



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:19 AM BST

PDB ID : 6UYM  
Title : Structure of Hepatitis C Virus Envelope Glycoprotein E2mc3-v6 redesigned core from genotype 1a bound to broadly neutralizing antibody AR3C  
Authors : Tzarum, N.; Wilson, I.A.; Zhu, J.  
Deposited on : 2019-11-13  
Resolution : 2.85 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](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

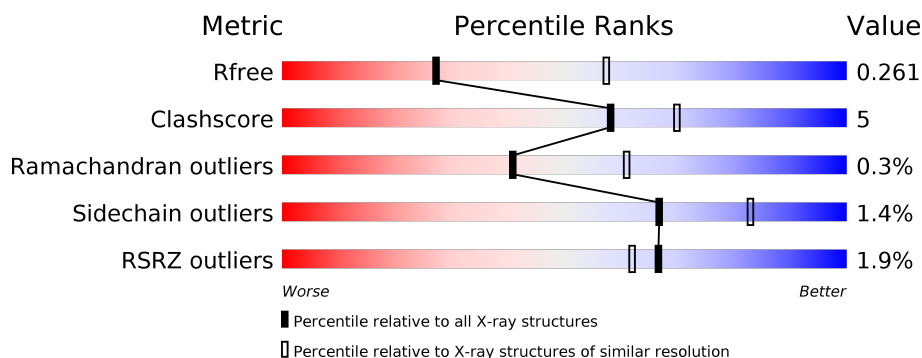
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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.




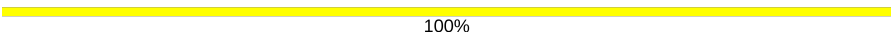
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	E	176	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>18%</div> <div>•</div> <div>18%</div> </div> </div>
1	F	176	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>10%</div> <div>•</div> <div>22%</div> </div> </div>
2	A	233	<div> <div></div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
2	H	233	<div> <div></div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
3	B	214	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>
3	L	214	<div> <div></div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	C	2	
4	D	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	E	701	-	-	-	X
5	NAG	E	703	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8859 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 Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	145	Total	C	N	O	S	0	0	0
			1143	735	192	203	13			
1	F	137	Total	C	N	O	S	0	0	0
			1075	692	181	190	12			

- Molecule 2 is a protein called Fab AR3C heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1650	1039	279	325	7			
2	A	223	Total	C	N	O	S	0	0	0
			1665	1047	282	329	7			

- Molecule 3 is a protein called Fab AR3C light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1612	1005	277	326	4			
3	B	208	Total	C	N	O	S	0	0	0
			1588	992	271	321	4			

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	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:  $C_8H_{15}NO_6$ ).

