



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 11:02 AM BST

PDB ID : 4O58  
Title : Crystal structure of broadly neutralizing antibody F045-092 in complex with A/Victoria/3/1975 (H3N2) influenza hemagglutinin  
Authors : Lee, P.S.; Wilson, I.A.  
Deposited on : 2013-12-19  
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	2.13.1
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

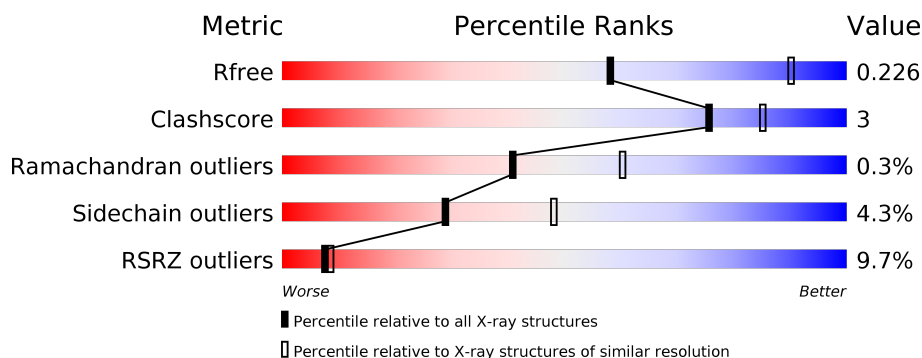
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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.



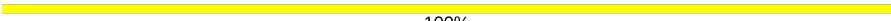
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	323	<div> <div>89%</div> <div>8%</div> <div>••</div> </div>
2	B	176	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
3	L	216	<div> <div>31%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>
4	H	240	<div> <div>9%</div> <div>83%</div> <div>9%</div> <div>• 7%</div> </div>
5	C	2	<div> <div>100%</div> </div>
5	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
6	D	5	 100%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7390 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2439	1526	430	470	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP P03435
A	8	ASP	-	expression tag	UNP P03435
A	9	PRO	-	expression tag	UNP P03435
A	10	GLY	-	expression tag	UNP P03435

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1393	864	246	277	6			

- Molecule 3 is a protein called Fab F045-092 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

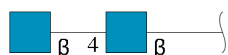
- Molecule 4 is a protein called Fab F045-092 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	223	Total	C	N	O	S	0	0	0
			1679	1065	275	331	8			

There are 6 discrepancies between the modelled and reference sequences:

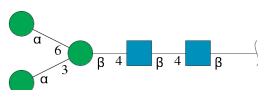
Chain	Residue	Modelled	Actual	Comment	Reference
H	217	HIS	-	expression tag	UNP S6C4S0
H	218	HIS	-	expression tag	UNP S6C4S0
H	219	HIS	-	expression tag	UNP S6C4S0
H	220	HIS	-	expression tag	UNP S6C4S0
H	221	HIS	-	expression tag	UNP S6C4S0
H	222	HIS	-	expression tag	UNP S6C4S0

- 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
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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
6	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



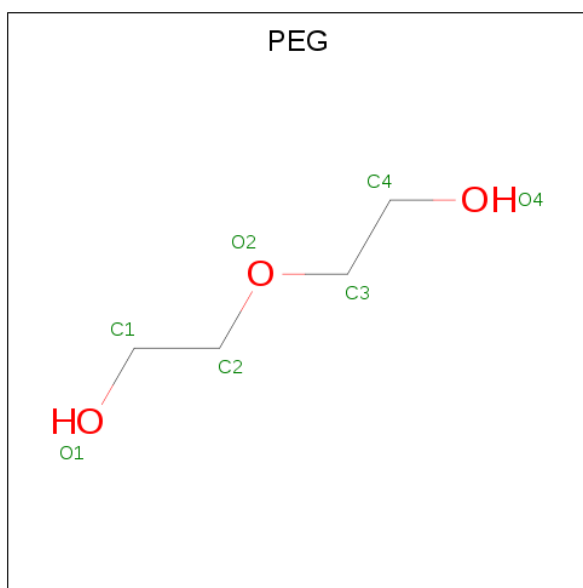
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	L	1	Total	C	O	0	0
			7	4	3		
9	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

