



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:45 PM BST

PDB ID : 3IYW  
EMDB ID: : EMD-5190  
Title : West Nile virus in complex with Fab fragments of MAb CR4354 (fitted coordinates of envelope proteins and Fab fragments of one icosahedral ASU)  
Authors : Rossmann, M.G.; Kaufmann, B.  
Deposited on : 2010-06-18  
Resolution : 13.70 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

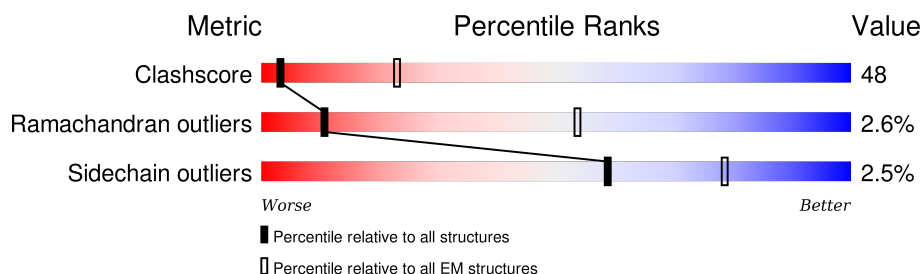
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.70 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	403	<div> <div>35%</div> <div>59%</div> <div>5% •</div> </div>
1	B	403	<div> <div>35%</div> <div>58%</div> <div>5% •</div> </div>
1	C	403	<div> <div>34%</div> <div>60%</div> <div>5% •</div> </div>
2	H	230	<div> <div>83%</div> <div>17%</div> </div>
2	K	230	<div> <div>81%</div> <div>18%</div> </div>
3	L	220	<div> <div>89%</div> <div>11%</div> </div>
3	M	220	<div> <div>90%</div> <div>10%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16202 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	400	Total	C	N	O	S	0	0
			3030	1908	519	581	22		
1	B	400	Total	C	N	O	S	0	0
			3030	1908	519	581	22		
1	C	400	Total	C	N	O	S	0	0
			3030	1908	519	581	22		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	NDG	-	EXPRESSION TAG	UNP Q9Q6P4
A	402	NDG	-	EXPRESSION TAG	UNP Q9Q6P4
A	403	FUL	-	EXPRESSION TAG	UNP Q9Q6P4
B	401	NDG	-	EXPRESSION TAG	UNP Q9Q6P4
B	402	NDG	-	EXPRESSION TAG	UNP Q9Q6P4
B	403	FUL	-	EXPRESSION TAG	UNP Q9Q6P4
C	401	NDG	-	EXPRESSION TAG	UNP Q9Q6P4
C	402	NDG	-	EXPRESSION TAG	UNP Q9Q6P4
C	403	FUL	-	EXPRESSION TAG	UNP Q9Q6P4

- Molecule 2 is a protein called CR4354 Fab fragment X1, heavy chain H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	230	Total	C	N	O	S	24	0
			1850	1172	309	356	13		
2	K	230	Total	C	N	O	S	24	0
			1850	1172	309	356	13		

- Molecule 3 is a protein called CR4354 Fab fragment X1, light chain L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	220	Total	C	N	O	S	9	0
			1649	1027	275	342	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	220	Total	C	N	O	S	9	0
			1649	1027	275	342	5		