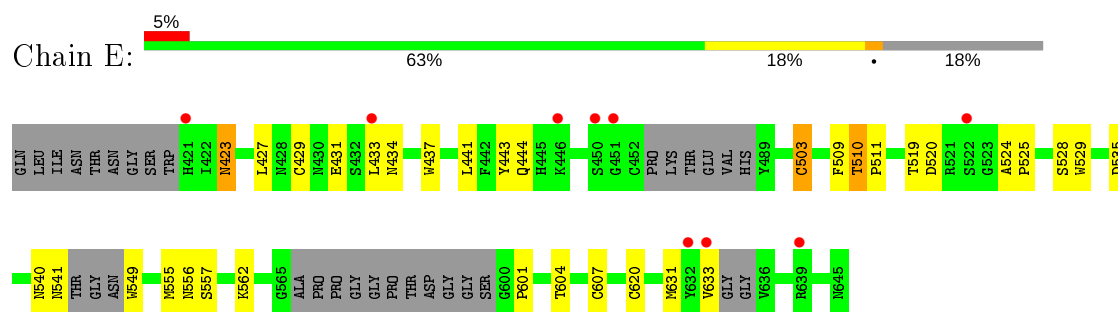


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

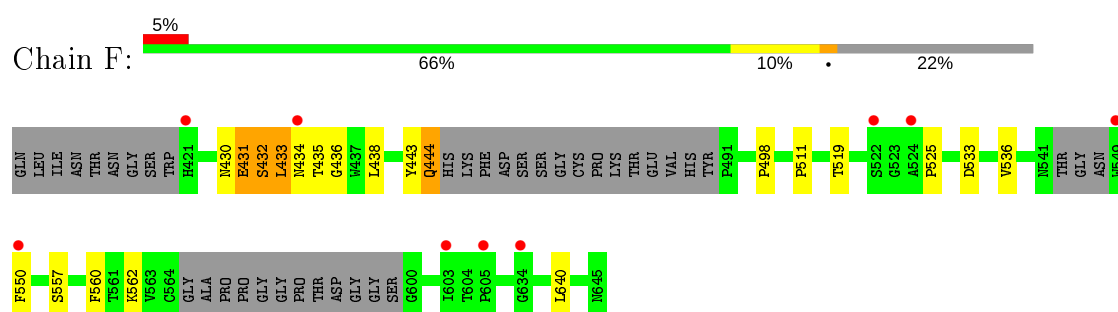
### 3 Residue-property plots

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.

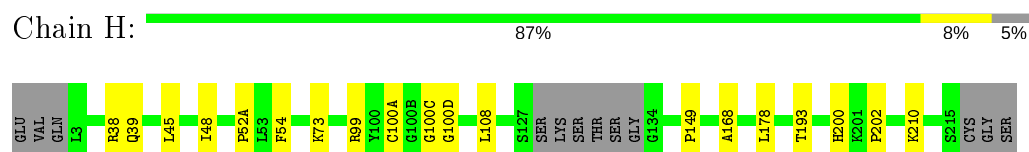
- Molecule 1: Envelope glycoprotein E2



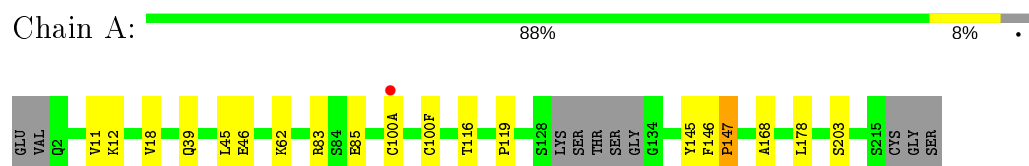
- Molecule 1: Envelope glycoprotein E2




- Molecule 2: Fab AR3C heavy chain



- Molecule 2: Fab AR3C heavy chain




- Molecule 3: Fab AR3C light chain

Chain L:  90% 8%




- Molecule 3: Fab AR3C light chain

Chain B:  % 86% 11%

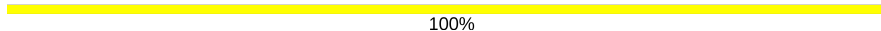


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  50% 50%



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

Chain D:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.10Å 90.84Å 94.03Å 84.50° 78.11° 77.09°	Depositor
Resolution (Å)	29.47 – 2.85 29.47 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.7 (29.47-2.85) 87.7 (29.47-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.214 , 0.260 0.216 , 0.261	Depositor DCC
$R_{free}$ test set	1551 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 21.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	E	0.25	0/1181	0.45	0/1613
1	F	0.25	0/1111	0.45	0/1520
2	A	0.26	0/1704	0.46	0/2318
2	H	0.25	0/1689	0.45	0/2298
3	B	0.24	0/1622	0.45	0/2204
3	L	0.24	0/1646	0.45	0/2235
All	All	0.25	0/8953	0.45	0/12188

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	E	1143	0	1059	21	0
1	F	1075	0	1007	14	0
2	A	1665	0	1619	12	0
2	H	1650	0	1606	12	0
3	B	1588	0	1548	16	0
3	L	1612	0	1570	10	0
4	C	28	0	25	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	28	0	25	5	0
5	E	42	0	39	1	0
5	F	28	0	26	1	0
All	All	8859	0	8524	84	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 5.

