Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 08:12 AM EDT

PDB ID	:	6E56
Title	:	Human antibody H2214 in complex with influenza hemagglutinin A/Aichi/2/1968 (X-31) (H3N2)
Authors	:	McCarthy, K.R.; Harrison, S.C.
Deposited on	:	2018-07-19
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

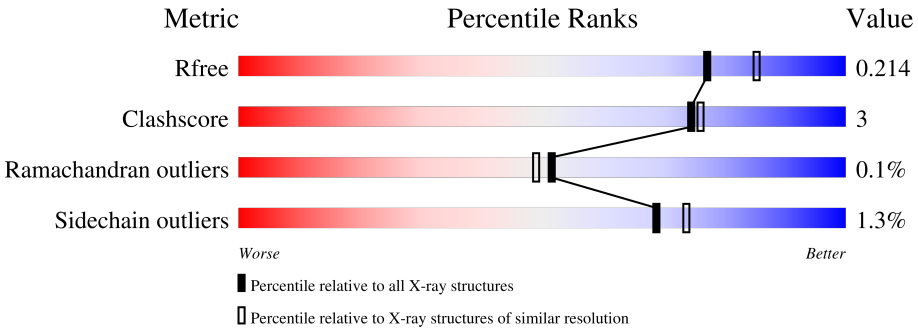
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Mol	Chain	Length	Quality of chain
1	A	290	87% 7% 6%
1	D	290	85% 9% 6%
2	G	253	83% 8% 9%
2	H	253	85% 6% 9%
3	I	215	92% 7% .
3	J	215	88% 10% .
4	B	2	100%

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	ACT	D	404	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11890 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	273	Total	C	N	O	S	0	0	0
			2124	1334	371	408	11			
1	A	272	Total	C	N	O	S	0	0	0
			2116	1330	369	406	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	ASP	ASN	conflict	UNP P03437
D	320	GLY	-	expression tag	UNP P03437
D	321	LEU	-	expression tag	UNP P03437
D	322	GLU	-	expression tag	UNP P03437
D	323	VAL	-	expression tag	UNP P03437
D	324	LEU	-	expression tag	UNP P03437
D	325	PHE	-	expression tag	UNP P03437
D	326	GLN	-	expression tag	UNP P03437
A	188	ASP	ASN	conflict	UNP P03437
A	320	GLY	-	expression tag	UNP P03437
A	321	LEU	-	expression tag	UNP P03437
A	322	GLU	-	expression tag	UNP P03437
A	323	VAL	-	expression tag	UNP P03437
A	324	LEU	-	expression tag	UNP P03437
A	325	PHE	-	expression tag	UNP P03437
A	326	GLN	-	expression tag	UNP P03437

- Molecule 2 is a protein called antibody H2214 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	229	Total	C	N	O	S	0	0	0
			1707	1068	288	344	7			
2	G	230	Total	C	N	O	S	0	0	0
			1716	1074	290	345	7			

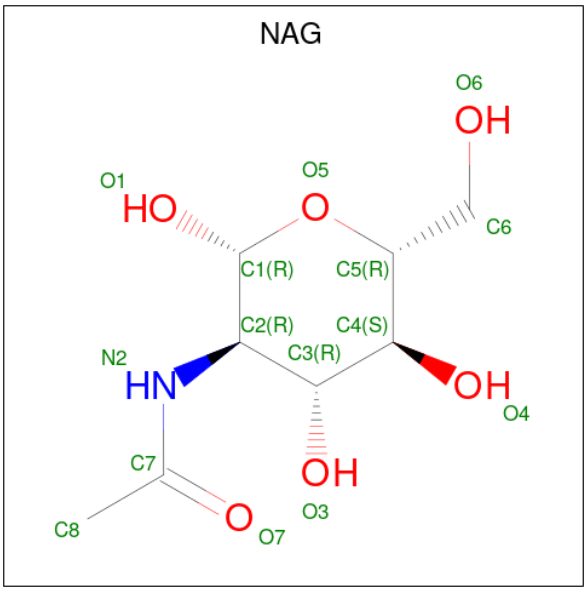
- Molecule 3 is a protein called antibody H2214 light chain, K1642.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	212	Total	C	N	O	S	0	0	0
			1637	1023	278	331	5			
3	J	212	Total	C	N	O	S	0	0	0
			1637	1023	278	331	5			

