



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 02:01 PM BST

PDB ID : 3LTF  
Title : Crystal Structure of the Drosophila Epidermal Growth Factor Receptor ectodomain in complex with Spitz  
Authors : Alvarado, D.; Klein, D.E.; Lemmon, M.A.  
Deposited on : 2010-02-15  
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 : 2.13.1  
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

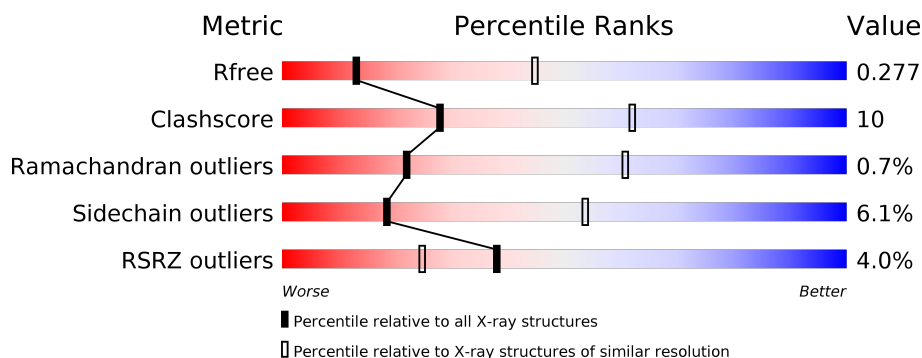
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



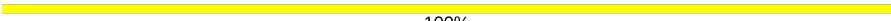
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	601	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	601	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	58	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
2	D	58	<div> <div></div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
3	E	6	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
4	F	2	<div> <div></div> <div> <div>100%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	G	4	 100%

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	MAN	E	3	X	-	-	-
3	MAN	E	4	X	-	-	-
3	MAN	E	5	X	-	-	-
3	MAN	E	6	X	-	-	X
5	MAN	G	3	X	-	-	-
5	MAN	G	4	X	-	-	-
6	NAG	C	596	X	-	-	-
7	MLI	A	596	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9221 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	522	Total	C	N	O	S	0	0	0
			4007	2495	707	757	48			
1	C	531	Total	C	N	O	S	0	1	0
			4109	2559	732	768	50			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P04412
A	-4	HIS	-	expression tag	UNP P04412
A	-3	HIS	-	expression tag	UNP P04412
A	-2	HIS	-	expression tag	UNP P04412
A	-1	HIS	-	expression tag	UNP P04412
A	0	HIS	-	expression tag	UNP P04412
A	38	GLU	LYS	conflict	UNP P04412
A	230	GLY	ALA	conflict	UNP P04412
A	232	CYS	SER	conflict	UNP P04412
A	359	LEU	ARG	conflict	UNP P04412
A	493	ASN	THR	conflict	UNP P04412
A	590	HIS	-	expression tag	UNP P04412
A	591	HIS	-	expression tag	UNP P04412
A	592	HIS	-	expression tag	UNP P04412
A	593	HIS	-	expression tag	UNP P04412
A	594	HIS	-	expression tag	UNP P04412
A	595	HIS	-	expression tag	UNP P04412
C	-5	HIS	-	expression tag	UNP P04412
C	-4	HIS	-	expression tag	UNP P04412
C	-3	HIS	-	expression tag	UNP P04412
C	-2	HIS	-	expression tag	UNP P04412
C	-1	HIS	-	expression tag	UNP P04412
C	0	HIS	-	expression tag	UNP P04412
C	38	GLU	LYS	conflict	UNP P04412
C	230	GLY	ALA	conflict	UNP P04412

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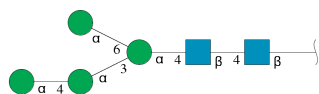
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Chain	Residue	Modelled	Actual	Comment	Reference
C	232	CYS	SER	conflict	UNP P04412
C	359	LEU	ARG	conflict	UNP P04412
C	493	ASN	THR	conflict	UNP P04412
C	590	HIS	-	expression tag	UNP P04412
C	591	HIS	-	expression tag	UNP P04412
C	592	HIS	-	expression tag	UNP P04412
C	593	HIS	-	expression tag	UNP P04412
C	594	HIS	-	expression tag	UNP P04412
C	595	HIS	-	expression tag	UNP P04412