All (84) 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:E:510:THR:HG22	1:E:549:TRP:HB3	1.70	0.72
3:L:103:LYS:NZ	3:L:165:GLU:OE2	2.20	0.71
1:F:557:SER:HB2	4:D:1:NAG:H82	1.73	0.71
1:F:562:LYS:NZ	4:D:1:NAG:O6	2.25	0.69
3:B:3:GLU:N	3:B:26:SER:HG	1.91	0.69
1:F:431:GLU:HG2	1:F:434:ASN:HA	1.79	0.65
2:A:83:ARG:NH1	2:A:85:GLU:OE2	2.31	0.62
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.80	0.62
3:B:27:GLN:CB	3:B:93:ARG:HH12	2.13	0.61
3:L:28:SER:O	3:L:93:ARG:NH1	2.32	0.59
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.84	0.58
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.84	0.58
2:A:39:GLN:HB2	2:A:45:LEU:HD23	1.85	0.58
1:F:444:GLN:N	1:F:444:GLN:OE1	2.27	0.57
1:F:430:ASN:HD22	5:F:702:NAG:H83	1.71	0.56
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.86	0.56
1:E:528:SER:OG	1:E:535:ASP:OD2	2.24	0.55
1:E:503:CYS:HB3	1:E:556:ASN:O	2.07	0.55
1:E:511:PRO:HG3	1:E:631:MET:HG2	1.88	0.55
2:A:11:VAL:HG22	2:A:147:PRO:HG3	1.89	0.55
3:B:63:SER:HB3	3:B:74:THR:HB	1.89	0.55
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.89	0.54
1:E:557:SER:HB2	4:C:1:NAG:H82	1.89	0.53
2:A:168:ALA:HA	2:A:178:LEU:HB3	1.91	0.53
3:B:27:GLN:HB2	3:B:93:ARG:HH12	1.73	0.53
2:H:108:LEU:HD23	2:H:149:PRO:HD3	1.91	0.53
3:B:120:PRO:HD3	3:B:132:VAL:HG22	1.90	0.53
1:E:604:THR:HB	1:E:607:CYS:HB2	1.91	0.52
2:H:52(A):PRO:HG2	2:H:73:LYS:HE2	1.92	0.52
3:B:27:GLN:HB2	3:B:93:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:702:NAG:H83	5:E:702:NAG:H3	1.91	0.51
2:H:200:HIS:CD2	2:H:202:PRO:HD2	2.45	0.51
3:B:33:LEU:HD22	3:B:71:PHE:CG	2.46	0.51
1:F:560:PHE:CD2	4:D:1:NAG:H5	2.46	0.50
3:B:145:LYS:HB3	3:B:197:THR:HB	1.93	0.50
2:A:168:ALA:HB2	2:A:178:LEU:HD23	1.94	0.50
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.47	0.50
1:F:560:PHE:CG	4:D:1:NAG:H5	2.47	0.50
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.44	0.48
1:F:431:GLU:OE2	1:F:436:GLY:N	2.36	0.48
1:E:429:CYS:HB2	2:H:100(A):CYS:HB2	1.94	0.48
3:B:27:GLN:CD	3:B:93:ARG:HH12	2.16	0.48
4:C:1:NAG:H61	4:C:2:NAG:H82	1.96	0.48
2:H:168:ALA:HB2	2:H:178:LEU:HD23	1.96	0.47
3:B:37:GLN:HB2	3:B:47:LEU:HD11	1.96	0.47