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

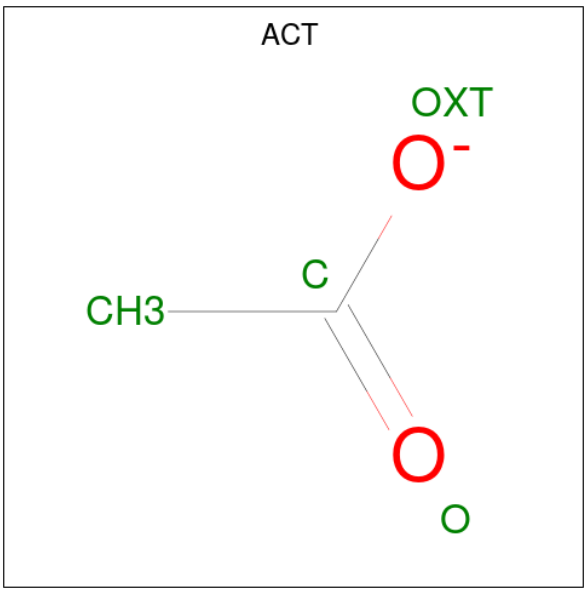
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

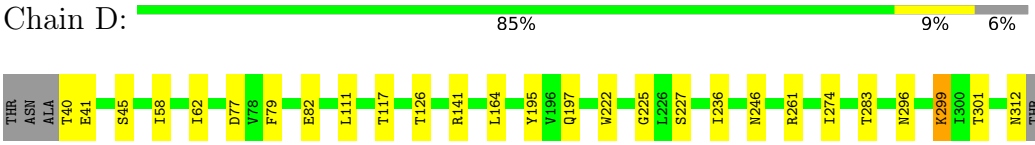
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	166	Total O 166 166	0	0
7	A	167	Total O 167 167	0	0
7	H	159	Total O 159 159	0	0
7	G	114	Total O 114 114	0	0
7	I	142	Total O 142 142	0	0
7	J	141	Total O 141 141	0	0

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. 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. 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.

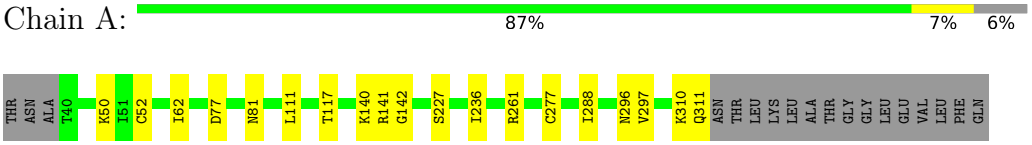
- Molecule 1: Hemagglutinin

Chain D:



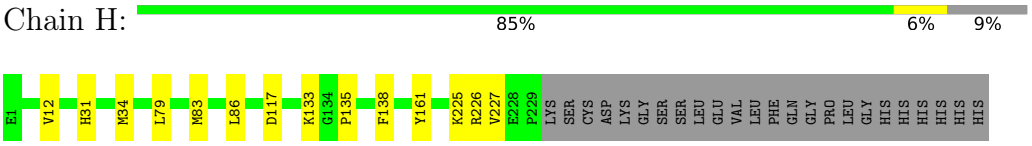
- Molecule 1: Hemagglutinin

Chain A:



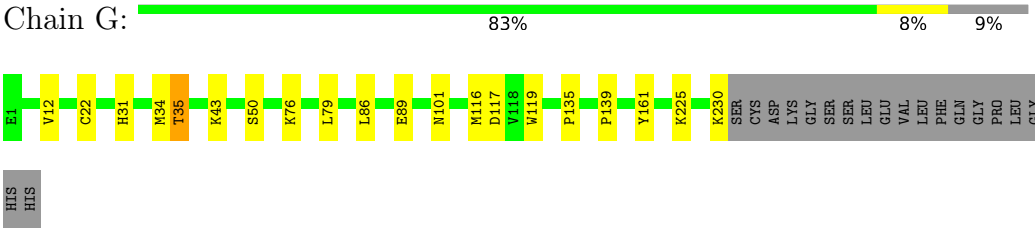
- Molecule 2: antibody H2214 heavy chain

Chain H:



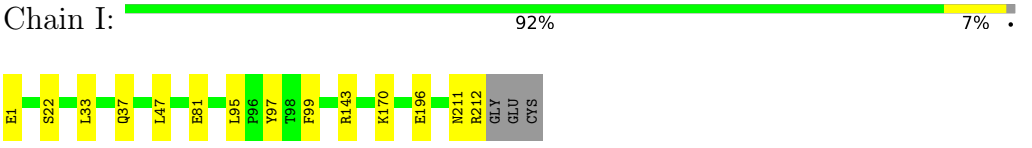
- Molecule 2: antibody H2214 heavy chain