- Molecule 2 is a protein called Protein spitz.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	57	Total	C	N	O	S	0	0	0
			450	290	70	83	7			
2	B	57	Total	C	N	O	S	0	0	0
			456	296	70	83	7			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



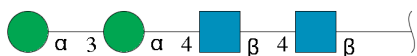
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



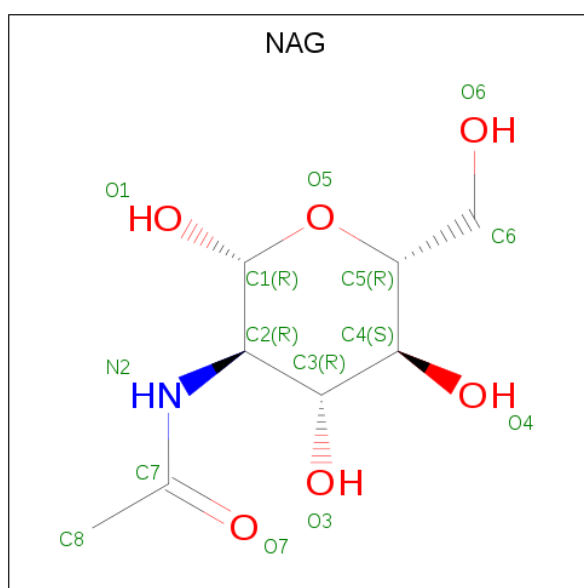
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



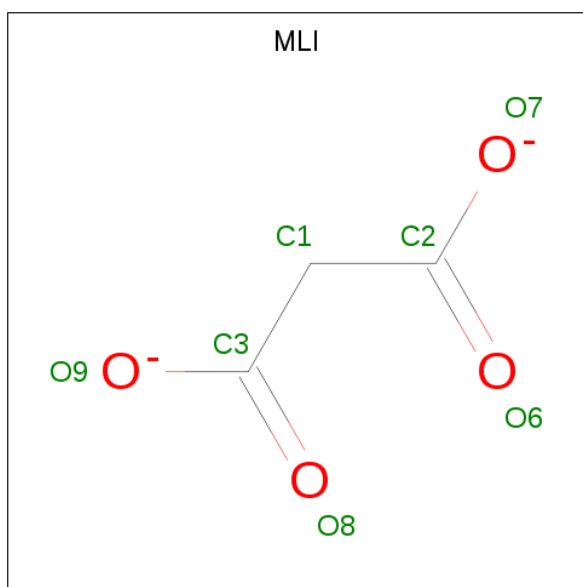
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).