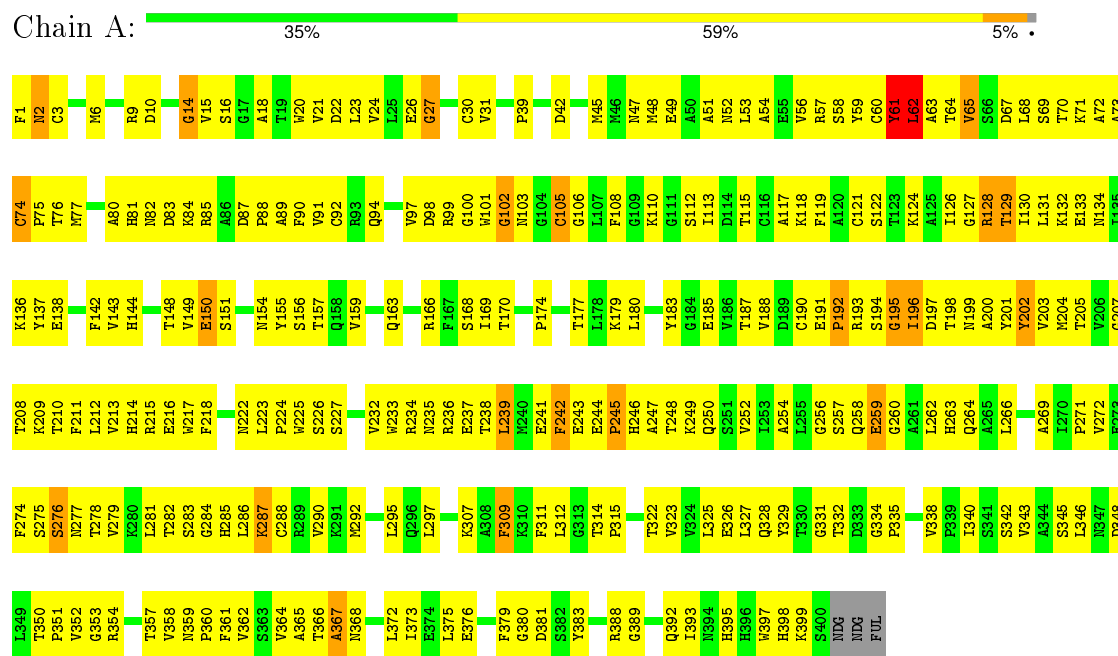
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				AltConf
4	A	3	Total	C	N	O	0
			38	22	2	14	
4	B	3	Total	C	N	O	0
			38	22	2	14	
4	C	3	Total	C	N	O	0
			38	22	2	14	

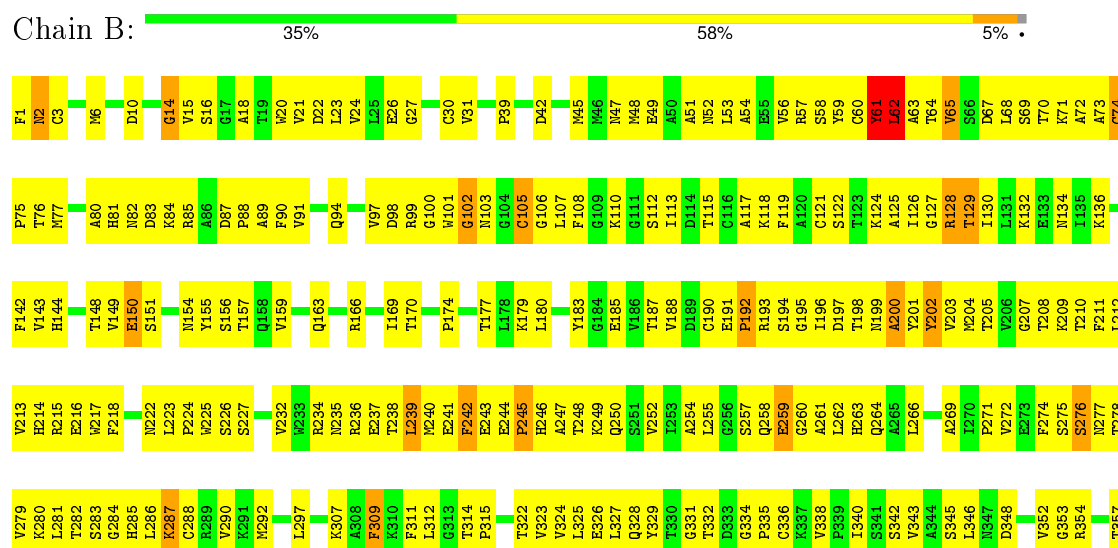
### 3 Residue-property plots

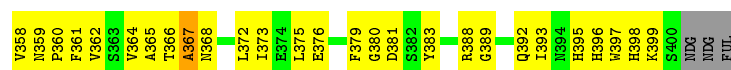
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Polyprotein



