C3	-2.14	105.86	110.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6

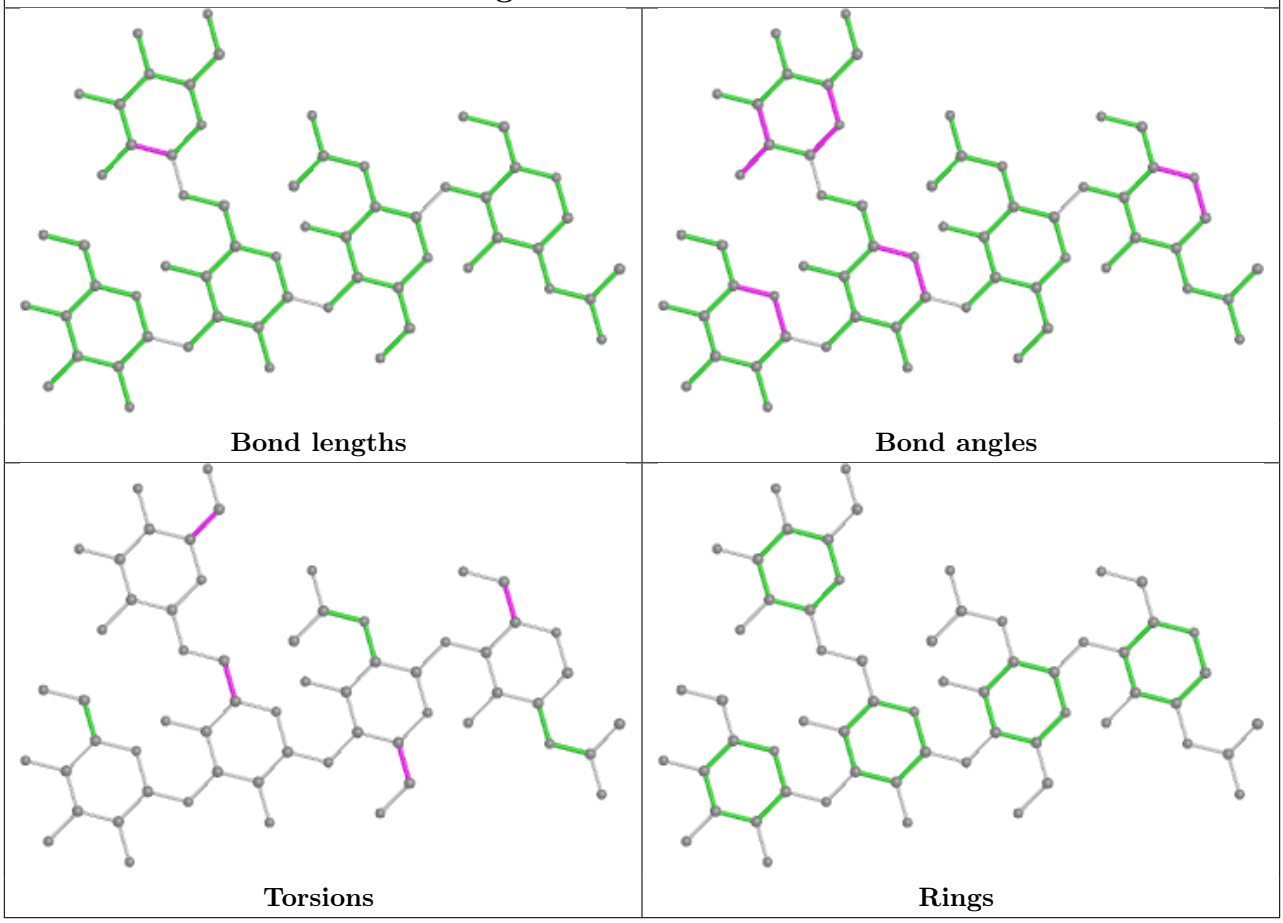
There are no ring outliers.

