



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 11:54 AM EST

PDB ID : 7LFR  
Title : Crystal structure of the epidermal growth factor receptor extracellular region with R84K mutation in complex with epiregulin crystallized with spermine  
Authors : Hu, C.; Leche II, C.A.; Stayrook, S.E.; Ferguson, K.M.; Lemmon, M.A.  
Deposited on : 2021-01-18  
Resolution : 3.20 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 : 2.23.2  
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) : 2.23.2

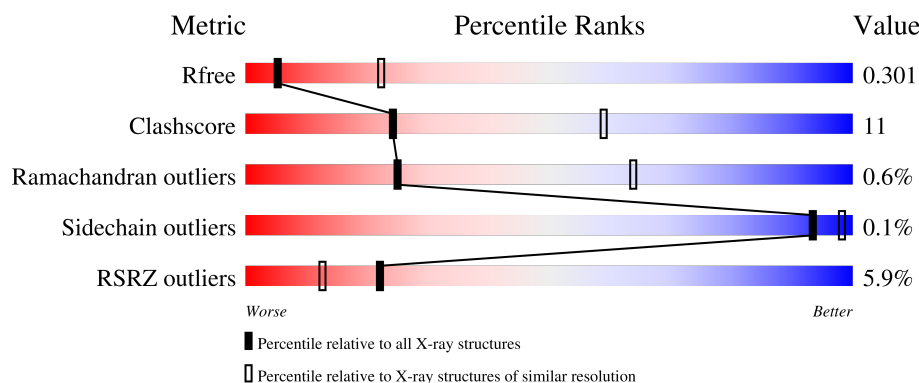
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	502	<div> <div>9%</div> <div>72%</div> <div>28%</div> </div>
1	B	502	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	C	48	<div> <div>8%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	D	48	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>

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
3	BMA	F	2	-	-	X	-
4	NAG	A	601	-	-	X	X
5	MAN	A	602	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8418 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			3773	2338	664	729	42			
1	B	499	Total	C	N	O	S	0	0	0
			3785	2345	661	737	42			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	LYS	ARG	engineered mutation	UNP P00533
A	502	HIS	-	expression tag	UNP P00533
B	84	LYS	ARG	engineered mutation	UNP P00533
B	502	HIS	-	expression tag	UNP P00533

- Molecule 2 is a protein called Proepiregulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	47	Total	C	N	O	S	0	0	0
			362	222	62	70	8			
2	D	47	Total	C	N	O	S	0	0	0
			370	230	62	70	8			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O		0	0	0
			25	14	1	10				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



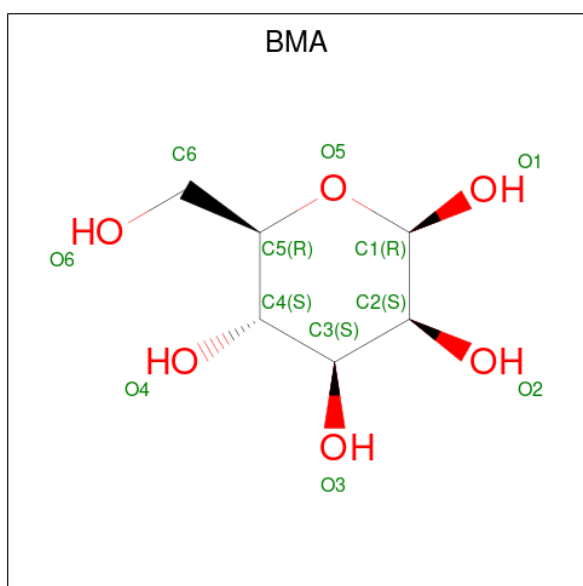
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

