Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 12:51 PM EDT

PDB ID	:	4FQI
Title	:	Crystal Structure of Fab CR9114 in Complex with a H5N1 influenza virus hemagglutinin
Authors	:	Dreyfus, C.; Wilson, I.A.
Deposited on	:	2012-06-25
Resolution	:	1.71 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:

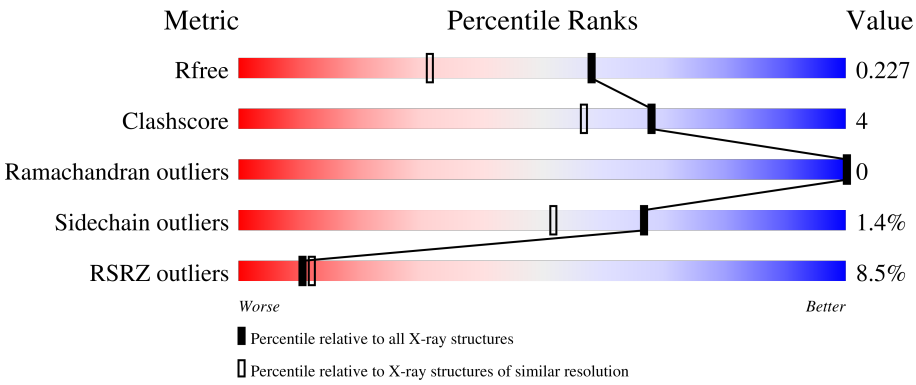
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	334	2%, 88%, 9%, •
2	B	177	%, 92%, 7%, ••
3	H	230	11%, 89%, 5%, 7%
4	L	216	22%, 87%, 10%, •
5	C	2	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
6	EDO	A	404	-	-	X	-
6	EDO	B	203	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 8532 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2658	1677	462	504	15	0	12	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q6DQ33
A	8	ASP	-	expression tag	UNP Q6DQ33
A	9	PRO	-	expression tag	UNP Q6DQ33
A	10	GLY	-	expression tag	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	176	1487	925	255	298	9	0	9	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q6DQ33
B	176	GLY	-	expression tag	UNP Q6DQ33
B	177	ARG	-	expression tag	UNP Q6DQ33

- Molecule 3 is a protein called antibody CR9114 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	215	1608	1013	268	320	7	0	2	0

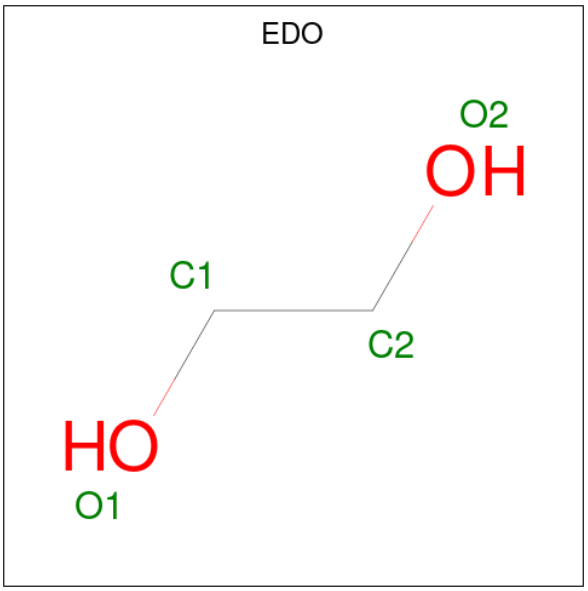
- Molecule 4 is a protein called antibody CR9114 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	211	1568	978	266	320	4	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0
6	A	1	4	2	2	0	0