1:F:498:PRO:HA	1:F:536:VAL:HG12	1.97	0.47
1:E:520:ASP:OD1	1:E:524:ALA:N	2.48	0.46
2:A:119:PRO:HB3	2:A:145:TYR:HB3	1.96	0.46
3:B:14:SER:HA	3:B:107:LYS:HB2	1.98	0.46
1:F:511:PRO:HB3	1:F:550:PHE:CE2	2.51	0.46
1:E:423:ASN:OD1	1:E:423:ASN:N	2.43	0.46
3:B:106:ILE:O	3:B:166:GLN:NE2	2.42	0.45
1:E:427:LEU:HD11	1:E:441:LEU:HD21	1.98	0.45
1:F:560:PHE:CE1	4:D:2:NAG:H82	2.52	0.45
1:E:431:GLU:HG2	1:E:433:LEU:O	2.17	0.45
2:H:100(C):GLY:HA2	2:H:100(D):GLY:HA2	1.54	0.45
2:A:12:LYS:HG3	2:A:18:VAL:HB	1.99	0.45
3:B:92:TYR:CD2	3:B:93:ARG:HG3	2.52	0.45
1:E:431:GLU:HG3	1:E:437:TRP:NE1	2.32	0.44
1:F:511:PRO:HB3	1:F:550:PHE:HE2	1.82	0.44
2:A:116:THR:HG22	2:A:203:SER:HB3	1.99	0.44
3:L:32:ASN:HD22	3:L:92:TYR:HA	1.83	0.44
2:A:100(A):CYS:HA	2:A:100(F):CYS:HA	2.00	0.44
3:B:18:ARG:HH11	3:B:74:THR:HG21	1.82	0.43
1:E:444:GLN:OE1	1:E:444:GLN:HA	2.17	0.43
1:F:519:THR:HG22	1:F:525:PRO:HA	2.01	0.43
1:F:432:SER:OG	1:F:433:LEU:N	2.50	0.43
1:E:511:PRO:HD3	1:E:633:VAL:HG21	2.00	0.43
3:L:24:ARG:HD3	3:L:70:GLU:OE2	2.18	0.43
1:E:519:THR:HG22	1:E:525:PRO:HA	2.01	0.43
1:E:509:PHE:CE1	1:E:601:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:CYS:O	1:E:555:MET:HB3	2.19	0.43
3:B:80:PRO:HA	3:B:106:ILE:HG21	2.00	0.42
1:E:562:LYS:HZ1	4:C:1:NAG:C6	2.27	0.42
3:B:89:GLN:NE2	3:B:96:LEU:HD23	2.34	0.42
2:A:46:GLU:OE2	2:A:62:LYS:HD3	2.20	0.42
1:E:557:SER:CB	4:C:1:NAG:H82	2.49	0.42
2:A:85:GLU:N	2:A:85:GLU:OE1	2.49	0.41
1:E:434:ASN:OD1	2:H:99:ARG:HD2	2.20	0.41
2:H:38:ARG:HB3	2:H:48:ILE:HD11	2.01	0.41
3:L:61:ARG:HH12	3:L:82:ASP:CG	2.24	0.41
2:A:146:PHE:HA	2:A:147:PRO:HA	1.83	0.40
1:E:529:TRP:CH2	2:H:54:PHE:HB3	2.56	0.40
3:L:18:ARG:NH1	3:L:76:SER:OG	2.55	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	E	135/176 (77%)	126 (93%)	8 (6%)	1 (1%)	22	42
1	F	129/176 (73%)	120 (93%)	8 (6%)	1 (1%)	19	38
2	A	219/233 (94%)	216 (99%)	2 (1%)	1 (0%)	29	51
2	H	217/233 (93%)	212 (98%)	5 (2%)	0	100	100
3	B	206/214 (96%)	198 (96%)	8 (4%)	0	100	100
3	L	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
All	All	1115/1246 (90%)	1072 (96%)	40 (4%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	432	SER
1	E	510	THR
2	A	147	PRO