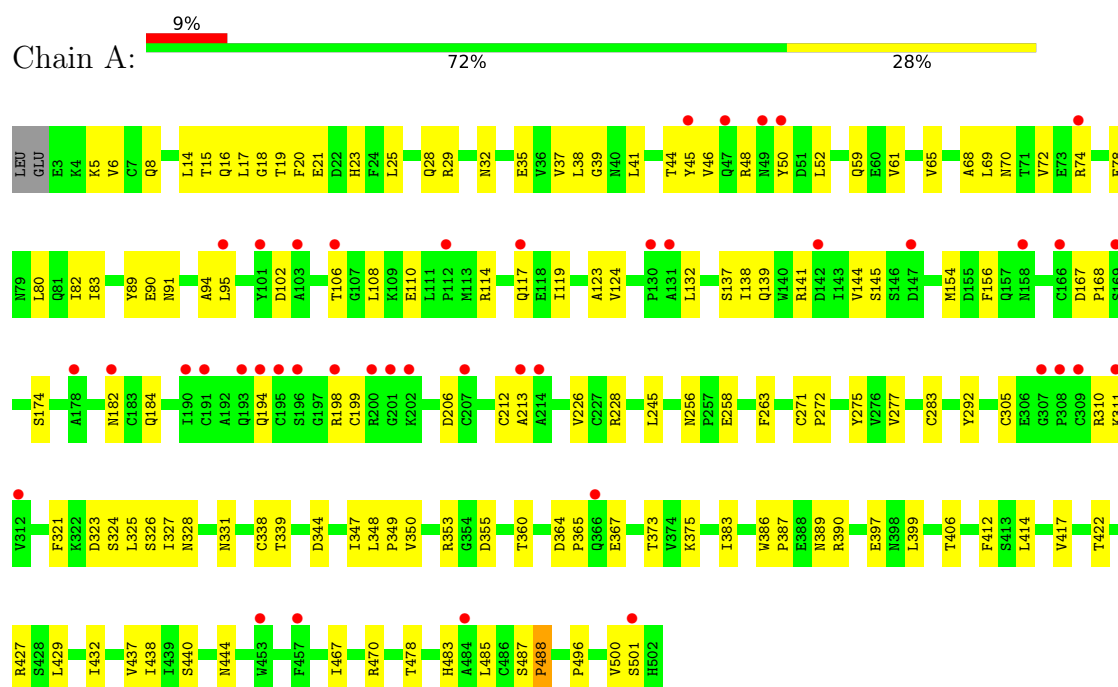


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		

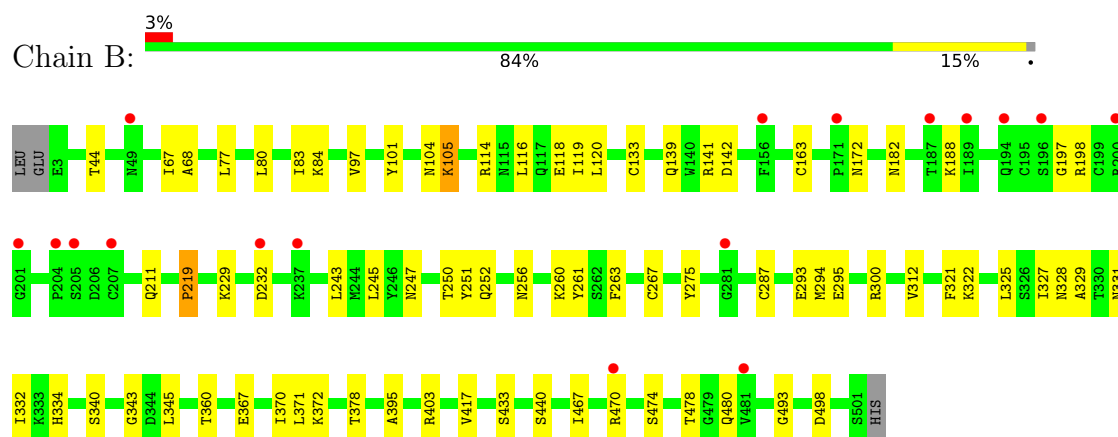
### 3 Residue-property plots [i](#)

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.

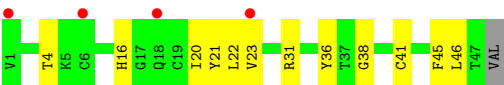
#### • Molecule 1: Epidermal growth factor receptor



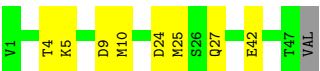
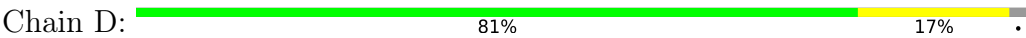
#### • Molecule 1: Epidermal growth factor receptor



#### • Molecule 2: Proepiregulin



• Molecule 2: Proepiregulin



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.59Å 87.21Å 198.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.60 – 3.20 43.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.60-3.20) 99.7 (43.60-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.250 , 0.303 0.250 , 0.301	Depositor DCC
$R_{free}$ test set	1114 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: BMA, NAG, MAN

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	0.27	0/3844	0.49	0/5216
1	B	0.26	0/3856	0.47	0/5229
2	C	0.31	0/368	0.64	1/495 (0.2%)
2	D	0.27	0/377	0.50	0/507
All	All	0.26	0/8445	0.49	1/11447 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	45	PHE	CB-CG-CD1	-5.39	117.03	120.80

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	3773	0	3569	114	0
1	B	3785	0	3592	50	0
2	C	362	0	329	11	0
2	D	370	0	343	5	0
3	F	25	0	22	10	0
4	A	14	0	13	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	56	0	52	1	0
5	A	11	0	10	10	0
5	B	11	0	10	0	0
6	B	11	0	10	0	0
All	All	8418	0	7950	180	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 11.