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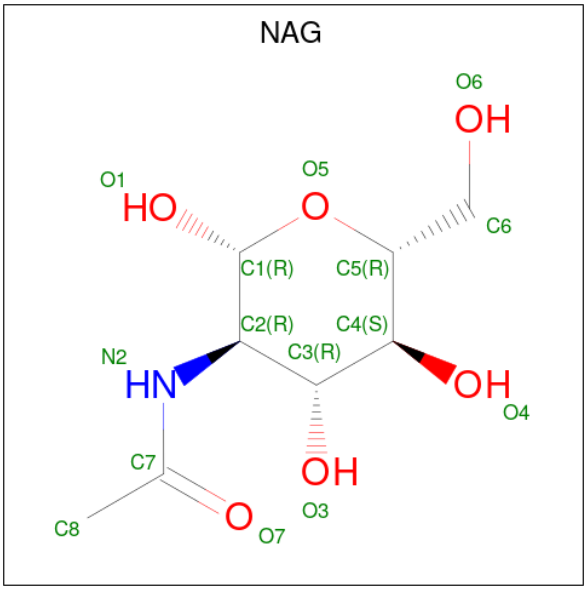
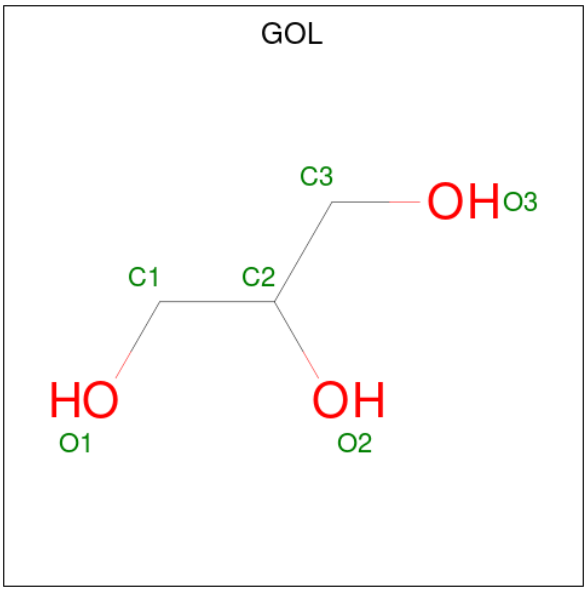
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	B	1	4	2	2		0	0
			Total	C	O			
6	H	1	4	2	2		0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	6	3	3	0	0

- Molecule 9 is water.

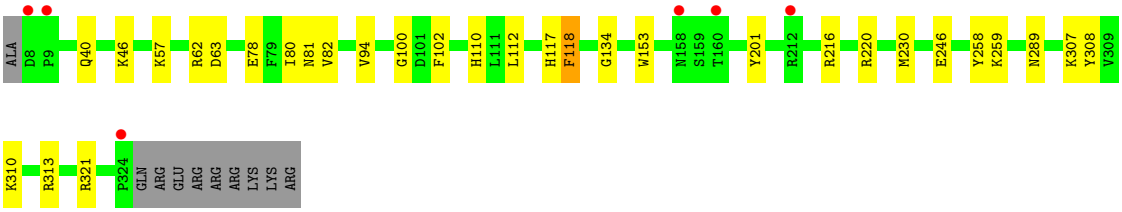
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	474	474	474	0	0
			Total	O		
9	B	242	242	242	0	0
			Total	O		
9	H	239	239	239	0	0
			Total	O		
9	L	136	136	136	0	0

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.

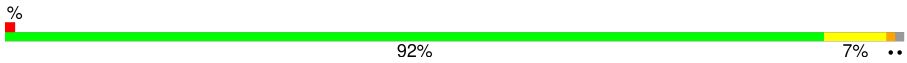
- Molecule 1: Hemagglutinin HA1

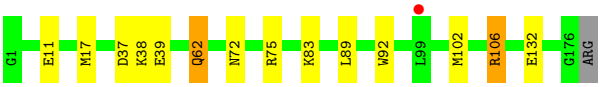
Chain A:



- Molecule 2: Hemagglutinin HA2

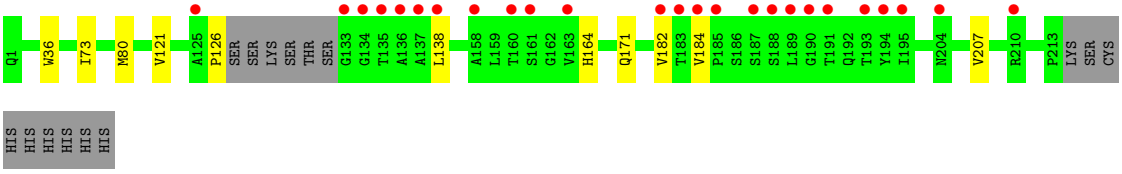
Chain B:





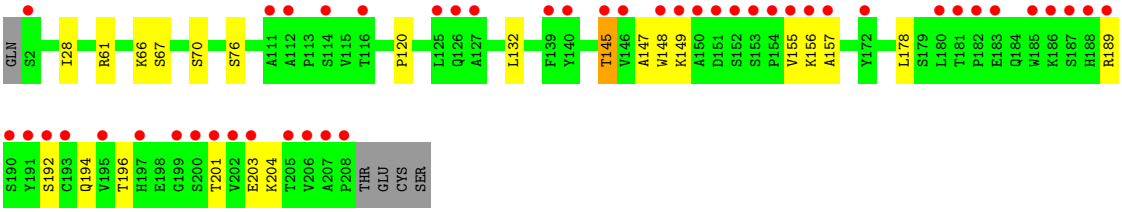
- Molecule 3: antibody CR9114 heavy chain

Chain H:



- Molecule 4: antibody CR9114 light chain

Chain L:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	141.64Å 141.64Å 382.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.55 – 1.71 36.55 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.55-1.71) 87.0 (36.55-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 1.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.198 , 0.232 0.195 , 0.227	Depositor DCC
R_{free} test set	7944 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: EDO, GOL, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.90	1/2740 (0.0%)	0.84	1/3719 (0.0%)
2	B	0.97	1/1526 (0.1%)	0.98	3/2048 (0.1%)
3	H	0.82	0/1647	0.83	0/2245
4	L	0.70	0/1606	0.71	0/2193
All	All	0.86	2/7519 (0.0%)	0.84	4/10205 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	HIS	C-N	11.38	1.60	1.34
2	B	132	GLU	CB-CG	-5.77	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	106	ARG	NE-CZ-NH1	12.23	126.42	120.30
2	B	106	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	112	LEU	CB-CG-CD1	-5.37	101.87	111.00
2	B	106	ARG	CD-NE-CZ	5.10	130.74	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	PHE	Peptide

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	2658	0	2599	27	0
2	B	1487	0	1395	12	0
3	H	1608	0	1556	8	0
4	L	1568	0	1517	14	0
5	C	28	0	25	0	0
6	A	20	0	30	7	0
6	B	20	0	30	3	0
6	H	4	0	6	0	0
7	A	28	0	26	0	0
7	B	14	0	13	0	0
8	B	6	0	8	0	0
9	A	474	0	0	8	0
9	B	242	0	0	0	0
9	H	239	0	0	1	0
9	L	136	0	0	1	0
All	All	8532	0	7205	56	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 4.

