



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2017 – 12:04 AM EDT

PDB ID : 4XLW  
Title : Complex of Notch1 (EGF11-13) bound to Delta-like 4 (N-EGF2)  
Authors : Luca, V.C.; Jude, K.M.; Garcia, K.C.  
Deposited on : unknown  
Resolution : 3.39 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

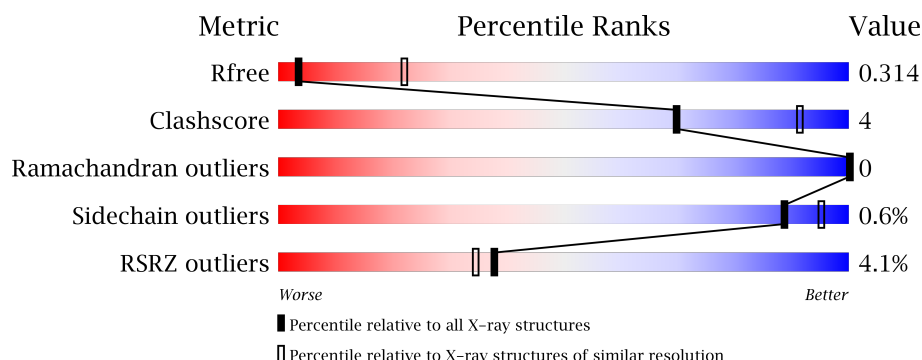
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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.



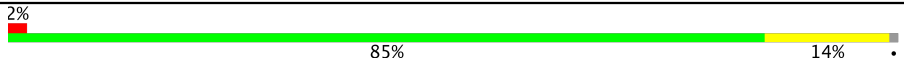
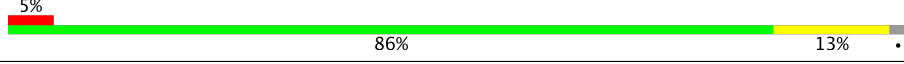
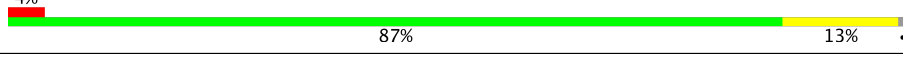
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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. 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	124	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
1	C	124	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	E	124	<div> <div>6%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	G	124	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
2	B	261	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	261	 2% 85% 14% .
2	F	261	 5% 86% 13% .
2	H	261	 4% 87% 13% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11773 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 Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			834	503	141	171	19			
1	C	118	Total	C	N	O	S	0	0	0
			872	525	149	179	19			
1	E	117	Total	C	N	O	S	0	0	0
			863	520	148	176	19			
1	G	117	Total	C	N	O	S	0	0	0
			863	520	148	176	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	SER	-	expression tag	UNP Q07008
A	528	GLY	-	expression tag	UNP Q07008
A	529	ARG	-	expression tag	UNP Q07008
A	530	LEU	-	expression tag	UNP Q07008
A	531	GLU	-	expression tag	UNP Q07008
A	532	VAL	-	expression tag	UNP Q07008
A	533	LEU	-	expression tag	UNP Q07008
A	534	PHE	-	expression tag	UNP Q07008
A	535	GLN	-	expression tag	UNP Q07008
C	527	SER	-	expression tag	UNP Q07008
C	528	GLY	-	expression tag	UNP Q07008
C	529	ARG	-	expression tag	UNP Q07008
C	530	LEU	-	expression tag	UNP Q07008
C	531	GLU	-	expression tag	UNP Q07008
C	532	VAL	-	expression tag	UNP Q07008
C	533	LEU	-	expression tag	UNP Q07008
C	534	PHE	-	expression tag	UNP Q07008
C	535	GLN	-	expression tag	UNP Q07008
E	527	SER	-	expression tag	UNP Q07008
E	528	GLY	-	expression tag	UNP Q07008
E	529	ARG	-	expression tag	UNP Q07008

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Chain	Residue	Modelled	Actual	Comment	Reference
E	530	LEU	-	expression tag	UNP Q07008
E	531	GLU	-	expression tag	UNP Q07008
E	532	VAL	-	expression tag	UNP Q07008
E	533	LEU	-	expression tag	UNP Q07008
E	534	PHE	-	expression tag	UNP Q07008
E	535	GLN	-	expression tag	UNP Q07008
G	527	SER	-	expression tag	UNP Q07008
G	528	GLY	-	expression tag	UNP Q07008
G	529	ARG	-	expression tag	UNP Q07008
G	530	LEU	-	expression tag	UNP Q07008
G	531	GLU	-	expression tag	UNP Q07008
G	532	VAL	-	expression tag	UNP Q07008
G	533	LEU	-	expression tag	UNP Q07008
G	534	PHE	-	expression tag	UNP Q07008
G	535	GLN	-	expression tag	UNP Q07008