All (180) 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:331:ASN:HD22	4:A:601:NAG:C6	1.04	1.60
1:A:331:ASN:ND2	4:A:601:NAG:C6	1.90	1.31
1:A:328:ASN:HD21	4:A:601:NAG:C1	1.46	1.29
1:A:331:ASN:ND2	4:A:601:NAG:O5	1.71	1.23
1:A:331:ASN:ND2	4:A:601:NAG:H62	1.48	1.21
1:A:328:ASN:ND2	4:A:601:NAG:C1	2.05	1.16
1:A:323:ASP:OD2	3:F:2:BMA:H62	1.46	1.15
1:A:328:ASN:OD1	4:A:601:NAG:C1	2.01	1.08
4:A:601:NAG:O4	3:F:1:NAG:C1	2.02	1.08
5:A:602:MAN:C1	3:F:2:BMA:O4	2.03	1.06
1:A:331:ASN:HD22	4:A:601:NAG:C5	1.72	1.03
1:A:331:ASN:ND2	4:A:601:NAG:C5	2.23	1.01
1:A:328:ASN:CG	4:A:601:NAG:C1	2.31	0.98
1:A:331:ASN:HD22	4:A:601:NAG:H62	0.81	0.97
5:A:602:MAN:C1	3:F:2:BMA:H61	1.95	0.95
5:A:602:MAN:C1	3:F:2:BMA:C4	2.56	0.84
1:A:91:ASN:HD21	5:A:602:MAN:H61	1.42	0.83
1:A:95:LEU:HB3	1:A:124:VAL:HG12	1.62	0.82
1:B:331:ASN:HB3	4:B:603:NAG:H62	1.63	0.80
1:A:16:GLN:NE2	1:A:20:PHE:CD1	2.51	0.77
1:A:16:GLN:HE22	1:A:20:PHE:HD1	1.30	0.76
1:A:328:ASN:HD21	4:A:601:NAG:C2	1.98	0.75
5:A:602:MAN:C1	3:F:2:BMA:C6	2.66	0.73
1:A:331:ASN:HB3	4:A:601:NAG:H62	1.68	0.73
1:A:414:LEU:HB3	1:A:437:VAL:HG22	1.70	0.72
1:A:331:ASN:CG	4:A:601:NAG:H62	2.09	0.72
1:A:331:ASN:CB	4:A:601:NAG:H62	2.19	0.71
2:C:20:ILE:HD11	2:C:31:ARG:HB2	1.72	0.70
1:A:331:ASN:ND2	4:A:601:NAG:O6	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG13	1:B:370:ILE:HD11	1.73	0.69
1:B:327:ILE:HD11	1:B:345:LEU:HD22	1.75	0.69
1:B:114:ARG:NH1	1:B:182:ASN:OD1	2.26	0.68
1:A:102:ASP:HB3	1:A:106:THR:H	1.60	0.67
1:A:91:ASN:ND2	5:A:602:MAN:H61	2.08	0.66
1:B:260:LYS:HG2	1:B:267:CYS:HB3	1.78	0.65
1:A:16:GLN:NE2	1:A:20:PHE:HD1	1.93	0.64
1:A:41:LEU:HB3	1:A:65:VAL:HG22	1.78	0.63
1:A:292:TYR:CD2	1:A:305:CYS:HB3	2.33	0.63
1:B:294:MET:O	1:B:300:ARG:HA	1.99	0.63
1:B:312:VAL:HG22	1:B:340:SER:HB2	1.79	0.63
1:A:326:SER:HB2	1:A:348:LEU:HB2	1.81	0.62
1:A:328:ASN:OD1	4:A:601:NAG:O5	2.17	0.62
1:A:91:ASN:ND2	5:A:602:MAN:C6	2.62	0.62
1:A:323:ASP:OD2	3:F:2:BMA:C6	2.36	0.62
1:B:141:ARG:HD2	1:B:141:ARG:H	1.62	0.62
1:B:232:ASP:HA	1:B:267:CYS:HB2	1.80	0.62
1:A:272:PRO:HB2	1:A:275:TYR:HD1	1.63	0.62
1:A:213:ALA:HB3	1:A:226:VAL:HB	1.81	0.61
1:B:478:THR:HG23	1:B:480:GLN:OE1	1.99	0.61
1:A:194:GLN:HG3	1:B:219:PRO:HB2	1.81	0.61
1:B:250:THR:O	1:B:252:GLN:N	2.31	0.61
1:B:77:LEU:HD22	1:B:80:LEU:HD12	1.82	0.60
1:A:83:ILE:HB	1:A:119:ILE:HG12	1.83	0.60
1:A:470:ARG:HH22	1:A:478:THR:HG21	1.66	0.60
1:B:372:LYS:HG2	1:B:395:ALA:HA	1.83	0.60
1:A:78:GLU:OE1	1:A:114:ARG:NH2	2.35	0.60
1:B:232:ASP:OD1	1:B:260:LYS:NZ	2.33	0.60
2:D:4:THR:HG22	2:D:5:LYS:H	1.67	0.59
1:A:485:LEU:HD11	1:A:496:PRO:HB3	1.85	0.58
1:A:117:GLN:O	1:A:198:ARG:NH1	2.37	0.58
1:B:321:PHE:HE1	1:B:334:HIS:HD1	1.50	0.57
1:B:295:GLU:HG2	1:B:300:ARG:HG2	1.86	0.57
1:A:108:LEU:HG	1:A:132:LEU:HD13	1.85	0.57
1:A:440:SER:HA	1:A:467:ILE:O	2.04	0.57
1:A:74:ARG:HG3	1:A:110:GLU:HB2	1.86	0.56