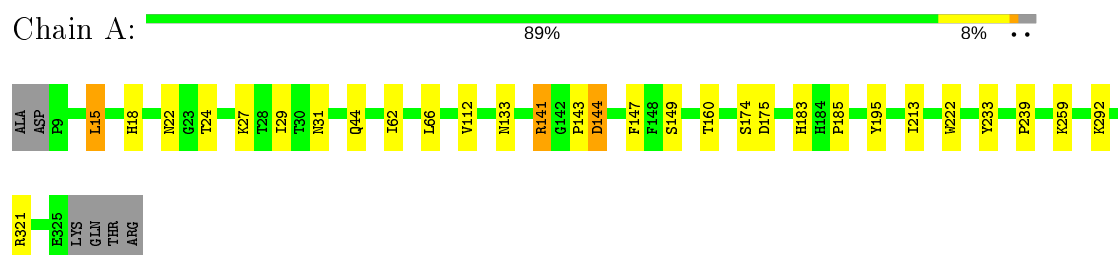
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	42	Total	O	0	0
			42	42		
10	B	16	Total	O	0	0
			16	16		
10	L	4	Total	O	0	0
			4	4		
10	H	14	Total	O	0	0
			14	14		



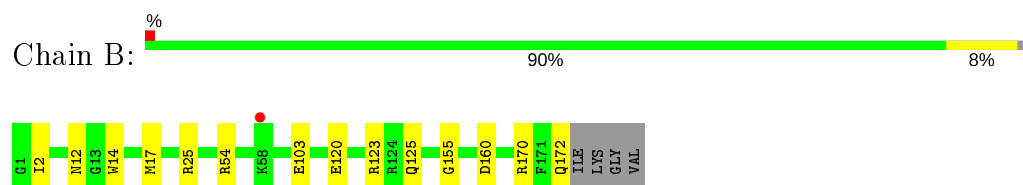
### 3 Residue-property plots [i](#)

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.

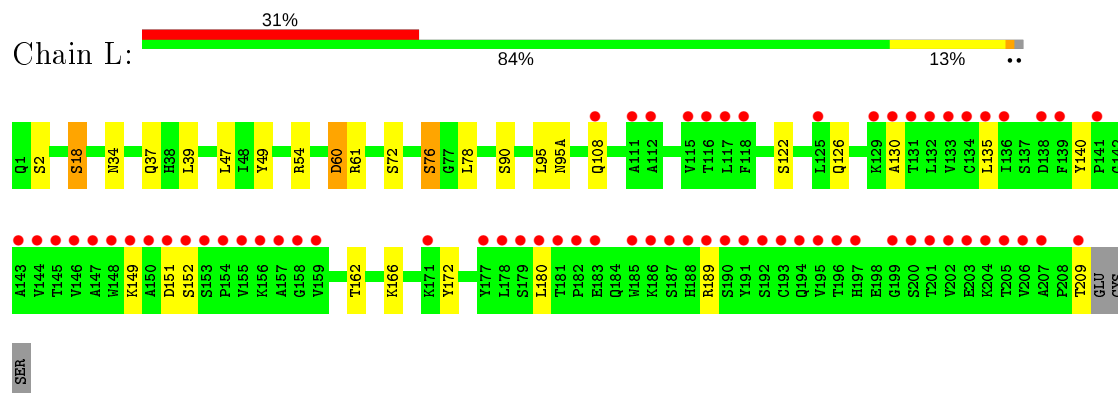
- Molecule 1: Hemagglutinin HA1 chain



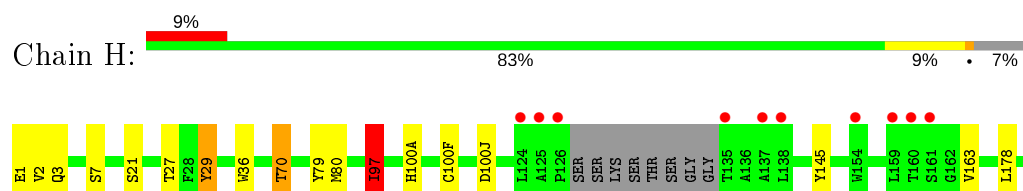
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 3: Fab F045-092 light chain



- Molecule 4: Fab F045-092 heavy chain





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

Chain C:  100%

MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2

- Molecule 6: 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 D:  100%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.10Å 99.10Å 336.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.02 – 2.75 49.02 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-2.75) 99.5 (49.02-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.177 , 0.224 0.180 , 0.226	Depositor DCC
$R_{free}$ test set	2583 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.2	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: PEG, MAN, BMA, NAG, SO4