Chain G:



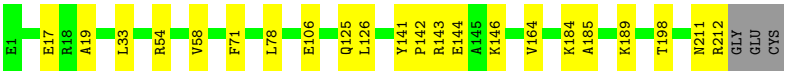
- Molecule 3: antibody H2214 light chain, K1642

Chain I:



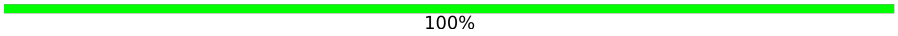
• Molecule 3: antibody H2214 light chain, K1642

Chain J:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	77.55Å 98.71Å 224.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.00 48.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.85-2.00) 99.4 (48.85-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.188 , 0.214 0.188 , 0.214	Depositor DCC
R_{free} test set	5842 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: NAG, ACT

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	0/2168	0.49	0/2952
1	D	0.28	0/2176	0.47	0/2963
2	G	0.27	0/1759	0.49	0/2395
2	H	0.28	0/1750	0.50	0/2384
3	I	0.29	0/1671	0.50	0/2270
3	J	0.29	0/1671	0.51	0/2270
All	All	0.28	0/11195	0.49	0/15234

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	2116	0	2059	10	0
1	D	2124	0	2064	18	0
2	G	1716	0	1650	16	0
2	H	1707	0	1637	6	0
3	I	1637	0	1597	10	0
3	J	1637	0	1597	13	0
4	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	13	0	0
5	D	14	0	13	0	0
6	A	4	0	3	1	0
6	D	4	0	3	2	0
7	A	167	0	0	3	0
7	D	166	0	0	2	0
7	G	114	0	0	4	0
7	H	159	0	0	1	0
7	I	142	0	0	3	0
7	J	141	0	0	3	0
All	All	11890	0	10661	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (69) 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:77:ASP:OD2	1:A:141:ARG:NH1	2.06	0.86
2:G:116:MET:SD	7:G:398:HOH:O	2.33	0.85
1:D:117:THR:HG21	1:D:261:ARG:HH11	1.41	0.84
1:A:81:ASN:ND2	7:A:501:HOH:O	2.09	0.81
2:H:227:VAL:O	7:H:301:HOH:O	2.11	0.68
3:J:126:LEU:O	3:J:184:LYS:NZ	2.22	0.68
1:A:117:THR:HG21	1:A:261:ARG:HH11	1.59	0.67
3:J:146:LYS:NZ	7:J:302:HOH:O	2.27	0.66
2:G:116:MET:HE3	2:G:119:TRP:CZ2	2.31	0.65
2:G:230:LYS:NZ	7:G:302:HOH:O	2.30	0.64
1:D:222:TRP:HD1	6:D:404:ACT:H2	1.63	0.64
1:D:40:THR:N	7:D:504:HOH:O	2.31	0.64
2:G:12:VAL:HG11	2:G:86:LEU:HD13	1.80	0.63
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.80	0.63
3:I:1:GLU:N	7:I:303:HOH:O	2.31	0.61
1:A:227:SER:OG	6:A:402:ACT:O	2.16	0.61
3:J:211:ASN:O	3:J:212:ARG:HB2	1.99	0.61
3:I:196:GLU:OE1	7:I:302:HOH:O	2.16	0.61
2:G:116:MET:HE1	3:I:99:PHE:HZ	1.68	0.59
2:G:135:PRO:HB3	2:G:161:TYR:HB3	1.84	0.58
1:D:227:SER:HG	6:D:404:ACT:C	2.17	0.57
3:I:143:ARG:NH2	7:I:305:HOH:O	2.38	0.56
3:J:146:LYS:HB3	3:J:198:THR:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:NZ	7:A:509:HOH:O	2.39	0.54
1:D:77:ASP:OD2	1:D:141:ARG:NH1	2.41	0.54
3:J:144:GLU:HG3	7:J:305:HOH:O	2.07	0.54
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.91	0.52
2:G:116:MET:HE1	3:I:99:PHE:CZ	2.44	0.52
1:D:117:THR:HG21	1:D:261:ARG:NH1	2.18	0.52
2:G:139:PRO:HD3	2:G:225:LYS:HD3	1.92	0.52
1:A:142:GLY:O	7:A:502:HOH:O	2.19	0.51