1:A:95:LEU:HB3	1:A:124:VAL:CG1	2.32	0.56
1:B:470:ARG:NH1	1:B:474:SER:OG	2.38	0.56
1:A:21:GLU:OE2	1:A:50:TYR:OH	2.20	0.56
1:A:69:LEU:HD11	2:C:22:LEU:HD21	1.86	0.56
1:A:16:GLN:NE2	1:A:18:GLY:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:601:NAG:HO4	3:F:1:NAG:C1	2.16	0.56
1:A:487:SER:N	1:A:488:PRO:HD3	2.21	0.56
1:A:364:ASP:HB3	1:A:367:GLU:HG3	1.86	0.56
1:A:344:ASP:OD1	1:A:406:THR:OG1	2.24	0.55
5:A:602:MAN:C1	3:F:2:BMA:H4	2.35	0.55
1:B:367:GLU:O	1:B:370:ILE:HG12	2.07	0.55
5:A:602:MAN:C1	3:F:2:BMA:HO4	2.20	0.54
1:B:378:THR:HA	1:B:403:ARG:HB2	1.89	0.54
1:B:141:ARG:HD2	1:B:141:ARG:N	2.23	0.54
1:A:375:LYS:HA	1:A:399:LEU:HA	1.89	0.53
1:B:440:SER:HA	1:B:467:ILE:O	2.08	0.53
1:A:347:ILE:HD12	1:A:383:ILE:HG12	1.91	0.53
1:B:118:GLU:OE2	1:B:198:ARG:NH1	2.41	0.53
1:A:17:LEU:HD22	2:C:36:TYR:O	2.11	0.51
1:A:321:PHE:HE1	1:A:331:ASN:HB2	1.76	0.50
1:B:211:GLN:HE22	1:B:229:LYS:HD2	1.75	0.50
1:B:44:THR:HA	1:B:68:ALA:O	2.12	0.49
1:A:19:THR:HG23	1:A:21:GLU:HB2	1.94	0.49
1:B:293:GLU:OE2	1:B:403:ARG:NH1	2.45	0.49
1:A:137:SER:HB2	1:A:174:SER:HA	1.94	0.49
1:A:5:LYS:N	1:A:35:GLU:OE2	2.40	0.48
1:A:327:ILE:HD11	1:A:347:ILE:HG12	1.96	0.48
2:C:20:ILE:HD11	2:C:31:ARG:CB	2.39	0.48
1:A:310:ARG:HG2	1:A:311:LYS:H	1.77	0.48
1:B:371:LEU:HB2	1:B:395:ALA:HB1	1.95	0.48
1:A:331:ASN:HB3	4:A:601:NAG:C6	2.42	0.48
2:C:16:HIS:H	2:C:41:CYS:HB2	1.78	0.48
2:C:4:THR:OG1	2:C:21:TYR:HB3	2.14	0.48
1:A:14:LEU:HD13	2:C:22:LEU:HD22	1.95	0.48
1:A:256:ASN:OD1	1:A:258:GLU:N	2.47	0.48
1:A:483:HIS:CD2	1:A:496:PRO:HD3	2.48	0.48
1:A:328:ASN:HD21	4:A:601:NAG:HN2	1.62	0.47
1:A:198:ARG:HD3	1:A:213:ALA:O	2.14	0.47
1:A:292:TYR:HD2	1:A:305:CYS:HB3	1.79	0.47
1:A:139:GLN:HG3	1:A:141:ARG:NH2	2.29	0.47
1:B:263:PHE:HE1	1:B:275:TYR:CE2	2.33	0.47
1:A:154:MET:O	1:A:154:MET:HG3	2.14	0.47
1:A:29:ARG:CZ	2:C:46:LEU:HD21	2.45	0.47
1:A:386:TRP:CG	1:A:387:PRO:HD2	2.50	0.46
1:A:6:VAL:HG13	1:A:38:LEU:HD23	1.97	0.46
1:B:325:LEU:HD22	2:D:42:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ASN:ND2	1:B:360:THR:HG21	2.31	0.46
2:D:9:ASP:OD1	2:D:10:MET:HG2	2.15	0.46
1:A:91:ASN:ND2	5:A:602:MAN:O6	2.48	0.46
1:B:104:ASN:O	1:B:105:LYS:HG3	2.15	0.46
1:B:142:ASP:HA	1:B:188:LYS:HD2	1.99	0.46
1:A:82:ILE:HG21	1:A:226:VAL:HG11	1.98	0.45
2:C:21:TYR:CE1	2:C:23:VAL:HA	2.51	0.45
1:A:412:PHE:CE1	1:A:438:ILE:HB	2.51	0.45
1:A:500:VAL:HG13	1:A:501:SER:N	2.31	0.45
1:B:84:LYS:HG2	1:B:120:LEU:HD12	1.98	0.45
1:B:245:LEU:HG	1:B:256:ASN:HB2	1.98	0.45
1:A:23:HIS:CD2	1:A:45:TYR:HB2	2.51	0.45
1:A:325:LEU:HB2	4:A:601:NAG:O7	2.17	0.45
1:A:37:VAL:HB	1:A:61:VAL:HG22	1.99	0.45
1:A:46:VAL:HG11	1:A:52:LEU:HD11	1.99	0.45
2:C:21:TYR:HE1	2:C:23:VAL:HA	1.82	0.44
1:B:417:VAL:HA	1:B:440:SER:O	2.18	0.44
1:A:212:CYS:O	1:A:228:ARG:NH2	2.51	0.44
1:A:94:ALA:N	1:A:123:ALA:O	2.45	0.44
1:B:83:ILE:HB	1:B:119:ILE:HG12	2.00	0.44