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	0.49	0/2496	0.63	1/3396 (0.0%)
2	B	0.58	0/1417	0.70	1/1904 (0.1%)
3	L	0.36	0/1604	0.54	0/2190
4	H	0.39	0/1721	0.55	1/2349 (0.0%)
All	All	0.46	0/7238	0.60	3/9839 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LEU	CA-CB-CG	-5.68	102.25	115.30
2	B	170	ARG	NE-CZ-NH1	-5.38	117.61	120.30
4	H	97	ILE	CB-CA-C	-5.06	101.48	111.60

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	2439	0	2384	13	0
2	B	1393	0	1312	5	0
3	L	1567	0	1515	15	0
4	H	1679	0	1628	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	28	0	25	0	0
5	E	28	0	25	0	0
6	D	61	0	52	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
8	A	25	0	0	1	0
8	B	15	0	0	0	0
8	H	20	0	0	0	0
8	L	10	0	0	0	0
9	A	7	0	10	0	0
9	L	14	0	20	0	0
10	A	42	0	0	0	0
10	B	16	0	0	0	0
10	H	14	0	0	1	0
10	L	4	0	0	0	0
All	All	7390	0	6997	45	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.

The worst 5 of 45 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)
4:H:70:THR:HG22	4:H:79:TYR:HB2	1.58	0.86
3:L:18:SER:HB3	3:L:76:SER:HA	1.62	0.80
1:A:321:ARG:NH2	8:A:515:SO4:O3	2.20	0.68
2:B:120:GLU:OE1	2:B:123:ARG:NH2	2.20	0.68
1:A:141:ARG:NH1	1:A:147:PHE:O	2.28	0.66

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	315/323 (98%)	303 (96%)	10 (3%)	2 (1%)	25	42
2	B	170/176 (97%)	161 (95%)	9 (5%)	0	100	100
3	L	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	29	47
4	H	219/240 (91%)	213 (97%)	6 (3%)	0	100	100
All	All	915/955 (96%)	879 (96%)	33 (4%)	3 (0%)	41	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	143	PRO
3	L	151	ASP

### 5.3.2 Protein sidechains ⓘ

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	277/282 (98%)	266 (96%)	11 (4%)	31	51
2	B	146/149 (98%)	141 (97%)	5 (3%)	37	58
3	L	178/181 (98%)	166 (93%)	12 (7%)	16	28
4	H	186/201 (92%)	180 (97%)	6 (3%)	39	59
All	All	787/813 (97%)	753 (96%)	34 (4%)	29	48

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	172	GLN
3	L	60	ASP
4	H	70	THR
3	L	18	SER
1	A	144	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	193	ASN
2	B	53	ASN
4	H	100(A)	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

9 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	1,5	14,14,15	0.64	0	17,19,21	2.05	4 (23%)
5	NAG	C	2	5	14,14,15	0.51	0	17,19,21	1.46	2 (11%)
6	NAG	D	1	1,6	14,14,15	0.73	0	17,19,21	1.22	1 (5%)
6	NAG	D	2	6	14,14,15	0.62	0	17,19,21	1.07	2 (11%)
6	BMA	D	3	6	11,11,12	0.82	0	15,15,17	1.48	3 (20%)
6	MAN	D	4	6	11,11,12	0.61	0	15,15,17	1.09	2 (13%)
6	MAN	D	5	6	11,11,12	0.61	0	15,15,17	1.18	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
5	NAG	E	2	5	14,14,15	0.46	0	17,19,21	1.15	1 (5%)

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	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	0/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
6	MAN	D	5	6	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C4-C3-C2	4.60	117.76	111.02
5	C	1	NAG	C1-O5-C5	4.41	118.17	112.19
5	C	1	NAG	C3-C4-C5	3.86	117.13	110.24
5	C	2	NAG	O5-C5-C6	3.85	113.24	107.20
6	D	5	MAN	O5-C5-C6	3.57	112.80	107.20