All (56) 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:82:VAL:H	6:A:404:EDO:H22	1.31	0.92
2:B:38[B]:LYS:HG2	6:B:206:EDO:H11	1.62	0.81
1:A:258:TYR:HE2	6:A:404:EDO:H12	1.43	0.80
1:A:82:VAL:N	6:A:404:EDO:H22	1.99	0.77
1:A:118:PHE:CD1	1:A:258:TYR:HB3	2.21	0.75
2:B:38[A]:LYS:HG2	6:B:206:EDO:H11	1.68	0.74
3:H:126:PRO:HG3	3:H:138:LEU:HB3	1.77	0.66
4:L:132:LEU:HB2	4:L:178:LEU:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HD2	2:B:62:GLN:HG2	1.76	0.65
4:L:149:LYS:HB2	4:L:192:SER:HB2	1.79	0.62
2:B:102:MET:HE3	2:B:106:ARG:NH2	2.16	0.61
4:L:145:THR:HG22	4:L:196:THR:OG1	2.00	0.60
1:A:289[A]:ASN:ND2	9:A:662:HOH:O	2.27	0.60
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.35	0.60
3:H:121:VAL:HG11	3:H:207:VAL:HG11	1.84	0.58
2:B:37:ASP:HA	6:B:206:EDO:H21	1.87	0.57
1:A:259:LYS:NZ	9:A:731:HOH:O	2.40	0.54
1:A:110:HIS:ND1	9:A:771:HOH:O	2.34	0.54
3:H:121:VAL:CG1	3:H:207:VAL:HG11	2.38	0.54
4:L:66:LYS:NZ	9:L:422:HOH:O	2.32	0.52
4:L:148:TRP:HB2	4:L:155:VAL:CG1	2.42	0.50
1:A:40[A]:GLN:HG2	3:H:73:ILE:HD11	1.95	0.49
4:L:61:ARG:HB2	4:L:76:SER:O	2.13	0.49
2:B:62:GLN:HB2	2:B:92:TRP:CD2	2.48	0.48
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.96	0.48
1:A:57:LYS:NZ	9:A:521:HOH:O	2.47	0.48
3:H:171:GLN:NE2	9:H:552:HOH:O	2.47	0.48
1:A:80:ILE:O	6:A:404:EDO:H11	2.13	0.47
4:L:155:VAL:HG22	4:L:157:ALA:H	1.78	0.47
1:A:216:ARG:O	1:A:220:ARG:NH2	2.48	0.47
2:B:106:ARG:HG3	2:B:106:ARG:HH11	1.82	0.45
3:H:36:TRP:CE2	3:H:80:MET:HB2	2.51	0.45
1:A:321[A]:ARG:HG2	9:A:675:HOH:O	2.16	0.45
4:L:28:ILE:O	4:L:66:LYS:HE3	2.17	0.45
4:L:203:GLU:O	4:L:204:LYS:HG2	2.18	0.44
1:A:63:ASP:HB3	1:A:94:VAL:HG22	2.00	0.44
1:A:82:VAL:HG22	6:A:404:EDO:H21	1.99	0.44
1:A:308:TYR:HE2	2:B:89[A]:LEU:HD21	1.83	0.44
1:A:258:TYR:CE2	6:A:404:EDO:H12	2.35	0.44
4:L:148:TRP:HB2	4:L:155:VAL:HG11	2.00	0.44
1:A:46:LYS:NZ	9:A:714:HOH:O	2.51	0.44
1:A:201:TYR:OH	1:A:246:GLU:OE1	2.23	0.43
1:A:81:ASN:HA	6:A:404:EDO:H11	2.01	0.43
1:A:62:ARG:HD3	1:A:78:GLU:OE2	2.19	0.43
1:A:100:GLY:HA3	1:A:230:MET:O	2.19	0.43
3:H:121:VAL:HG11	3:H:207:VAL:CG1	2.49	0.42
4:L:196:THR:HG22	4:L:201:THR:OG1	2.18	0.42
2:B:102:MET:HE3	2:B:102:MET:HB3	1.86	0.42
1:A:310:LYS:HE3	2:B:89[A]:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:HE3	2:B:89[A]:LEU:CD2	2.50	0.41
4:L:147:ALA:HB3	4:L:194:GLN:HB2	2.03	0.41
1:A:321[D]:ARG:HD3	9:A:846:HOH:O	2.21	0.40
1:A:313:ARG:NH2	9:A:762:HOH:O	2.55	0.40
3:H:182:VAL:HG22	3:H:184:VAL:HG13	2.03	0.40
4:L:120:PRO:HD3	4:L:132:LEU:HG	2.03	0.40
4:L:156:LYS:HE3	4:L:156:LYS:HB2	1.72	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	334/334 (100%)	325 (97%)	9 (3%)	0	100	100
2	B	183/177 (103%)	180 (98%)	3 (2%)	0	100	100
3	H	213/230 (93%)	211 (99%)	2 (1%)	0	100	100
4	L	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
All	All	939/957 (98%)	920 (98%)	19 (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	303/300 (101%)	302 (100%)	1 (0%)	92	89
2	B	159/151 (105%)	153 (96%)	6 (4%)	33	13
3	H	180/193 (93%)	179 (99%)	1 (1%)	86	80
4	L	175/180 (97%)	171 (98%)	4 (2%)	50	31
All	All	817/824 (99%)	805 (98%)	12 (2%)	67	49