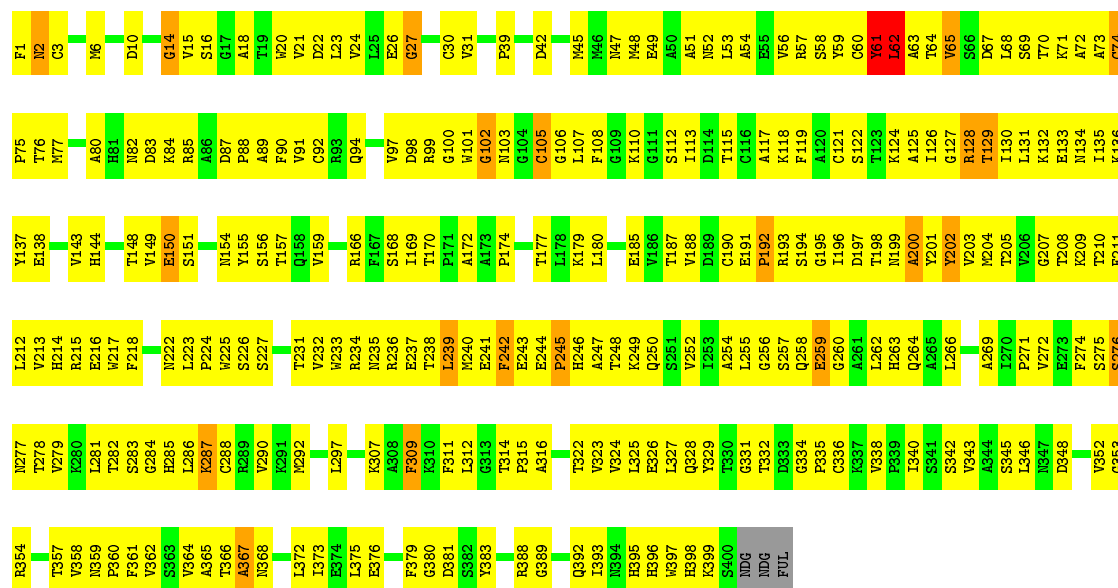
#### • Molecule 1: Polyprotein





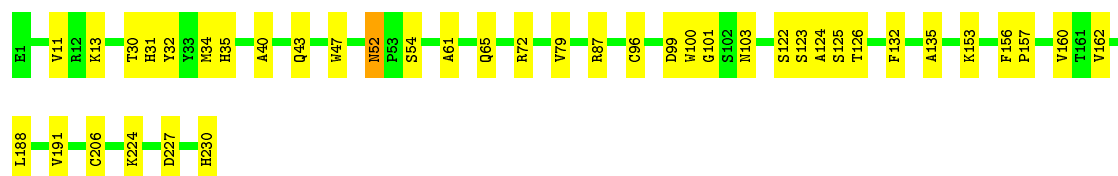
• Molecule 1: Polyprotein

Chain C: 34% 60% 5%



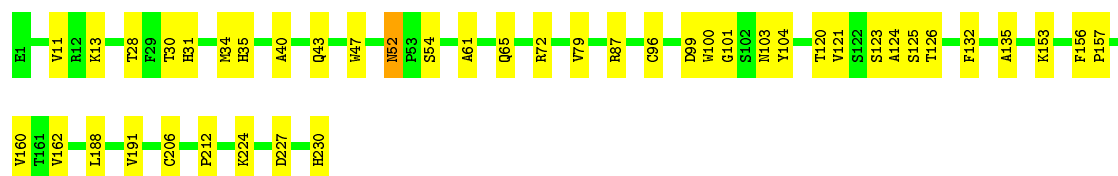
• Molecule 2: CR4354 Fab fragment X1, heavy chain H