3 monomers are involved in 4 short contacts:

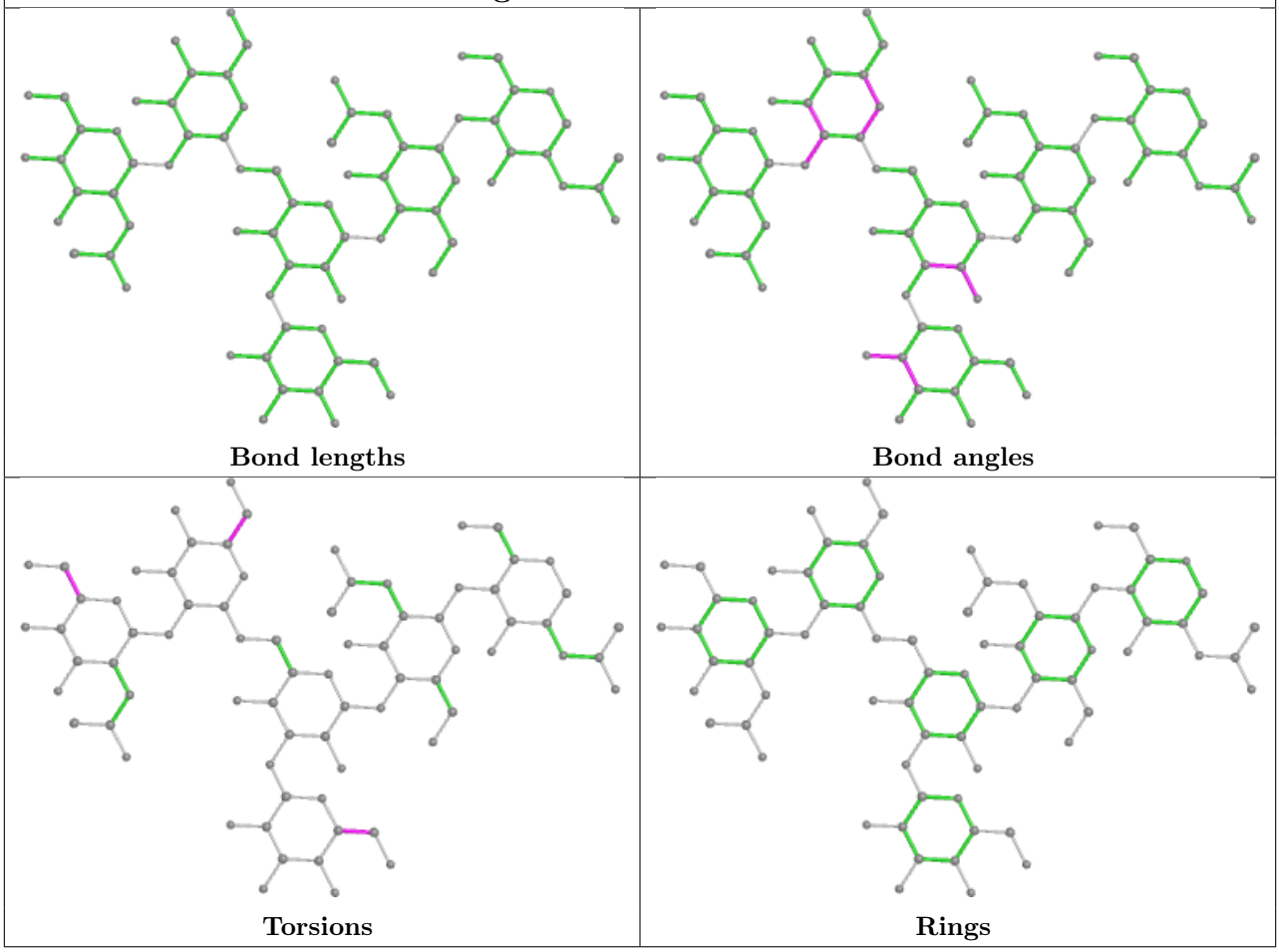
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	3	0
2	C	3	BMA	1	0
2	C	2	NAG	3	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	507	-	5,5,5	0.43	0	5,5,5	0.28	0
4	GOL	B	508	-	5,5,5	0.36	0	5,5,5	0.26	0
5	MES	A	507	-	12,12,12	2.25	1 (8%)	14,16,16	1.66	2 (14%)
4	GOL	A	506	-	5,5,5	0.35	0	5,5,5	0.20	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
4	GOL	B	507	-	-	2/4/4/4	-
4	GOL	B	508	-	-	2/4/4/4	-
5	MES	A	507	-	-	3/6/14/14	0/1/1/1
4	GOL	A	506	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	507	MES	C8-S	-7.53	1.66	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	507	MES	O3S-S-C8	3.36	111.20	105.77
5	A	507	MES	C6-C5-N4	-3.01	105.54	110.10