1:D:79:PHE:HA	1:D:82:GLU:HG3	1.92	0.51
1:D:45:SER:HB3	1:D:296:ASN:HD21	1.76	0.50
1:A:296:ASN:OD1	1:A:311:GLN:HA	2.11	0.50
1:D:58:ILE:HG21	1:D:274:ILE:HD12	1.94	0.49
1:D:283:THR:HG22	1:D:301:THR:HG22	1.95	0.49
3:J:54:ARG:HG2	3:J:58:VAL:HB	1.95	0.48
1:D:111:LEU:HD21	1:D:236:ILE:HD11	1.95	0.48
2:H:138:PHE:CE2	3:J:125:GLN:HG3	2.49	0.48
3:J:185:ALA:O	3:J:189:LYS:HG3	2.13	0.48
2:G:35:THR:HB	2:G:50:SER:OG	2.14	0.47
3:I:37:GLN:HB2	3:I:47:LEU:HD11	1.96	0.47
1:A:111:LEU:HD21	1:A:236:ILE:HD11	1.98	0.46
3:I:211:ASN:O	3:I:212:ARG:HG2	2.16	0.45
2:H:135:PRO:HB3	2:H:161:TYR:HB3	1.98	0.45
3:J:17:GLU:OE1	7:J:301:HOH:O	2.20	0.44
3:I:81:GLU:H	3:I:81:GLU:CD	2.20	0.44
2:H:12:VAL:HG11	2:H:86:LEU:HD13	2.00	0.44
1:D:222:TRP:NE1	1:D:225:GLY:HA2	2.33	0.44
1:D:126:THR:O	7:D:501:HOH:O	2.20	0.44
2:G:34:MET:HB3	2:G:79:LEU:HD22	2.00	0.43
3:J:143:ARG:CZ	3:J:164:VAL:HG21	2.48	0.43
1:D:164:LEU:O	1:D:246:ASN:HA	2.19	0.43
2:G:89:GLU:HG3	7:G:366:HOH:O	2.17	0.43
2:G:101:ASN:ND2	7:G:312:HOH:O	2.52	0.43
1:D:40:THR:HG22	1:D:41:GLU:H	1.84	0.43
1:D:296:ASN:ND2	1:D:312:ASN:HA	2.34	0.43
1:A:52:CYS:HB3	1:A:277:CYS:O	2.19	0.42
3:J:33:LEU:HD22	3:J:71:PHE:CG	2.55	0.42
2:G:22:CYS:HB3	2:G:79:LEU:HB3	2.01	0.42
2:G:43:LYS:HE3	2:G:43:LYS:HB3	1.73	0.41
2:G:35:THR:HG21	3:I:97:TYR:CE1	2.55	0.41
1:A:288:ILE:HG21	1:A:297:VAL:HG21	2.03	0.41
1:D:195:TYR:O	1:D:197:GLN:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:LYS:HB2	1:D:299:LYS:HE2	1.83	0.41
3:I:95:LEU:HD23	3:I:95:LEU:HA	1.97	0.41
3:J:19:ALA:HB2	3:J:78:LEU:HD11	2.02	0.41
2:G:230:LYS:HA	2:G:230:LYS:HD2	1.74	0.41
3:J:141:TYR:CG	3:J:142:PRO:HA	2.57	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	270/290 (93%)	259 (96%)	10 (4%)	1 (0%)	34	30
1	D	271/290 (93%)	261 (96%)	9 (3%)	1 (0%)	34	30
2	G	228/253 (90%)	225 (99%)	3 (1%)	0	100	100
2	H	227/253 (90%)	223 (98%)	4 (2%)	0	100	100
3	I	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
3	J	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
All	All	1416/1516 (93%)	1375 (97%)	39 (3%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	D	62	ILE

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	241/255 (94%)	239 (99%)	2 (1%)	81 86
1	D	242/255 (95%)	241 (100%)	1 (0%)	91 93
2	G	192/212 (91%)	188 (98%)	4 (2%)	53 57
2	H	191/212 (90%)	186 (97%)	5 (3%)	46 48
3	I	186/188 (99%)	183 (98%)	3 (2%)	62 67
3	J	186/188 (99%)	185 (100%)	1 (0%)	88 92
All	All	1238/1310 (94%)	1222 (99%)	16 (1%)	69 74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	299	LYS
1	A	50	LYS
1	A	310	LYS
2	H	31	HIS
2	H	117	ASP
2	H	133	LYS
2	H	225	LYS
2	H	226	ARG
2	G	31	HIS
2	G	35	THR
2	G	76	LYS
2	G	117	ASP
3	I	22	SER
3	I	33	LEU
3	I	170	LYS
3	J	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	296	ASN
2	H	215	ASN