- Molecule 2 is a protein called Delta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2012	1251	362	376	23			
2	D	258	Total	C	N	O	S	0	0	0
			2021	1256	363	379	23			
2	F	257	Total	C	N	O	S	0	0	0
			2016	1253	362	378	23			
2	H	259	Total	C	N	O	S	0	0	0
			2026	1259	364	380	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	SER	-	expression tag	UNP D3ZHH1
B	28	SER	GLY	engineered mutation	UNP D3ZHH1
B	107	LEU	PHE	engineered mutation	UNP D3ZHH1
B	206	PRO	LEU	engineered mutation	UNP D3ZHH1
B	257	LYS	ASN	engineered mutation	UNP D3ZHH1
B	284	ALA	-	expression tag	UNP D3ZHH1
B	285	ALA	-	expression tag	UNP D3ZHH1
B	286	ALA	-	expression tag	UNP D3ZHH1
D	26	SER	-	expression tag	UNP D3ZHH1
D	28	SER	GLY	engineered mutation	UNP D3ZHH1
D	107	LEU	PHE	engineered mutation	UNP D3ZHH1

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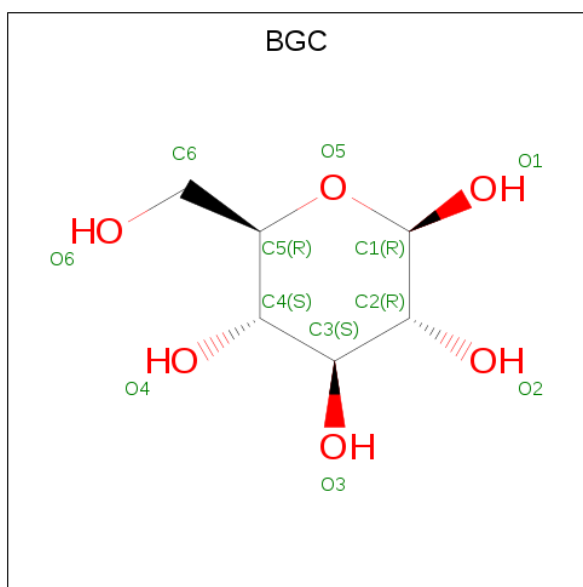
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Chain	Residue	Modelled	Actual	Comment	Reference
D	206	PRO	LEU	engineered mutation	UNP D3ZHH1
D	257	LYS	ASN	engineered mutation	UNP D3ZHH1
D	284	ALA	-	expression tag	UNP D3ZHH1
D	285	ALA	-	expression tag	UNP D3ZHH1
D	286	ALA	-	expression tag	UNP D3ZHH1
F	26	SER	-	expression tag	UNP D3ZHH1
F	28	SER	GLY	engineered mutation	UNP D3ZHH1
F	107	LEU	PHE	engineered mutation	UNP D3ZHH1
F	206	PRO	LEU	engineered mutation	UNP D3ZHH1
F	257	LYS	ASN	engineered mutation	UNP D3ZHH1
F	284	ALA	-	expression tag	UNP D3ZHH1
F	285	ALA	-	expression tag	UNP D3ZHH1
F	286	ALA	-	expression tag	UNP D3ZHH1
H	26	SER	-	expression tag	UNP D3ZHH1
H	28	SER	GLY	engineered mutation	UNP D3ZHH1
H	107	LEU	PHE	engineered mutation	UNP D3ZHH1
H	206	PRO	LEU	engineered mutation	UNP D3ZHH1
H	257	LYS	ASN	engineered mutation	UNP D3ZHH1
H	284	ALA	-	expression tag	UNP D3ZHH1
H	285	ALA	-	expression tag	UNP D3ZHH1
H	286	ALA	-	expression tag	UNP D3ZHH1