1:B:287:CYS:SG	1:B:293:GLU:HG2	2.58	0.44
1:A:199:CYS:HB2	1:A:206:ASP:O	2.18	0.43
1:B:139:GLN:HE22	1:B:172:ASN:HD22	1.66	0.43
1:A:48:ARG:HA	1:A:72:VAL:HA	2.00	0.43
1:A:328:ASN:ND2	1:A:360:THR:HG21	2.33	0.43
1:A:28:GLN:O	1:A:32:ASN:HB2	2.18	0.43
1:B:67:ILE:O	1:B:97:VAL:HA	2.18	0.43
1:A:397:GLU:HB2	1:A:427:ARG:NH1	2.34	0.43
1:A:365:PRO:HB3	1:A:387:PRO:HB3	2.01	0.43
1:B:80:LEU:HD22	1:B:116:LEU:HD13	2.01	0.43
1:A:338:CYS:O	1:A:373:THR:HG23	2.19	0.43
1:B:403:ARG:O	1:B:433:SER:HB2	2.19	0.43
1:A:429:LEU:HD21	1:A:432:ILE:HD11	2.01	0.42
1:A:144:VAL:HG12	1:A:145:SER:O	2.19	0.42
1:A:389:ASN:OD1	1:A:389:ASN:N	2.51	0.42
1:A:349:PRO:O	1:A:353:ARG:HG2	2.20	0.42
1:A:386:TRP:CD2	1:A:387:PRO:HD2	2.54	0.42
1:A:422:THR:HA	1:A:444:ASN:O	2.19	0.42
1:B:343:GLY:N	1:B:378:THR:OG1	2.52	0.42
1:A:70:ASN:HB3	1:A:72:VAL:HG12	2.01	0.42
1:A:245:LEU:HD11	1:A:256:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:HA	1:A:80:LEU:HA	2.02	0.42
1:A:387:PRO:HG2	1:A:390:ARG:HG3	2.02	0.42
1:A:15:THR:HG21	2:C:38:GLY:O	2.20	0.41
1:A:44:THR:HA	1:A:68:ALA:O	2.20	0.41
2:D:25:MET:O	2:D:27:GLN:HG3	2.20	0.41
1:A:21:GLU:O	1:A:25:LEU:HD23	2.20	0.41
1:A:95:LEU:O	1:A:124:VAL:HA	2.20	0.41
1:A:8:GLN:O	1:A:39:GLY:N	2.52	0.41
1:A:263:PHE:HB2	1:A:283:CYS:SG	2.60	0.41
1:B:243:LEU:HD21	1:B:261:TYR:CE1	2.55	0.41
1:A:310:ARG:HG2	1:A:311:LYS:N	2.36	0.41
1:A:310:ARG:HD2	1:A:339:THR:H	1.85	0.41
1:B:101:TYR:OH	2:D:24:ASP:OD2	2.32	0.41
1:B:133:CYS:HB3	1:B:163:CYS:HB3	1.83	0.41
1:B:247:ASN:HB3	1:B:250:THR:O	2.20	0.41
1:A:114:ARG:HB3	1:A:182:ASN:HA	2.03	0.41
1:A:167:ASP:CG	1:A:168:PRO:HD2	2.41	0.41
1:A:321:PHE:CE1	1:A:331:ASN:HB2	2.56	0.41
1:A:324:SER:OG	4:A:601:NAG:H4	2.21	0.41
1:A:271:CYS:SG	1:A:277:VAL:HG22	2.60	0.40
1:A:350:VAL:CG2	1:A:355:ASP:HB2	2.51	0.40
1:A:138:ILE:HA	1:A:184:GLN:OE1	2.22	0.40
1:A:89:TYR:CD2	1:A:90:GLU:HG2	2.55	0.40
1:B:142:ASP:OD1	1:B:198:ARG:NH2	2.54	0.40
1:B:321:PHE:HZ	1:B:334:HIS:HB2	1.86	0.40
1:B:493:GLY:N	1:B:498:ASP:HB3	2.36	0.40
1:B:328:ASN:OD1	1:B:329:ALA:N	2.50	0.40
1:A:417:VAL:HA	1:A:440:SER:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	498/502 (99%)	457 (92%)	39 (8%)	2 (0%)	34	69
1	B	497/502 (99%)	461 (93%)	32 (6%)	4 (1%)	19	58
2	C	45/48 (94%)	42 (93%)	3 (7%)	0	100	100
2	D	45/48 (94%)	42 (93%)	3 (7%)	0	100	100
All	All	1085/1100 (99%)	1002 (92%)	77 (7%)	6 (1%)	25	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	TYR
1	A	156	PHE
1	B	219	PRO
1	B	322	LYS
1	B	197	GLY
1	A	488	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	A	415/441 (94%)	415 (100%)	0	100	100
1	B	421/441 (96%)	420 (100%)	1 (0%)	93	98
2	C	41/44 (93%)	41 (100%)	0	100	100
2	D	43/44 (98%)	43 (100%)	0	100	100
All	All	920/970 (95%)	919 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	91	ASN
1	A	252	GLN
1	A	328	ASN
1	A	331	ASN
1	B	172	ASN
1	B	420	ASN
1	B	444	ASN