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	$\#\|Z\| > 2$
4	NAG	B	1	1,4	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	B	2	4	14,14,15	0.26	0	17,19,21	0.52	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	NAG	B	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

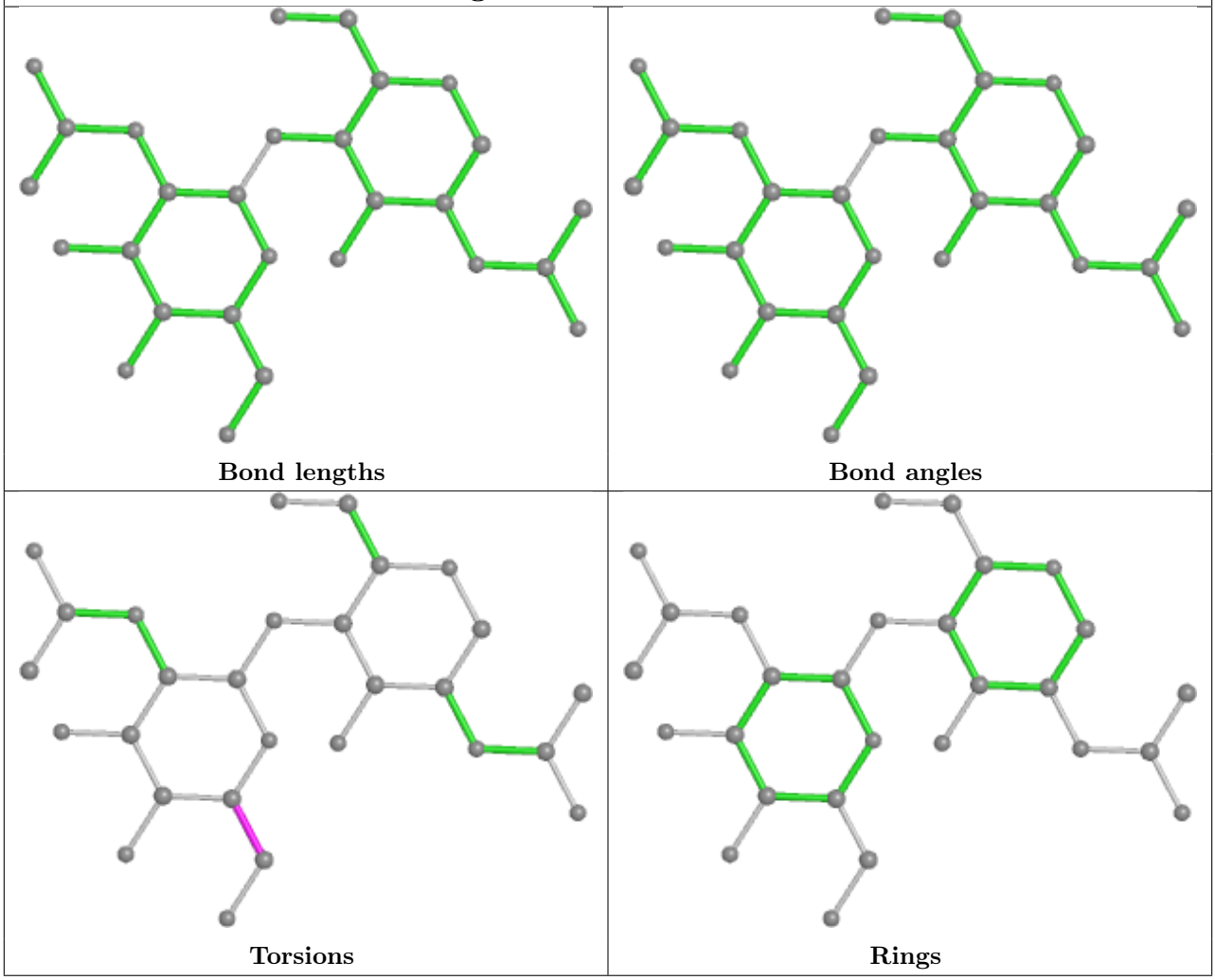
Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain B