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

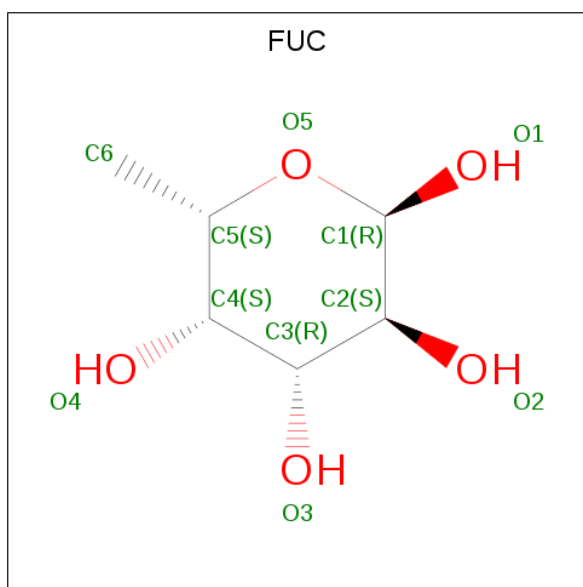
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Ca 2 2	0	0
3	A	3	Total Ca 3 3	0	0
3	C	3	Total Ca 3 3	0	0
3	E	2	Total Ca 2 2	0	0

- Molecule 4 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



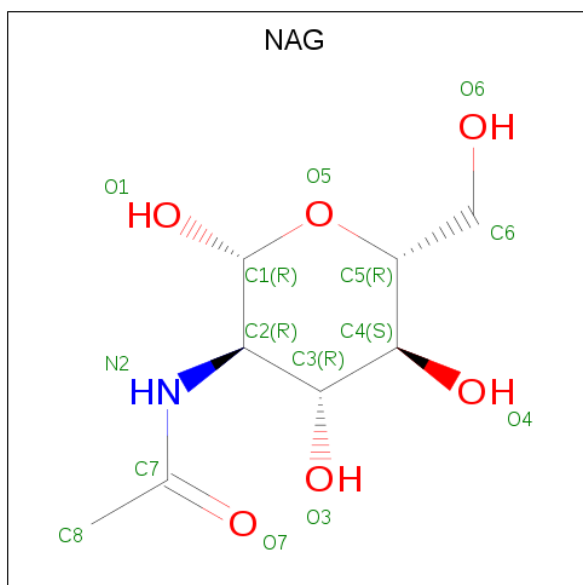
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	E	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		
4	G	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



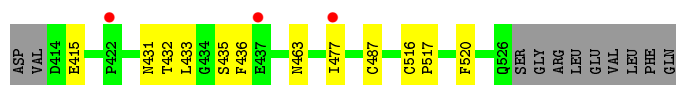
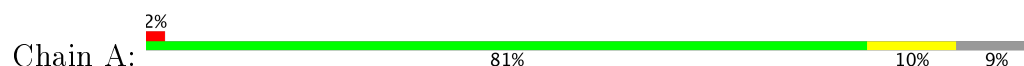


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		

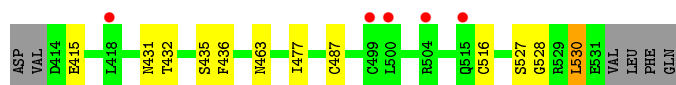
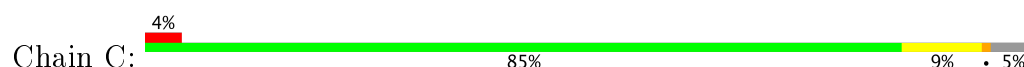
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

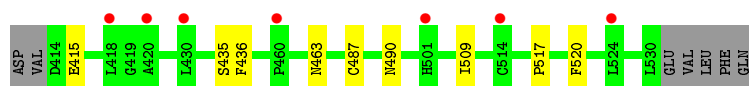
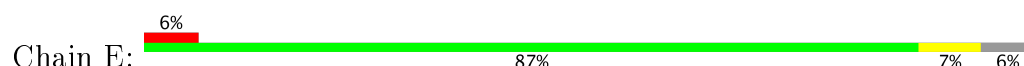
- Molecule 1: Neurogenic locus notch homolog protein 1



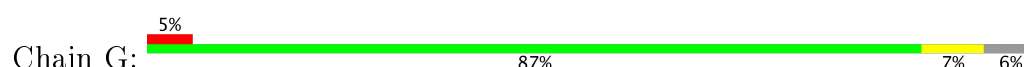
- Molecule 1: Neurogenic locus notch homolog protein 1