### 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 ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	F	1	3	14,14,15	0.41	0	17,19,21	0.60	0
3	BMA	F	2	3	11,11,12	0.21	0	15,15,17	0.83	1 (6%)

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
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	BMA	F	2	3	-	2/2/19/22	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(°)
3	F	2	BMA	O5-C1-C2	-2.13	107.49	110.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

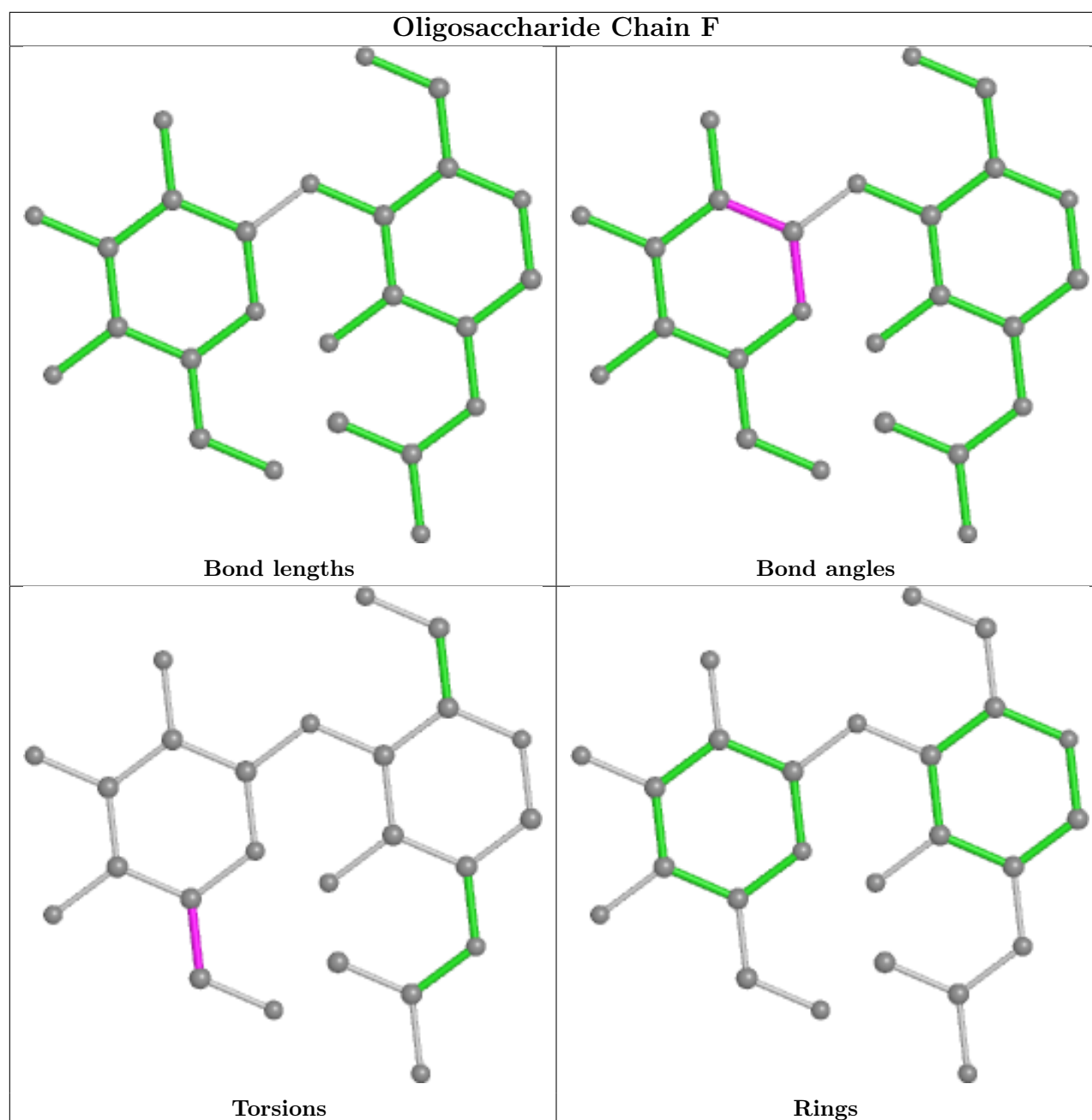
Mol	Chain	Res	Type	Atoms
3	F	2	BMA	O5-C5-C6-O6
3	F	2	BMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	BMA	8	0
3	F	1	NAG	2	0