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

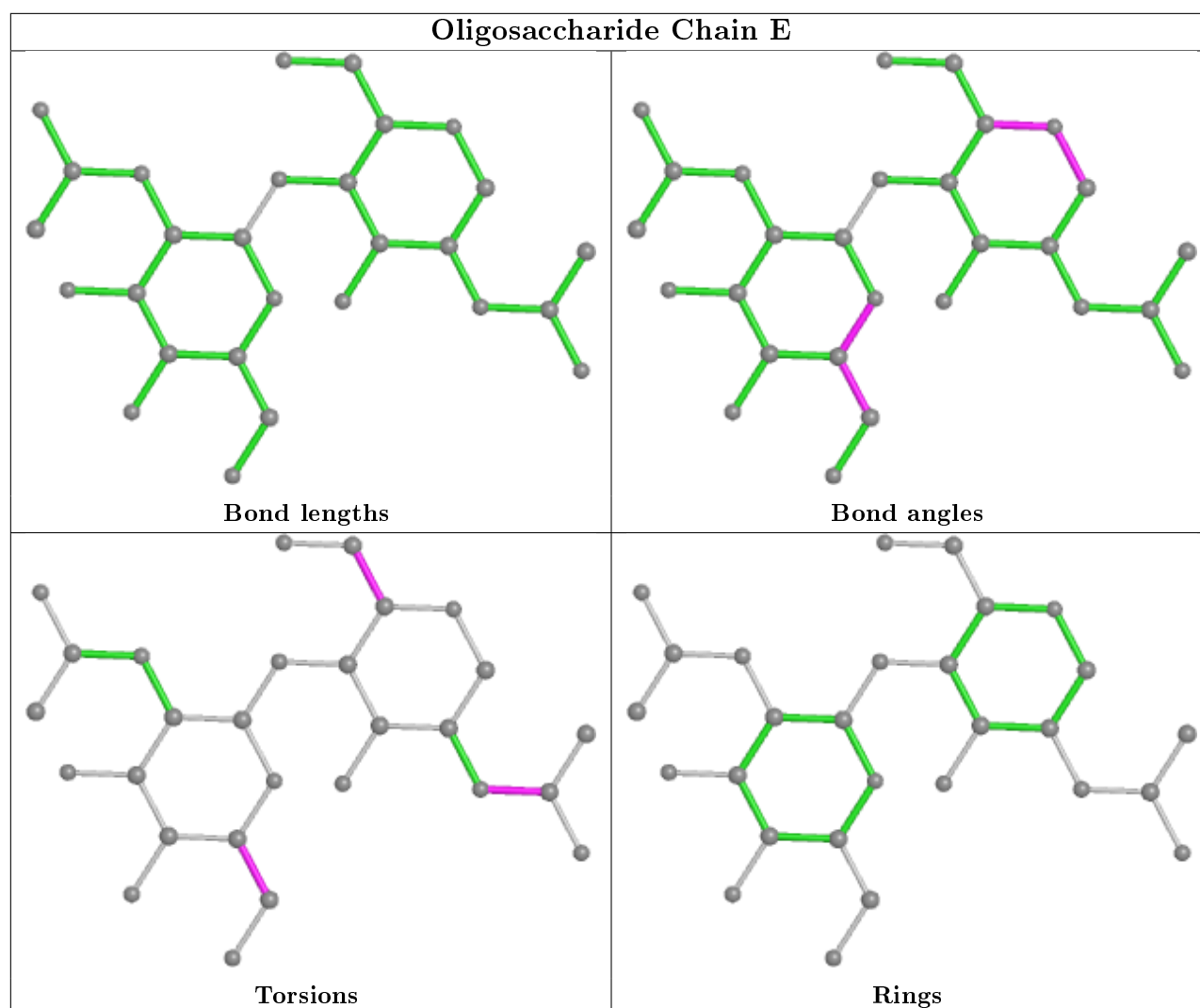
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2

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.