Chain H: 83% 17%



• Molecule 2: CR4354 Fab fragment X1, heavy chain H

Chain K: 81% 18%

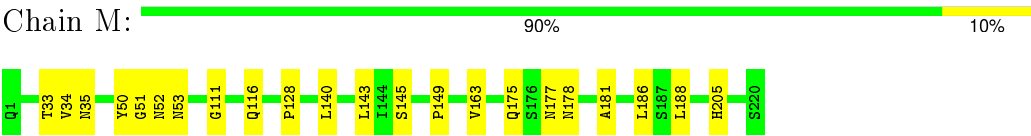


• Molecule 3: CR4354 Fab fragment X1, light chain L

Chain L: 89% 11%



- Molecule 3: CR4354 Fab fragment X1, light chain L



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FCS at 0.5 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	22	Depositor
Minimum defocus (nm)	1450	Depositor
Maximum defocus (nm)	3530	Depositor
Magnification	45000	Depositor
Image detector	Kodak SO163 film	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, PCA, NDG

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.65	1/3092 (0.0%)	1.22	6/4193 (0.1%)
1	B	0.39	0/3091	0.74	3/4190 (0.1%)
1	C	0.39	0/3091	0.74	3/4190 (0.1%)
2	H	0.35	0/1959	0.56	0/2661
2	K	0.35	0/1959	0.56	0/2661
3	L	0.32	0/1712	0.54	0/2334
3	M	0.32	0/1712	0.54	0/2334
All	All	0.43	1/16616 (0.0%)	0.78	12/22563 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	GLY	C-N	28.70	2.00	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	GLY	CA-C-N	-46.34	15.26	117.20
1	A	195	GLY	C-N-CA	-41.68	17.49	121.70
1	A	195	GLY	O-C-N	7.06	134.00	122.70
1	C	61	TYR	N-CA-C	-6.72	92.84	111.00
1	B	61	TYR	N-CA-C	-6.72	92.85	111.00

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	3030	0	2976	419	0
1	B	3030	0	2968	529	0
1	C	3030	0	2966	570	0
2	H	1850	0	1858	99	0
2	K	1850	0	1862	160	0
3	L	1649	0	1620	32	0
3	M	1649	0	1620	18	0
4	A	38	0	34	5	0
4	B	38	0	34	5	0
4	C	38	0	34	5	0
All	All	16202	0	15972	1535	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 48.

The worst 5 of 1535 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:C:136:LYS:HD3	2:K:31:HIS:CA	1.26	1.58
1:B:263:HIS:CB	1:C:258:GLN:HG3	1.23	1.56
2:K:11:VAL:CG2	2:K:157:PRO:HG3	1.13	1.55
2:H:11:VAL:CG2	2:H:157:PRO:HG3	1.36	1.54
1:A:136:LYS:CD	2:H:31:HIS:HA	1.29	1.54

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	392/403 (97%)	328 (84%)	46 (12%)	18 (5%)	3	33
1	B	390/403 (97%)	327 (84%)	45 (12%)	18 (5%)	3	33
1	C	390/403 (97%)	327 (84%)	45 (12%)	18 (5%)	3	33
2	H	249/230 (108%)	246 (99%)	3 (1%)	0	100	100
2	K	249/230 (108%)	246 (99%)	3 (1%)	0	100	100
3	L	225/220 (102%)	217 (96%)	8 (4%)	0	100	100
3	M	225/220 (102%)	217 (96%)	8 (4%)	0	100	100
All	All	2120/2109 (100%)	1908 (90%)	158 (8%)	54 (2%)	11	46

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ILE
1	A	227	SER
1	A	276	SER
1	A	367	ALA
1	B	227	SER