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

Mol	Chain	Res	Type
1	A	102	PHE
2	B	11	GLU
2	B	17	MET
2	B	39[A]	GLU
2	B	39[B]	GLU
2	B	62	GLN
2	B	83	LYS
3	H	164	HIS
4	L	67	SER
4	L	70	SER
4	L	145	THR
4	L	189	ARG

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)

2 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	C	1	5,1	14,14,15	0.68	0	17,19,21	1.75	3 (17%)
5	NAG	C	2	5	14,14,15	0.48	0	17,19,21	0.89	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
5	NAG	C	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1	NAG	C1-O5-C5	5.83	120.00	112.19
5	C	1	NAG	C6-C5-C4	-2.28	107.43	113.02
5	C	1	NAG	C1-C2-N2	2.01	113.60	110.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

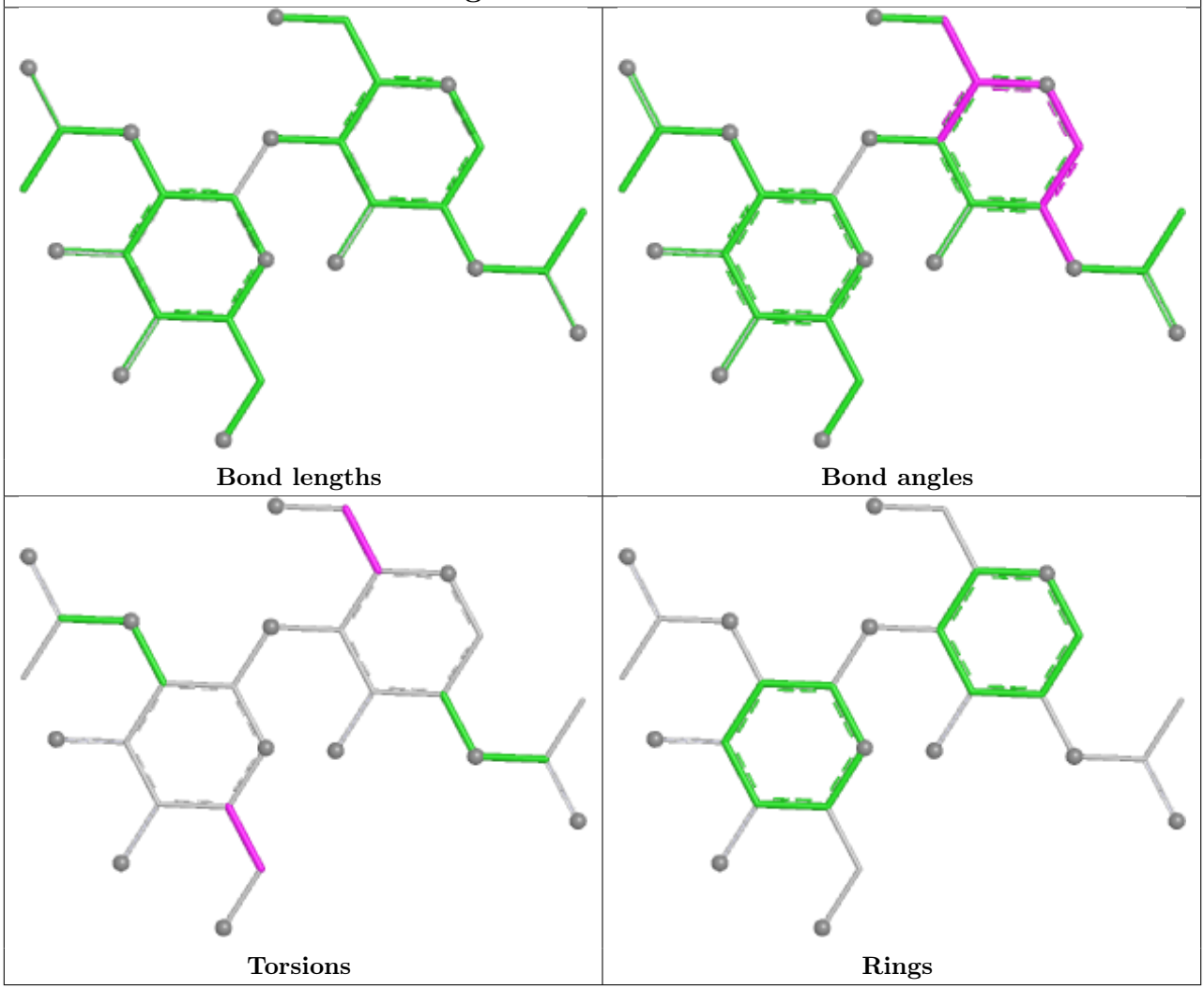
Mol	Chain	Res	Type	Atoms
5	C	2	NAG	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain C