## 5.6 Ligand geometry [i](#)

19 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	PEG	L	303	-	6,6,6	0.43	0	5,5,5	0.33	0
9	PEG	A	516	-	6,6,6	0.78	0	5,5,5	0.54	0
8	SO4	H	304	-	4,4,4	0.13	0	6,6,6	0.23	0
8	SO4	A	514	-	4,4,4	0.13	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	L	301	-	4,4,4	0.12	0	6,6,6	0.21	0
8	SO4	H	302	-	4,4,4	0.22	0	6,6,6	0.23	0
8	SO4	B	203	-	4,4,4	0.22	0	6,6,6	0.43	0
8	SO4	B	204	-	4,4,4	0.22	0	6,6,6	0.41	0
7	NAG	B	201	2	14,14,15	0.53	0	17,19,21	0.98	2 (11%)
8	SO4	A	511	-	4,4,4	0.12	0	6,6,6	0.30	0
9	PEG	L	304	-	6,6,6	0.68	0	5,5,5	0.45	0
8	SO4	A	515	-	4,4,4	0.17	0	6,6,6	0.25	0
8	SO4	B	202	-	4,4,4	0.14	0	6,6,6	0.21	0
7	NAG	A	503	1	14,14,15	0.57	0	17,19,21	2.02	3 (17%)
8	SO4	L	302	-	4,4,4	0.15	0	6,6,6	0.13	0
8	SO4	H	303	-	4,4,4	0.12	0	6,6,6	0.20	0
8	SO4	A	512	-	4,4,4	0.15	0	6,6,6	0.24	0
8	SO4	H	301	-	4,4,4	0.11	0	6,6,6	0.27	0
8	SO4	A	513	-	4,4,4	0.15	0	6,6,6	0.04	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	PEG	L	304	-	-	1/4/4/4	-
9	PEG	L	303	-	-	0/4/4/4	-
9	PEG	A	516	-	-	1/4/4/4	-
7	NAG	B	201	2	-	1/6/23/26	0/1/1/1
7	NAG	A	503	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	503	NAG	C1-O5-C5	6.78	121.37	112.19
7	A	503	NAG	O5-C5-C6	-2.89	102.67	107.20
7	B	201	NAG	O5-C5-C6	2.11	110.51	107.20
7	B	201	NAG	C1-C2-N2	-2.05	106.98	110.49
7	A	503	NAG	O4-C4-C5	2.05	114.38	109.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	516	PEG	O2-C3-C4-O4
9	L	304	PEG	C4-C3-O2-C2
7	B	201	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	515	SO4	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/323 (98%)	-0.10	0 100 100	20, 38, 59, 85	0
2	B	172/176 (97%)	-0.01	1 (0%) 89 92	16, 27, 53, 95	0
3	L	213/216 (98%)	1.32	67 (31%) 0 0	36, 85, 151, 170	0
4	H	223/240 (92%)	0.55	22 (9%) 7 8	31, 63, 135, 169	0
All	All	925/955 (96%)	0.40	90 (9%) 7 8	16, 43, 130, 170	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	193	CYS	7.1
3	L	132	LEU	6.0
3	L	146	VAL	5.8
3	L	117	LEU	5.4
3	L	157	ALA	5.3

### 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<sup>th</sup> 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.