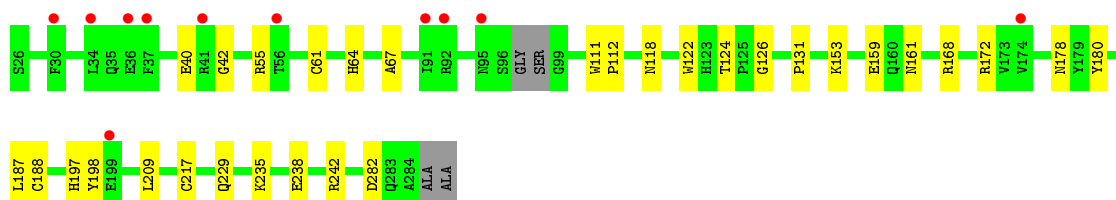
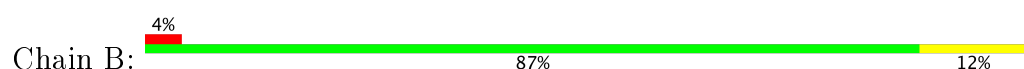
- Molecule 1: Neurogenic locus notch homolog protein 1



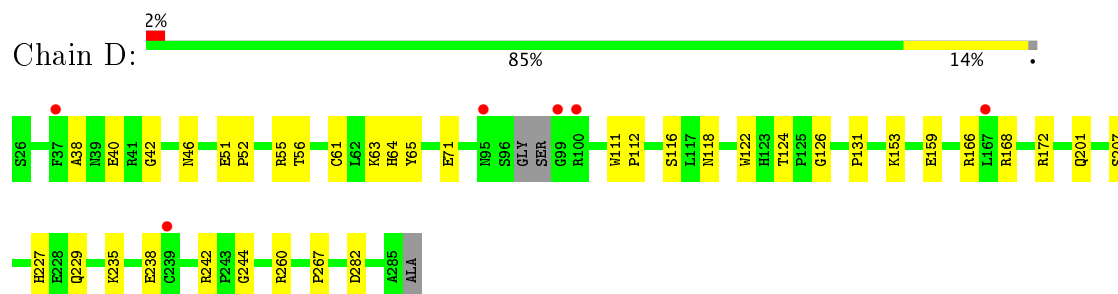
- Molecule 1: Neurogenic locus notch homolog protein 1