5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
6	EDO	A	406	-	3,3,3	0.45	0	2,2,2	0.64	0
7	NAG	B	207	2	14,14,15	0.87	1 (7%)	17,19,21	1.80	3 (17%)
8	GOL	B	201	-	5,5,5	0.21	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	B	205	-	3,3,3	0.56	0	2,2,2	0.60	0
6	EDO	B	206	-	3,3,3	0.78	0	2,2,2	0.78	0
7	NAG	A	405	1	14,14,15	0.47	0	17,19,21	0.88	1 (5%)
6	EDO	H	301	-	3,3,3	0.86	0	2,2,2	0.64	0
6	EDO	B	204	-	3,3,3	0.48	0	2,2,2	0.63	0
6	EDO	A	402	-	3,3,3	0.72	0	2,2,2	0.65	0
6	EDO	B	203	-	3,3,3	0.47	0	2,2,2	0.43	0
6	EDO	B	202	-	3,3,3	0.34	0	2,2,2	0.77	0
7	NAG	A	409	1	14,14,15	0.56	0	17,19,21	1.20	3 (17%)
6	EDO	A	404	-	3,3,3	0.44	0	2,2,2	0.59	0
6	EDO	A	401	-	3,3,3	0.46	0	2,2,2	0.29	0
6	EDO	A	403	-	3,3,3	0.34	0	2,2,2	0.56	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
6	EDO	A	406	-	-	1/1/1/1	-
7	NAG	B	207	2	-	2/6/23/26	0/1/1/1
8	GOL	B	201	-	-	2/4/4/4	-
6	EDO	B	205	-	-	0/1/1/1	-
6	EDO	B	206	-	-	1/1/1/1	-
7	NAG	A	405	1	-	1/6/23/26	0/1/1/1
6	EDO	H	301	-	-	1/1/1/1	-
6	EDO	B	204	-	-	1/1/1/1	-
6	EDO	A	402	-	-	1/1/1/1	-
6	EDO	B	203	-	-	0/1/1/1	-
6	EDO	B	202	-	-	1/1/1/1	-
7	NAG	A	409	1	-	0/6/23/26	0/1/1/1
6	EDO	A	404	-	-	1/1/1/1	-
6	EDO	A	401	-	-	0/1/1/1	-
6	EDO	A	403	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	207	NAG	O5-C1	-2.07	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	207	NAG	C1-O5-C5	5.63	119.73	112.19
7	A	409	NAG	C1-O5-C5	2.58	115.64	112.19
7	A	405	NAG	C2-N2-C7	-2.52	119.52	122.90
7	A	409	NAG	C6-C5-C4	-2.13	107.80	113.02
7	B	207	NAG	C2-N2-C7	2.08	125.69	122.90
7	A	409	NAG	O5-C5-C6	2.07	111.70	107.66
7	B	207	NAG	C6-C5-C4	-2.07	107.94	113.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	207	NAG	O5-C5-C6-O6
7	B	207	NAG	C4-C5-C6-O6
8	B	201	GOL	O1-C1-C2-C3
6	A	403	EDO	O1-C1-C2-O2
6	B	206	EDO	O1-C1-C2-O2
8	B	201	GOL	O1-C1-C2-O2
6	A	406	EDO	O1-C1-C2-O2
7	A	405	NAG	C4-C5-C6-O6
6	A	404	EDO	O1-C1-C2-O2
6	B	202	EDO	O1-C1-C2-O2
6	B	204	EDO	O1-C1-C2-O2
6	A	402	EDO	O1-C1-C2-O2
6	H	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	206	EDO	3	0
6	A	404	EDO	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/334 (97%)	-0.31	6 (1%)	66	70	19, 29, 45, 83	0
2	B	176/177 (99%)	-0.15	1 (0%)	89	91	17, 25, 44, 60	0
3	H	215/230 (93%)	0.36	25 (11%)	4	5	17, 29, 80, 100	0
4	L	211/216 (97%)	0.78	47 (22%)	0	0	20, 46, 93, 101	0
All	All	926/957 (96%)	0.12	79 (8%)	10	12	17, 30, 75, 101	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	188	SER	7.4
4	L	156	LYS	7.1
4	L	154	PRO	6.7
4	L	155	VAL	6.6
3	H	195	ILE	6.1
3	H	133	GLY	5.9
4	L	189	ARG	5.9
4	L	187	SER	5.8
3	H	134	GLY	5.3
4	L	188	HIS	5.3
4	L	186	LYS	4.9
3	H	185	PRO	4.9
4	L	150	ALA	4.9
1	A	324	PRO	4.6
3	H	184	VAL	4.5
4	L	185	TRP	4.5
4	L	206	VAL	4.5
4	L	207	ALA	4.5
3	H	138	LEU	4.4
4	L	193	CYS	4.2
4	L	190	SER	4.1