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	GOL	O1-C1-C2-C3
4	B	507	GOL	O1-C1-C2-C3
4	B	508	GOL	O1-C1-C2-O2
4	B	508	GOL	O1-C1-C2-C3
5	A	507	MES	C7-C8-S-O1S
5	A	507	MES	C7-C8-S-O3S
4	A	506	GOL	O1-C1-C2-O2
4	B	507	GOL	O1-C1-C2-O2
5	A	507	MES	C7-C8-S-O2S

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	213/228 (93%)	1.55	60 (28%)	0	0	42, 93, 209, 248	0
1	B	213/228 (93%)	0.63	15 (7%)	16	12	42, 80, 157, 202	0
All	All	426/456 (93%)	1.09	75 (17%)	1	1	42, 84, 196, 248	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	VAL	7.9
1	A	281	GLY	7.8
1	A	296	TYR	7.6
1	A	301	ARG	7.1
1	A	269	GLU	7.0
1	A	302	VAL	7.0
1	A	305	VAL	7.0
1	A	278	TYR	6.7
1	A	275	PHE	6.1
1	A	237	GLY	6.0
1	A	265	ASP	5.7
1	A	326	LYS	5.7
1	A	273	VAL	5.6
1	A	267	SER	5.5
1	A	306	LEU	5.0
1	A	298	SER	4.7
1	A	322	LYS	4.5
1	A	328	LEU	4.5
1	A	294	GLU	4.3
1	A	239	SER	4.3
1	A	293	GLU	4.3
1	A	274	LYS	4.1
1	A	331	PRO	4.0
1	A	323	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	333	GLU	3.9
1	A	290	LYS	3.8
1	A	266	VAL	3.8
1	A	332	ILE	3.8
1	A	321	CYS	3.7
1	A	300	TYR	3.7
1	A	268	HIS	3.7
1	A	277	TRP	3.6
1	A	264	VAL	3.6
1	B	296	TYR	3.4
1	A	282	VAL	3.4
1	A	307	THR	3.3
1	A	263	VAL	3.3
1	A	236	GLY	3.3
1	B	269	GLU	3.3
1	B	326	LYS	3.3
1	A	276	ASN	3.2
1	A	324	SER	3.1
1	A	286	ASN	3.0
1	A	262	VAL	3.0
1	B	298	SER	2.9
1	A	284	VAL	2.9
1	A	280	ASP	2.8
1	A	330	ALA	2.8
1	A	329	PRO	2.8
1	B	294	GLU	2.8
1	B	268	HIS	2.7
1	A	271	PRO	2.7
1	A	319	TYR	2.6
1	A	295	GLN	2.6
1	B	271	PRO	2.5
1	A	279	VAL	2.5
1	A	325	ASN	2.5
1	B	278	TYR	2.4
1	A	238	PRO	2.4
1	A	242	LEU	2.4
1	A	320	LYS	2.4
1	A	291	PRO	2.4
1	B	266	VAL	2.4
1	B	299	THR	2.4
1	A	304	SER	2.4
1	B	265	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	262	VAL	2.3
1	A	283	GLU	2.2
1	A	297	ASN	2.2
1	B	272	GLU	2.2
1	A	240	VAL	2.1
1	A	308	VAL	2.1
1	B	305	VAL	2.1
1	B	346	PRO	2.0
1	A	270	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)