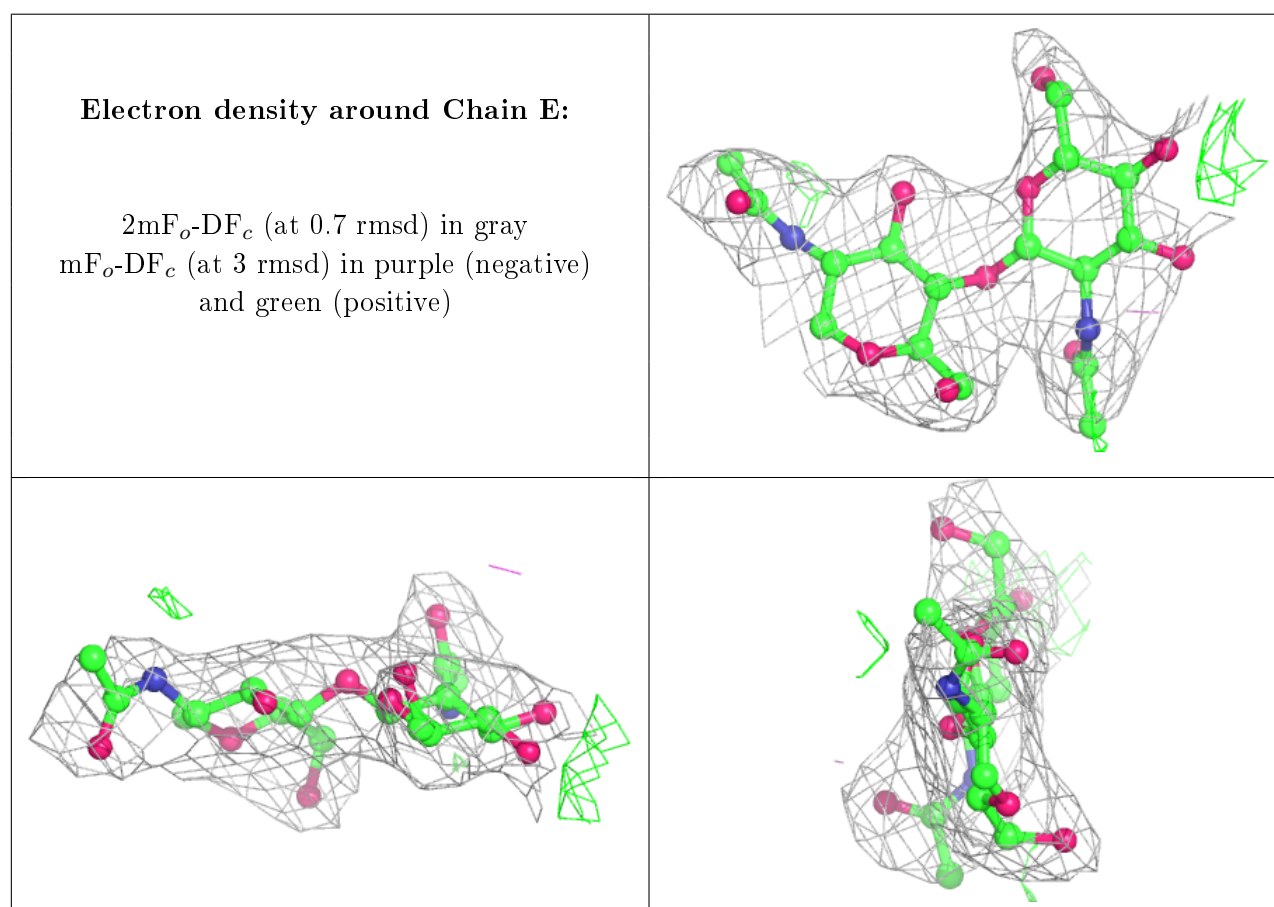
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	C	2	14/15	0.70	0.34	98,112,120,124	0
6	MAN	D	4	11/12	0.79	0.25	111,117,122,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	1	14/15	0.81	0.20	71,80,91,96	0
6	MAN	D	5	11/12	0.87	0.23	106,116,121,124	0
6	BMA	D	3	11/12	0.87	0.13	82,95,104,111	0
5	NAG	E	2	14/15	0.89	0.17	66,95,99,101	0
5	NAG	E	1	14/15	0.95	0.14	42,52,67,72	0
6	NAG	D	2	14/15	0.96	0.15	49,55,67,70	0
6	NAG	D	1	14/15	0.97	0.16	41,51,63,64	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.



## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	SO4	H	304	5/5	0.81	0.26	117,119,122,122	0
7	NAG	B	201	14/15	0.85	0.31	81,97,111,112	0
8	SO4	A	512	5/5	0.86	0.22	108,109,110,111	0
8	SO4	L	302	5/5	0.87	0.20	119,122,123,125	0
9	PEG	L	304	7/7	0.87	0.23	56,68,73,74	0
8	SO4	B	204	5/5	0.88	0.27	83,93,98,99	0
9	PEG	A	516	7/7	0.90	0.18	30,45,50,53	0
8	SO4	H	301	5/5	0.90	0.18	97,97,103,106	0
8	SO4	A	513	5/5	0.91	0.23	122,122,125,126	0
8	SO4	A	511	5/5	0.92	0.33	104,107,110,111	0
8	SO4	A	514	5/5	0.92	0.36	141,142,142,143	0
8	SO4	H	303	5/5	0.92	0.17	103,103,105,109	0
8	SO4	H	302	5/5	0.93	0.24	83,87,89,92	0
9	PEG	L	303	7/7	0.94	0.21	59,60,71,73	0
8	SO4	A	515	5/5	0.94	0.12	76,78,82,83	0
7	NAG	A	503	14/15	0.96	0.15	45,51,60,60	0
8	SO4	L	301	5/5	0.97	0.13	80,81,83,83	0
8	SO4	B	203	5/5	0.98	0.13	30,36,45,56	0
8	SO4	B	202	5/5	0.98	0.14	56,61,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.