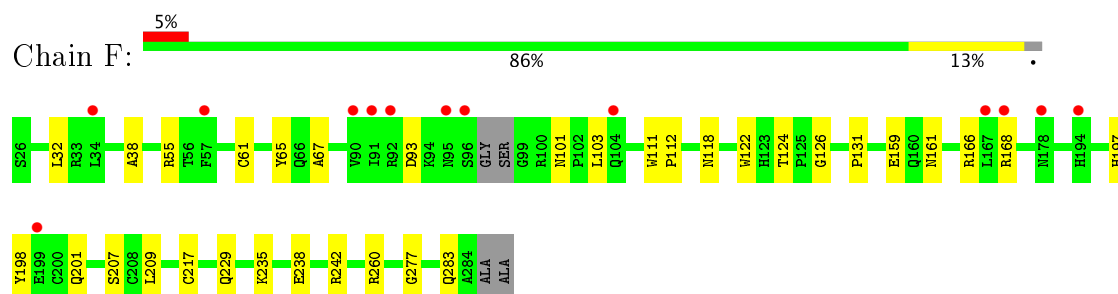
- Molecule 2: Delta-like protein



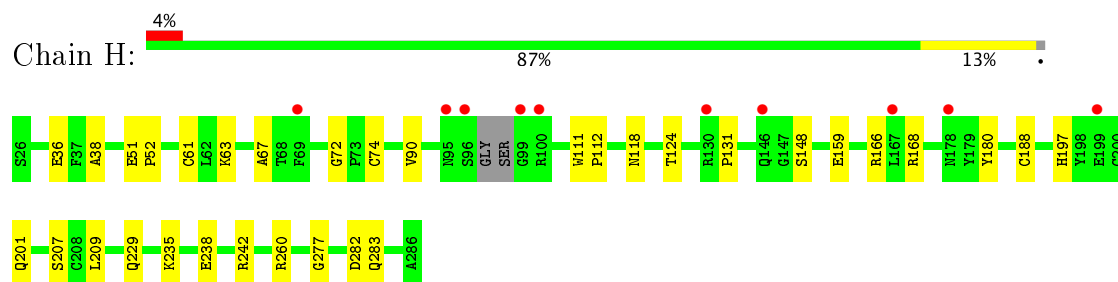
- Molecule 2: Delta-like protein



- Molecule 2: Delta-like protein



- Molecule 2: Delta-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.56 Å 95.57 Å 122.90 Å 90.00° 96.21° 90.00°	Depositor
Resolution (Å)	84.06 – 3.39 84.06 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (84.06-3.39) 99.2 (84.06-3.39)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.41 Å)	Xtriage
Refinement program	PHENIX DEV-1839	Depositor
R, $R_{free}$	0.257 , 0.310 0.259 , 0.314	Depositor DCC
$R_{free}$ test set	1329 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.0	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 74.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5689e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CA, BGC, NAG, MLY, FUC

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	0.23	0/849	0.46	0/1150
1	C	0.22	0/887	0.45	1/1200 (0.1%)
1	E	0.23	0/878	0.43	0/1188
1	G	0.22	0/878	0.42	0/1188
2	B	0.21	0/2014	0.39	0/2739
2	D	0.21	0/2023	0.39	0/2751
2	F	0.21	0/2018	0.39	0/2744
2	H	0.21	0/2028	0.39	0/2758
All	All	0.21	0/11575	0.40	1/15718 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	530	LEU	CA-CB-CG	5.05	126.92	115.30

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	834	0	729	8	0
1	C	872	0	768	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	863	0	762	4	0
1	G	863	0	762	4	0
2	B	2012	0	1864	19	0
2	D	2021	0	1873	24	0
2	F	2016	0	1867	19	0
2	H	2026	0	1877	20	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	2	0	0	0	0
3	G	2	0	0	0	0
4	A	33	0	30	1	0
4	C	33	0	30	0	0
4	E	33	0	30	0	0
4	G	33	0	30	0	0
5	A	10	0	10	0	0
5	C	10	0	10	1	0
5	E	10	0	10	1	0
5	G	10	0	10	1	0
6	B	14	0	13	0	0
6	D	14	0	13	0	0
6	F	28	0	25	0	0
6	H	28	0	25	0	0
All	All	11773	0	10738	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 94 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:431:ASN:OD1	1:A:432:THR:O	1.78	1.01
1:E:435:SER:OG	1:E:436:PHE:N	2.21	0.72
2:D:122:TRP:HH2	2:H:67:ALA:HB1	1.54	0.71
1:A:435:SER:OG	1:A:436:PHE:N	2.24	0.70
1:G:435:SER:OG	1:G:436:PHE:N	2.20	0.69

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 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	111/124 (90%)	102 (92%)	9 (8%)	0	100	100
1	C	116/124 (94%)	103 (89%)	13 (11%)	0	100	100
1	E	115/124 (93%)	108 (94%)	7 (6%)	0	100	100
1	G	115/124 (93%)	108 (94%)	7 (6%)	0	100	100
2	B	248/261 (95%)	231 (93%)	17 (7%)	0	100	100
2	D	249/261 (95%)	229 (92%)	20 (8%)	0	100	100
2	F	248/261 (95%)	229 (92%)	19 (8%)	0	100	100
2	H	250/261 (96%)	232 (93%)	18 (7%)	0	100	100
All	All	1452/1540 (94%)	1342 (92%)	110 (8%)	0	100	100

There are no Ramachandran outliers to report.

### 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	95/107 (89%)	93 (98%)	2 (2%)	59	83
1	C	99/107 (92%)	96 (97%)	3 (3%)	46	78
1	E	98/107 (92%)	97 (99%)	1 (1%)	80	91
1	G	98/107 (92%)	96 (98%)	2 (2%)	60	84
2	B	218/220 (99%)	218 (100%)	0	100	100
2	D	219/220 (100%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	219/220 (100%)	219 (100%)	0	100	100
2	H	219/220 (100%)	219 (100%)	0	100	100
All	All	1265/1308 (97%)	1257 (99%)	8 (1%)	89	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	516	CYS
1	G	516	CYS
1	E	415	GLU
1	C	415	GLU
1	C	530	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 ⓘ