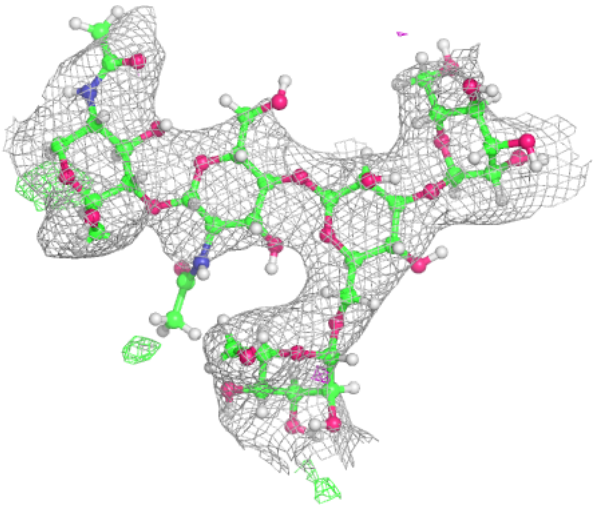
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

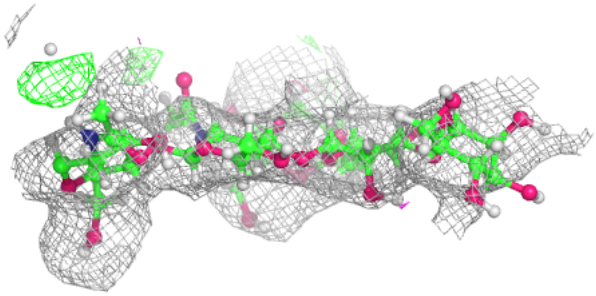
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	5	11/12	0.62	0.20	113,136,153,166	0
2	MAN	C	4	11/12	0.71	0.21	122,143,165,169	0
2	NAG	C	1	14/15	0.74	0.21	112,141,167,174	0
2	BMA	C	3	11/12	0.84	0.21	116,132,156,158	0
3	NAG	D	1	14/15	0.85	0.12	125,143,171,171	0
3	MAN	D	6	11/12	0.86	0.12	108,126,146,151	0
2	NAG	C	2	14/15	0.91	0.40	0,152,182,182	0
3	MAN	D	4	11/12	0.92	0.11	86,98,117,117	0
3	BMA	D	3	11/12	0.92	0.09	82,94,110,112	0
3	NAG	D	5	14/15	0.93	0.10	85,103,124,144	0
3	NAG	D	2	14/15	0.94	0.16	96,118,138,149	0

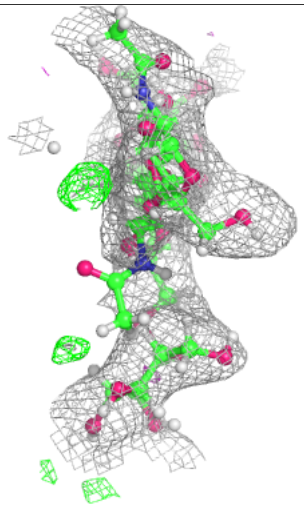
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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







Electron density around Chain D:

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

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	507	6/6	0.54	0.37	84,102,115,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MES	A	507	12/12	0.56	0.49	128,154,183,190	0
4	GOL	A	506	6/6	0.85	0.27	84,103,124,126	0
4	GOL	B	508	6/6	0.92	0.25	79,104,125,130	0

6.5 Other polymers (i)

There are no such residues in this entry.