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Mol	Chain	Res	Type	RSRZ
4	L	195	VAL	4.1
3	H	194	TYR	4.0
4	L	152	SER	4.0
3	H	191	THR	4.0
4	L	183	GLU	3.9
3	H	136	ALA	3.8
4	L	200	SER	3.7
3	H	190	GLY	3.7
3	H	135	THR	3.7
4	L	201	THR	3.6
3	H	158	ALA	3.6
4	L	202	VAL	3.6
3	H	137	ALA	3.3
3	H	187	SER	3.3
4	L	192	SER	3.3
3	H	125	ALA	3.1
4	L	191	TYR	3.1
4	L	2	SER	3.1
4	L	112	ALA	3.0
3	H	182	VAL	3.0
3	H	189	LEU	2.9
4	L	151	ASP	2.8
4	L	153	SER	2.8
3	H	163	VAL	2.8
4	L	203	GLU	2.8
4	L	146	VAL	2.7
4	L	180	LEU	2.7
4	L	205	THR	2.7
1	A	160	THR	2.7
3	H	193	THR	2.7
4	L	127	ALA	2.6
4	L	116	THR	2.6
4	L	139	PHE	2.6
4	L	157	ALA	2.6
4	L	199	GLY	2.5
1	A	8	ASP	2.4
4	L	208	PRO	2.4
3	H	204	ASN	2.4
3	H	160	THR	2.4
3	H	183	THR	2.4
4	L	140	TYR	2.3
3	H	210	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	158	ASN	2.3
4	L	111	ALA	2.3
4	L	197	HIS	2.3
4	L	148	TRP	2.2
4	L	114	SER	2.2
4	L	182	PRO	2.2
4	L	181	THR	2.2
3	H	161	SER	2.2
4	L	172	TYR	2.2
1	A	9	PRO	2.2
2	B	99	LEU	2.1
4	L	125	LEU	2.1
4	L	149	LYS	2.1
1	A	212[A]	ARG	2.0
4	L	145	THR	2.0
4	L	126	GLN	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)