20 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	MLY	B	153	2	10,10,11	0.83	1 (10%)	8,11,13	0.99	0
2	MLY	B	189	2	10,10,11	0.74	0	8,11,13	0.96	0
2	MLY	B	190	2	10,10,11	0.86	1 (10%)	8,11,13	0.85	0
2	MLY	B	215	2	10,10,11	0.78	0	8,11,13	0.91	0
2	MLY	B	235	2	10,10,11	0.87	1 (10%)	8,11,13	1.01	0
2	MLY	D	153	2	10,10,11	0.86	1 (10%)	8,11,13	0.98	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MLY	D	189	2	10,10,11	0.79	1 (10%)	8,11,13	0.95	0
2	MLY	D	190	2	10,10,11	0.91	1 (10%)	8,11,13	0.83	0
2	MLY	D	215	2	10,10,11	0.86	1 (10%)	8,11,13	0.87	0
2	MLY	D	235	2	10,10,11	0.86	1 (10%)	8,11,13	1.02	0
2	MLY	F	153	2	10,10,11	0.81	1 (10%)	8,11,13	1.00	0
2	MLY	F	189	2	10,10,11	0.73	0	8,11,13	0.97	0
2	MLY	F	190	2	10,10,11	0.87	1 (10%)	8,11,13	0.83	0
2	MLY	F	215	2	10,10,11	0.81	1 (10%)	8,11,13	0.89	0
2	MLY	F	235	2	10,10,11	0.85	1 (10%)	8,11,13	1.02	0
2	MLY	H	153	2	10,10,11	0.80	1 (10%)	8,11,13	1.00	0
2	MLY	H	189	2	10,10,11	0.78	0	8,11,13	0.96	0
2	MLY	H	190	2	10,10,11	0.86	1 (10%)	8,11,13	0.85	0
2	MLY	H	215	2	10,10,11	0.81	1 (10%)	8,11,13	0.89	0
2	MLY	H	235	2	10,10,11	0.90	1 (10%)	8,11,13	0.98	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
2	MLY	B	153	2	-	0/7/9/11	0/0/0/0
2	MLY	B	189	2	-	0/7/9/11	0/0/0/0
2	MLY	B	190	2	-	0/7/9/11	0/0/0/0
2	MLY	B	215	2	-	0/7/9/11	0/0/0/0
2	MLY	B	235	2	-	0/7/9/11	0/0/0/0
2	MLY	D	153	2	-	0/7/9/11	0/0/0/0
2	MLY	D	189	2	-	0/7/9/11	0/0/0/0
2	MLY	D	190	2	-	0/7/9/11	0/0/0/0
2	MLY	D	215	2	-	0/7/9/11	0/0/0/0
2	MLY	D	235	2	-	0/7/9/11	0/0/0/0
2	MLY	F	153	2	-	0/7/9/11	0/0/0/0
2	MLY	F	189	2	-	0/7/9/11	0/0/0/0
2	MLY	F	190	2	-	0/7/9/11	0/0/0/0
2	MLY	F	215	2	-	0/7/9/11	0/0/0/0
2	MLY	F	235	2	-	0/7/9/11	0/0/0/0
2	MLY	H	153	2	-	0/7/9/11	0/0/0/0
2	MLY	H	189	2	-	0/7/9/11	0/0/0/0
2	MLY	H	190	2	-	0/7/9/11	0/0/0/0
2	MLY	H	215	2	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	H	235	2	-	0/7/9/11	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	215	MLY	CA-C	2.05	1.52	1.50
2	D	189	MLY	CA-C	2.07	1.53	1.50
2	H	153	MLY	CA-C	2.08	1.53	1.50
2	F	215	MLY	CA-C	2.10	1.53	1.50
2	F	153	MLY	CA-C	2.15	1.53	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	153	MLY	2	0
2	B	235	MLY	1	0
2	D	153	MLY	1	0
2	D	235	MLY	1	0
2	F	235	MLY	1	0
2	H	235	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 for Mogul analysis.