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](#)

8 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
4	NAG	A	601	-	14,14,15	0.56	1 (7%)	17,19,21	0.52	0
4	NAG	B	602	1	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	B	603	-	14,14,15	0.24	0	17,19,21	0.45	0
5	MAN	A	602	-	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
5	MAN	B	606	-	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
4	NAG	B	604	-	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	601	1	14,14,15	0.23	0	17,19,21	0.51	0
6	BMA	B	605	-	11,11,12	0.61	0	15,15,17	0.73	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	A	601	-	-	1/6/23/26	0/1/1/1
4	NAG	B	602	1	-	1/6/23/26	0/1/1/1
4	NAG	B	603	-	-	0/6/23/26	0/1/1/1
5	MAN	A	602	-	-	1/2/19/22	0/1/1/1
5	MAN	B	606	-	-	0/2/19/22	0/1/1/1
4	NAG	B	604	-	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
6	BMA	B	605	-	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	-2.05	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	MAN	C1-O5-C5	2.46	115.53	112.19
5	A	602	MAN	C1-O5-C5	2.39	115.43	112.19
5	A	602	MAN	O2-C2-C3	-2.25	105.63	110.14
5	B	606	MAN	O2-C2-C3	-2.17	105.78	110.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O5-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
5	A	602	MAN	O5-C5-C6-O6
4	A	601	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	23	0
4	B	603	NAG	1	0
5	A	602	MAN	10	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	A	500/502 (99%)	0.66	43 (8%) 10 5	57, 100, 138, 160	0
1	B	499/502 (99%)	0.37	17 (3%) 45 29	54, 82, 114, 139	0
2	C	47/48 (97%)	0.61	4 (8%) 10 6	78, 99, 119, 128	0
2	D	47/48 (97%)	0.29	0 100 100	56, 71, 87, 102	0
All	All	1093/1100 (99%)	0.51	64 (5%) 22 13	54, 90, 130, 160	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	GLY	6.0
1	A	194	GLN	5.6
1	A	195	CYS	5.5
1	B	196	SER	3.8
1	A	202	LYS	3.7
1	A	169	SER	3.6
1	A	309	CYS	3.5
1	A	213	ALA	3.5
1	A	49	ASN	3.5
1	A	190	ILE	3.5
1	A	130	PRO	3.3
1	A	366	GLN	3.2
1	A	103	ALA	3.1
1	B	49	ASN	3.1
1	A	182	ASN	3.0
1	A	308	PRO	3.0
1	A	178	ALA	3.0
1	B	207	CYS	3.0
1	A	166	CYS	2.9
1	A	207	CYS	2.9
1	A	196	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	2.8
1	B	481	VAL	2.8
1	A	484	ALA	2.8
1	A	106	THR	2.8
1	A	200	ARG	2.8
2	C	18	GLN	2.7
1	B	281	GLY	2.7
2	C	1	VAL	2.7
1	A	312	VAL	2.7
1	A	47	GLN	2.4
1	A	193	GLN	2.4
1	B	200	ARG	2.4
1	A	214	ALA	2.4
2	C	6	CYS	2.4
1	A	45	TYR	2.4
1	B	156	PHE	2.3
1	B	187	THR	2.3
1	A	311	LYS	2.3
1	B	470	ARG	2.3
1	B	201	GLY	2.3
1	A	457	PHE	2.3
1	A	74	ARG	2.3
1	B	171	PRO	2.3
1	B	194	GLN	2.2
1	A	501	SER	2.2
1	A	142	ASP	2.2
1	A	307	GLY	2.2
1	A	131	ALA	2.2
1	A	112	PRO	2.2
2	C	23	VAL	2.2
1	A	453	TRP	2.2
1	B	205	SER	2.1
1	A	101	TYR	2.1
1	B	232	ASP	2.1
1	A	158	ASN	2.1
1	A	117	GLN	2.1
1	B	189	ILE	2.1
1	B	237	LYS	2.0
1	A	191	CYS	2.0
1	A	147	ASP	2.0
1	A	198	ARG	2.0
1	B	204	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	95	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