### 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	E	126/148 (85%)	120 (95%)	6 (5%)	25	49
1	F	118/148 (80%)	110 (93%)	8 (7%)	16	31
2	A	187/195 (96%)	187 (100%)	0	100	100
2	H	185/195 (95%)	185 (100%)	0	100	100
3	B	179/184 (97%)	179 (100%)	0	100	100
3	L	181/184 (98%)	181 (100%)	0	100	100
All	All	976/1054 (93%)	962 (99%)	14 (1%)	67	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	423	ASN
1	E	443	TYR
1	E	503	CYS
1	E	540	ASN
1	E	541	ASN
1	E	620	CYS
1	F	431	GLU
1	F	433	LEU
1	F	435	THR
1	F	438	LEU
1	F	443	TYR
1	F	444	GLN
1	F	533	ASP
1	F	640	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 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 ⓘ

4 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	C	1	1,4	14,14,15	1.25	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	C	2	4	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	D	1	1,4	14,14,15	0.46	0	17,19,21	0.57	0
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.44	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	C	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	-4.59	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C3-C4-C5	3.11	115.79	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	C1-C2-N2-C7
4	C	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	C	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NAG	1	0
4	D	1	NAG	4	0
4	C	1	NAG	4	0
4	C	2	NAG	1	0

## 5.6 Ligand geometry [i](#)

5 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	F	701	1	14,14,15	0.44	0	17,19,21	0.38	0
5	NAG	E	702	1	14,14,15	0.46	0	17,19,21	1.30	2 (11%)
5	NAG	F	702	1	14,14,15	0.37	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	701	1	14,14,15	0.62	0	17,19,21	0.64	1 (5%)
5	NAG	E	703	1	14,14,15	0.48	0	17,19,21	0.57	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	F	701	1	-	4/6/23/26	0/1/1/1
5	NAG	E	702	1	-	5/6/23/26	0/1/1/1
5	NAG	F	702	1	-	4/6/23/26	0/1/1/1
5	NAG	E	701	1	-	2/6/23/26	0/1/1/1
5	NAG	E	703	1	-	4/6/23/26	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(°)	Ideal(°)
5	E	702	NAG	C2-N2-C7	4.27	128.99	122.90
5	E	702	NAG	C1-C2-N2	2.20	114.25	110.49
5	E	701	NAG	C1-O5-C5	2.13	115.07	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	702	NAG	O5-C5-C6-O6
5	F	701	NAG	O5-C5-C6-O6
5	E	702	NAG	C4-C5-C6-O6
5	F	702	NAG	O5-C5-C6-O6
5	E	703	NAG	O5-C5-C6-O6
5	F	702	NAG	C4-C5-C6-O6
5	E	703	NAG	C4-C5-C6-O6
5	F	701	NAG	C4-C5-C6-O6
5	F	702	NAG	C8-C7-N2-C2
5	F	702	NAG	O7-C7-N2-C2
5	E	702	NAG	C8-C7-N2-C2
5	E	702	NAG	O7-C7-N2-C2
5	F	701	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	E	701	NAG	C1-C2-N2-C7
5	E	703	NAG	C1-C2-N2-C7
5	E	702	NAG	C3-C2-N2-C7
5	F	701	NAG	C3-C2-N2-C7
5	E	701	NAG	C3-C2-N2-C7
5	E	703	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	702	NAG	1	0
5	F	702	NAG	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	E	145/176 (82%)	0.28	9 (6%) 20 15	30, 67, 105, 126	0
1	F	137/176 (77%)	0.47	9 (6%) 18 12	45, 73, 98, 107	0
2	A	223/233 (95%)	-0.23	1 (0%) 92 91	40, 55, 77, 94	0
2	H	221/233 (94%)	-0.20	0 100 100	41, 61, 82, 97	0
3	B	208/214 (97%)	-0.05	3 (1%) 75 71	46, 67, 86, 94	0
3	L	211/214 (98%)	-0.14	0 100 100	45, 67, 86, 96	0
All	All	1145/1246 (91%)	-0.03	22 (1%) 66 62	30, 63, 90, 126	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	550	PHE	4.3
1	E	450	SER	4.2
1	F	421	HIS	4.0
1	F	605	PRO	2.8
1	E	451	GLY	2.8
1	E	639	ARG	2.7
1	E	421	HIS	2.7
1	E	446	LYS	2.7
3	B	187	GLU	2.6
1	F	603	ILE	2.6
1	F	434	ASN	2.6
3	B	188	LYS	2.6
1	F	522	SER	2.6
1	F	524	ALA	2.4
1	E	433	LEU	2.3
2	A	100(A)	CYS	2.2
1	E	522	SER	2.1
1	E	633	VAL	2.1
3	B	184	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	632	TYR	2.1
1	F	634	GLY	2.0
1	F	549	TRP	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, 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
4	NAG	D	2	14/15	0.70	0.36	109,119,131,137	0
4	NAG	C	2	14/15	0.73	0.30	93,111,115,116	0
4	NAG	C	1	14/15	0.83	0.23	72,83,98,104	0
4	NAG	D	1	14/15	0.85	0.16	77,90,96,108	0

## 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, 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	E	701	14/15	0.63	0.41	105,113,120,132	0
5	NAG	E	703	14/15	0.74	0.49	111,123,128,131	0
5	NAG	F	702	14/15	0.82	0.27	78,90,98,104	0
5	NAG	F	701	14/15	0.85	0.30	97,108,114,114	0
5	NAG	E	702	14/15	0.87	0.26	79,92,98,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.