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	$\#\|Z\|>2$
5	NAG	A	401	1	14,14,15	0.28	0	17,19,21	0.43	0
6	ACT	D	404	-	3,3,3	1.16	0	3,3,3	1.30	0
6	ACT	A	402	-	3,3,3	1.39	0	3,3,3	1.27	0
5	NAG	D	403	1	14,14,15	0.51	0	17,19,21	0.50	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	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	D	403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	403	NAG	C1-C2-N2-C7
5	D	403	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	404	ACT	2	0
6	A	402	ACT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

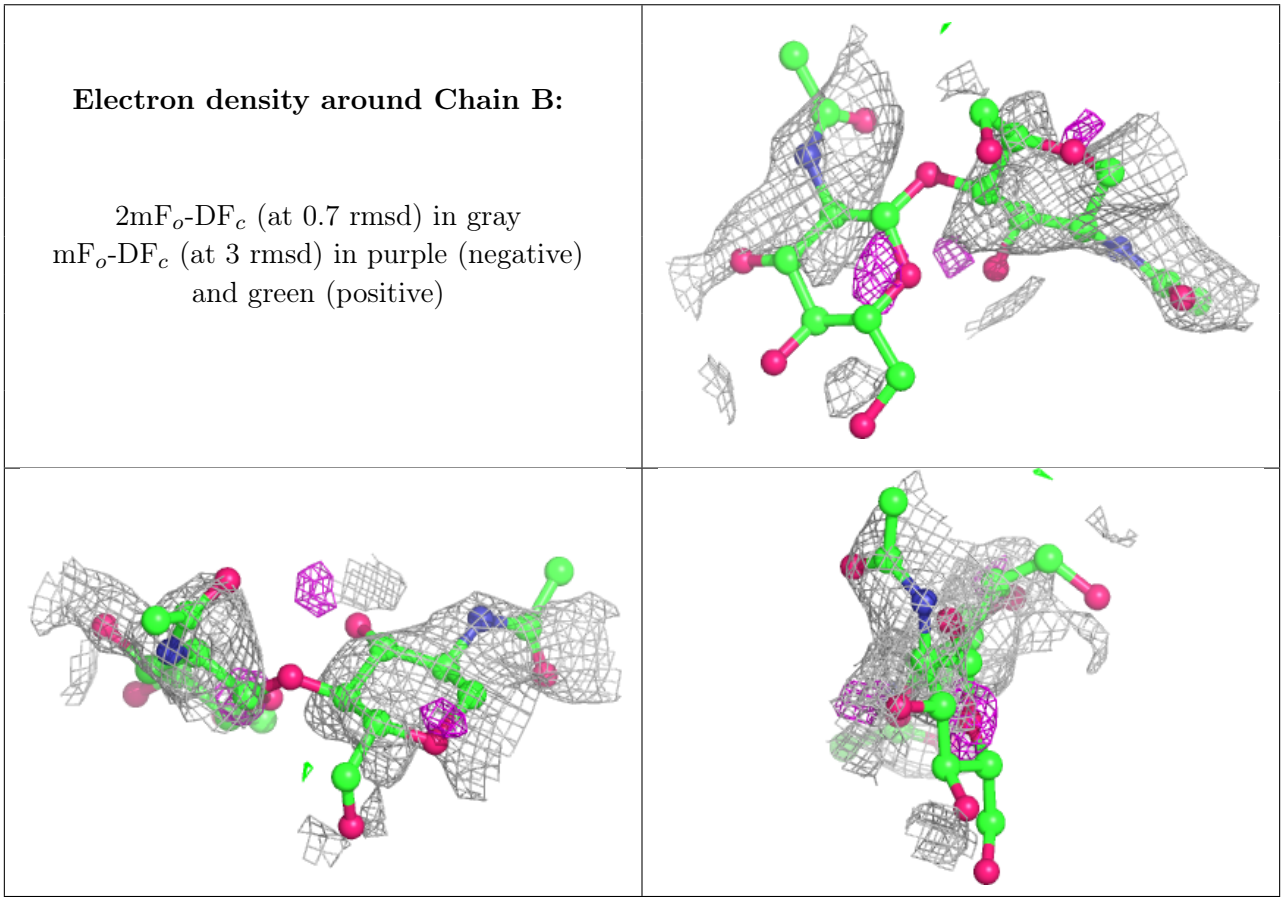
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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 B:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.