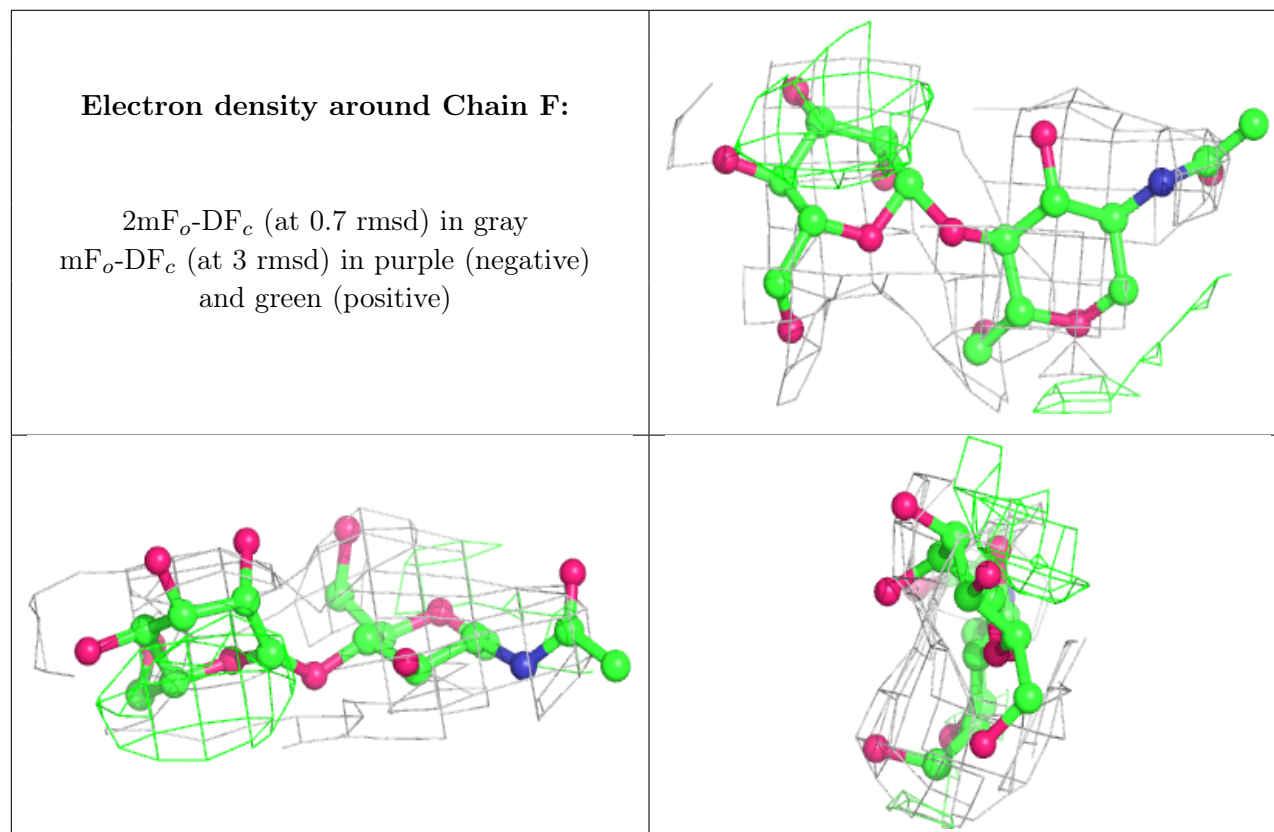
There are no non-standard protein/DNA/RNA residues in this entry.

## 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
3	BMA	F	2	11/12	0.63	0.32	117,124,130,149	0
3	NAG	F	1	14/15	0.86	0.30	90,104,115,121	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 [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	MAN	A	602	11/12	0.59	0.38	102,114,122,130	0
4	NAG	B	602	14/15	0.68	0.33	85,115,122,127	0
4	NAG	A	601	14/15	0.68	0.43	69,83,95,97	0
4	NAG	B	601	14/15	0.70	0.27	96,110,120,122	0
6	BMA	B	605	11/12	0.77	0.19	96,117,121,122	0
5	MAN	B	606	11/12	0.82	0.25	109,117,123,126	0
4	NAG	B	603	14/15	0.89	0.32	60,72,88,94	0
4	NAG	B	604	14/15	0.90	0.22	81,93,106,115	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.