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	BGC	A	604	1	11,11,12	0.28	0	13,15,17	0.61	0
5	FUC	A	605	1	9,10,11	0.67	0	13,14,16	0.73	0
4	BGC	A	606	1	11,11,12	0.34	0	13,15,17	0.73	0
4	BGC	A	607	1	11,11,12	0.27	0	13,15,17	0.64	0
6	NAG	B	301	2	14,14,15	0.24	0	15,19,21	0.57	0
4	BGC	C	601	1	11,11,12	0.30	0	13,15,17	0.54	0
5	FUC	C	602	1	9,10,11	0.75	0	13,14,16	0.69	0
4	BGC	C	603	1	11,11,12	0.34	0	13,15,17	0.83	0
4	BGC	C	604	1	11,11,12	0.29	0	13,15,17	0.82	1 (7%)
6	NAG	D	301	2	14,14,15	0.34	0	15,19,21	0.54	0
4	BGC	E	903	1	11,11,12	0.30	0	13,15,17	0.62	0
5	FUC	E	904	1	9,10,11	0.70	0	13,14,16	0.73	0
4	BGC	E	905	1	11,11,12	0.35	0	13,15,17	0.79	0
4	BGC	E	906	1	11,11,12	0.27	0	13,15,17	0.68	0
6	NAG	F	301	2	14,14,15	0.25	0	15,19,21	0.46	0
6	NAG	F	302	2	14,14,15	0.20	0	15,19,21	0.56	0
4	BGC	G	903	1	11,11,12	0.31	0	13,15,17	0.74	0
5	FUC	G	904	1	9,10,11	0.73	0	13,14,16	0.71	0
4	BGC	G	905	1	11,11,12	0.35	0	13,15,17	0.96	0
4	BGC	G	906	1	11,11,12	0.26	0	13,15,17	0.61	0
6	NAG	H	301	2	14,14,15	0.22	0	15,19,21	0.45	0
6	NAG	H	302	2	14,14,15	0.27	0	15,19,21	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
4	BGC	A	604	1	-	0/2/19/22	0/1/1/1
5	FUC	A	605	1	-	0/0/17/20	0/1/1/1
4	BGC	A	606	1	-	0/2/19/22	0/1/1/1
4	BGC	A	607	1	-	0/2/19/22	0/1/1/1
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
4	BGC	C	601	1	-	0/2/19/22	0/1/1/1
5	FUC	C	602	1	-	0/0/17/20	0/1/1/1
4	BGC	C	603	1	-	0/2/19/22	0/1/1/1
4	BGC	C	604	1	-	0/2/19/22	0/1/1/1
6	NAG	D	301	2	-	0/6/23/26	0/1/1/1
4	BGC	E	903	1	-	0/2/19/22	0/1/1/1
5	FUC	E	904	1	-	0/0/17/20	0/1/1/1
4	BGC	E	905	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	E	906	1	-	0/2/19/22	0/1/1/1
6	NAG	F	301	2	-	0/6/23/26	0/1/1/1
6	NAG	F	302	2	-	0/6/23/26	0/1/1/1
4	BGC	G	903	1	-	0/2/19/22	0/1/1/1
5	FUC	G	904	1	-	0/0/17/20	0/1/1/1
4	BGC	G	905	1	-	0/2/19/22	0/1/1/1
4	BGC	G	906	1	-	0/2/19/22	0/1/1/1
6	NAG	H	301	2	-	0/6/23/26	0/1/1/1
6	NAG	H	302	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	604	BGC	C1-C2-C3	2.19	112.42	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	BGC	1	0
5	C	602	FUC	1	0
5	E	904	FUC	1	0
5	G	904	FUC	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	113/124 (91%)	0.19	3 (2%) 55 51	101, 160, 220, 298	0
1	C	118/124 (95%)	0.14	5 (4%) 37 34	76, 145, 207, 247	0
1	E	117/124 (94%)	0.28	7 (5%) 23 22	119, 174, 225, 243	0
1	G	117/124 (94%)	0.26	6 (5%) 29 26	94, 138, 203, 241	0
2	B	252/261 (96%)	0.24	11 (4%) 35 32	93, 139, 226, 310	0
2	D	253/261 (96%)	0.14	6 (2%) 59 55	60, 117, 175, 271	0
2	F	252/261 (96%)	0.37	13 (5%) 28 26	84, 162, 215, 291	0
2	H	254/261 (97%)	0.15	10 (3%) 40 36	67, 129, 181, 232	0
All	All	1476/1540 (95%)	0.22	61 (4%) 38 34	60, 142, 213, 310	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	95	ASN	5.6
2	H	99	GLY	5.3
2	B	36	GLU	5.2
2	B	37	PHE	4.8