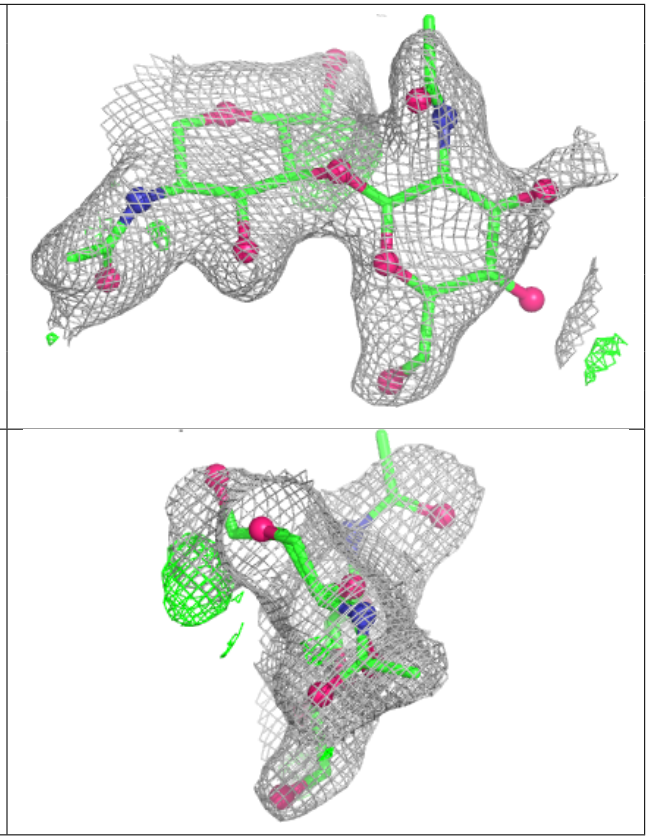
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	C	2	14/15	0.88	0.33	67,74,83,93	0
5	NAG	C	1	14/15	0.95	0.08	33,43,60,72	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)



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
6	EDO	B	203	4/4	0.63	0.48	70,89,100,101	0
7	NAG	A	409	14/15	0.83	0.24	54,66,79,84	0
6	EDO	B	206	4/4	0.85	0.15	33,38,44,47	0
6	EDO	H	301	4/4	0.88	0.13	29,31,32,42	0
8	GOL	B	201	6/6	0.88	0.18	53,60,64,67	0
7	NAG	A	405	14/15	0.90	0.30	41,63,82,86	0
7	NAG	B	207	14/15	0.91	0.15	40,58,66,67	0
6	EDO	A	402	4/4	0.91	0.08	39,40,41,45	0
6	EDO	B	202	4/4	0.92	0.12	46,46,54,69	0
6	EDO	A	403	4/4	0.93	0.18	20,37,38,45	0
6	EDO	A	404	4/4	0.93	0.24	33,36,42,43	0
6	EDO	A	406	4/4	0.96	0.13	28,36,38,42	0
6	EDO	B	204	4/4	0.96	0.09	35,36,36,47	0
6	EDO	B	205	4/4	0.96	0.06	36,37,38,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	401	4/4	0.99	0.07	19,20,23,25	0

6.5 Other polymers (i)

There are no such residues in this entry.