### 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 PDB entries followed by that with respect to all EM entries.

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	331/331 (100%)	320 (97%)	11 (3%)	45	76
1	B	331/331 (100%)	320 (97%)	11 (3%)	45	76
1	C	331/331 (100%)	320 (97%)	11 (3%)	45	76
2	H	219/195 (112%)	215 (98%)	4 (2%)	66	87
2	K	219/195 (112%)	215 (98%)	4 (2%)	66	87
3	L	190/181 (105%)	188 (99%)	2 (1%)	80	91
3	M	190/181 (105%)	188 (99%)	2 (1%)	80	91
All	All	1811/1745 (104%)	1766 (98%)	45 (2%)	59	81

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	287	LYS
1	C	74	CYS
2	K	87[A]	ARG
1	C	2	ASN
1	C	128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	152	HIS
2	H	35	HIS
3	M	53	ASN
1	C	328	GLN
2	H	52	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	PCA	H	1	2	7,8,9	1.50	1 (14%)	9,10,12	1.64	3 (33%)
2	PCA	K	1	2	7,8,9	1.51	1 (14%)	9,10,12	1.64	3 (33%)

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	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	K	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	3.84	1.45	1.33
2	K	1	PCA	CD-N	3.86	1.45	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	PCA	CA-N-CD	-2.52	104.57	113.53
2	H	1	PCA	CA-N-CD	-2.51	104.58	113.53
2	K	1	PCA	O-C-CA	-2.04	120.12	125.69
2	H	1	PCA	O-C-CA	-2.03	120.13	125.69
2	H	1	PCA	CB-CA-N	2.23	110.11	103.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

9 carbohydrates 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	NDG	A	409	4	14,14,15	0.58	0	15,19,21	1.10	2 (13%)
4	NDG	A	410	4	14,14,15	0.62	0	15,19,21	0.95	1 (6%)
4	FUL	A	411	4	10,10,11	0.66	0	13,14,16	0.55	0
4	NDG	B	409	4	14,14,15	0.58	0	15,19,21	1.10	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NDG	B	410	4	14,14,15	0.62	0	15,19,21	0.95	1 (6%)
4	FUL	B	411	4	10,10,11	0.65	0	13,14,16	0.55	0
4	NDG	C	409	4	14,14,15	0.58	0	15,19,21	1.11	2 (13%)
4	NDG	C	410	4	14,14,15	0.62	0	15,19,21	0.96	1 (6%)
4	FUL	C	411	4	10,10,11	0.66	0	13,14,16	0.55	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	NDG	A	409	4	-	0/6/23/26	0/1/1/1
4	NDG	A	410	4	-	1/6/23/26	0/1/1/1
4	FUL	A	411	4	-	0/0/17/20	0/1/1/1
4	NDG	B	409	4	-	0/6/23/26	0/1/1/1
4	NDG	B	410	4	-	1/6/23/26	0/1/1/1
4	FUL	B	411	4	-	0/0/17/20	0/1/1/1
4	NDG	C	409	4	-	0/6/23/26	0/1/1/1
4	NDG	C	410	4	-	1/6/23/26	0/1/1/1
4	FUL	C	411	4	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	410	NDG	C2-N2-C7	-2.66	119.65	123.11
4	B	410	NDG	C2-N2-C7	-2.65	119.66	123.11
4	A	410	NDG	C2-N2-C7	-2.64	119.67	123.11
4	C	409	NDG	C2-N2-C7	-2.60	119.72	123.11
4	A	409	NDG	C2-N2-C7	-2.57	119.76	123.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	410	NDG	O7-C7-N2-C2
4	A	410	NDG	O7-C7-N2-C2
4	B	410	NDG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	409	NDG	5	0
4	A	410	NDG	4	0
4	A	411	FUL	1	0
4	B	409	NDG	5	0
4	B	410	NDG	4	0
4	B	411	FUL	1	0
4	C	409	NDG	5	0
4	C	410	NDG	4	0
4	C	411	FUL	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.