2	F	96	SER	4.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MLY	B	190	11/12	0.76	0.51	-	143,160,186,187	0
2	MLY	D	189	11/12	0.86	0.25	-	102,109,123,127	0
2	MLY	B	189	11/12	0.74	0.52	-	122,132,136,138	0
2	MLY	F	190	11/12	0.81	0.32	-	167,173,177,178	0
2	MLY	F	153	11/12	0.70	0.31	-	155,169,186,188	0
2	MLY	H	190	11/12	0.81	0.39	-	124,132,147,151	0
2	MLY	H	189	11/12	0.78	0.59	-	145,154,164,169	0
2	MLY	D	190	11/12	0.89	0.21	-	113,129,148,149	0
2	MLY	D	235	11/12	0.95	0.36	-	106,118,140,150	0
2	MLY	F	235	11/12	0.88	0.33	-	177,188,198,200	0
2	MLY	H	215	11/12	0.81	0.35	-	141,156,163,164	0
2	MLY	F	215	11/12	0.84	0.52	-	168,178,188,197	0
2	MLY	B	153	11/12	0.89	0.14	-	140,142,149,152	0
2	MLY	D	215	11/12	0.81	0.36	-	136,145,155,160	0
2	MLY	B	235	11/12	0.93	0.34	-	93,107,134,138	0
2	MLY	B	215	11/12	0.90	0.38	-	110,119,134,138	0
2	MLY	H	153	11/12	0.75	0.25	-	132,145,158,158	0
2	MLY	H	235	11/12	0.85	0.38	-	79,121,143,144	0
2	MLY	F	189	11/12	0.82	0.38	-	156,167,184,185	0
2	MLY	D	153	11/12	0.67	0.30	-	109,119,137,139	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	H	301	14/15	0.83	0.30	1.06	101,124,132,137	0
4	BGC	A	606	11/12	0.75	0.28	1.02	136,146,177,181	0
6	NAG	H	302	14/15	0.82	0.22	0.83	94,118,123,129	0
4	BGC	A	607	11/12	0.73	0.31	0.70	180,186,193,194	0
6	NAG	B	301	14/15	0.85	0.23	0.63	115,134,143,151	0
4	BGC	C	603	11/12	0.81	0.25	0.62	100,113,135,137	0
4	BGC	G	905	11/12	0.86	0.25	0.39	100,114,155,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	D	301	14/15	0.80	0.24	0.16	92,112,122,144	0
4	BGC	G	906	11/12	0.85	0.27	-0.02	99,116,130,142	0
4	BGC	E	906	11/12	0.80	0.21	-0.05	103,113,118,121	0
4	BGC	G	903	11/12	0.83	0.25	-0.16	63,91,102,105	0
4	BGC	C	604	11/12	0.79	0.21	-0.18	108,124,129,131	0
4	BGC	C	601	11/12	0.85	0.22	-0.21	81,91,110,115	0
3	CA	G	901	1/1	0.92	0.19	-0.42	123,123,123,123	0
4	BGC	E	905	11/12	0.92	0.20	-0.50	99,116,122,122	0
5	FUC	C	602	10/11	0.95	0.20	-0.71	79,87,111,114	0
5	FUC	A	605	10/11	0.92	0.18	-0.74	107,118,135,143	0
4	BGC	A	604	11/12	0.86	0.22	-0.77	108,113,118,120	0
5	FUC	E	904	10/11	0.91	0.14	-1.10	87,110,121,121	0
3	CA	C	605	1/1	0.73	0.17	-1.23	277,277,277,277	0
3	CA	A	602	1/1	0.84	0.16	-1.31	116,116,116,116	0
4	BGC	E	903	11/12	0.89	0.17	-1.37	95,100,108,108	0
3	CA	C	606	1/1	0.95	0.14	-1.37	102,102,102,102	0
3	CA	G	902	1/1	0.98	0.10	-1.63	188,188,188,188	0
5	FUC	G	904	10/11	0.94	0.14	-1.64	71,80,88,89	0
3	CA	E	901	1/1	0.97	0.12	-1.68	107,107,107,107	0
3	CA	A	601	1/1	0.77	0.13	-1.93	382,382,382,382	0
3	CA	A	603	1/1	0.77	0.09	-2.03	261,261,261,261	0
3	CA	C	607	1/1	0.94	0.09	-2.09	185,185,185,185	0
3	CA	E	902	1/1	0.94	0.07	-2.35	152,152,152,152	0
6	NAG	F	302	14/15	0.85	0.17	-	118,130,140,141	0
6	NAG	F	301	14/15	0.80	0.32	-	114,129,140,145	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.