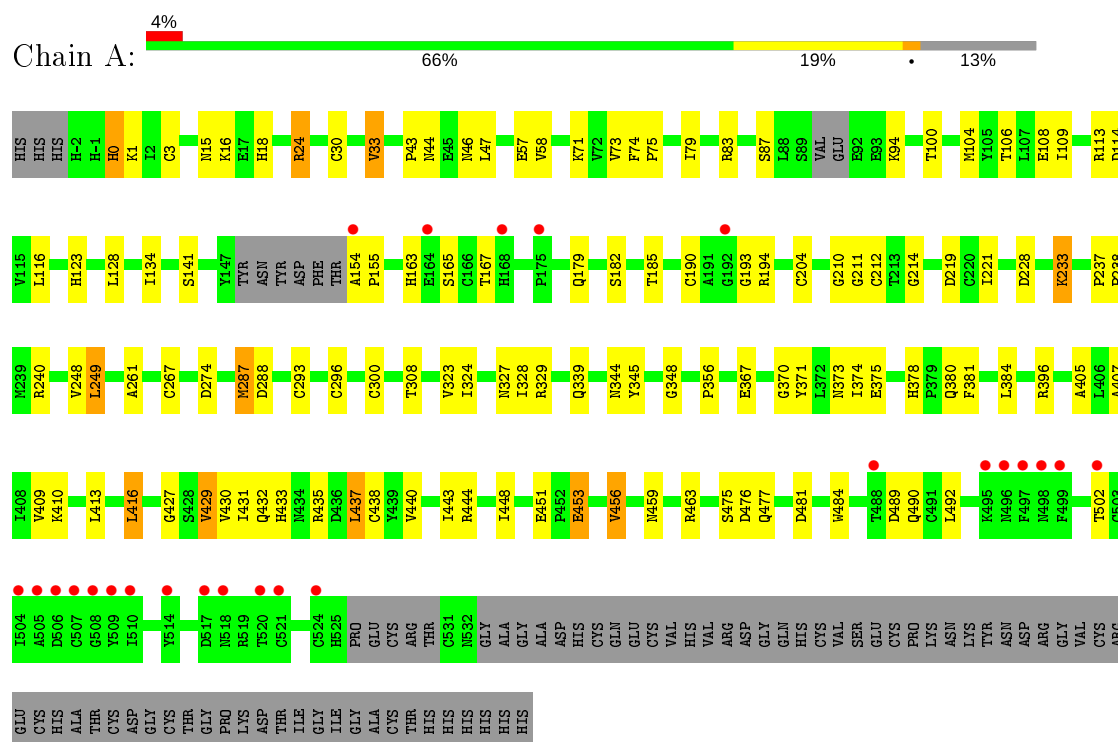


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		

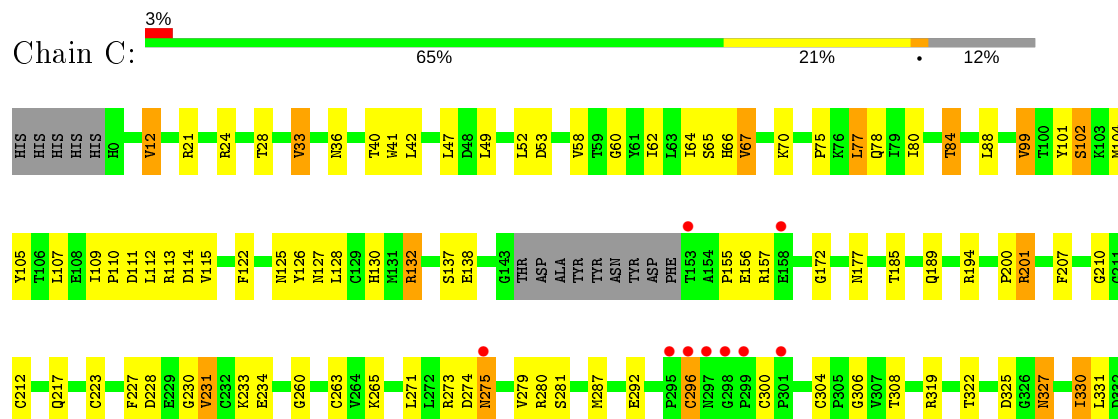
### 3 Residue-property plots

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.

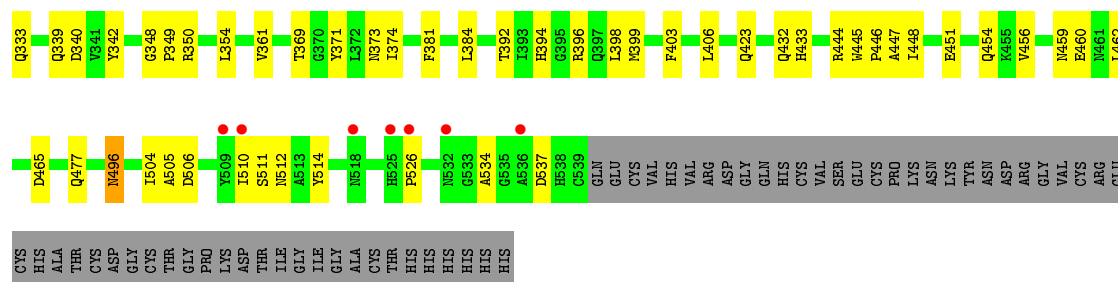
- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor







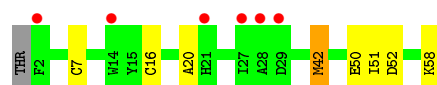
- Molecule 2: Protein spitiz

Chain D: 83% 12% . .



- Molecule 2: Protein spitiz

Chain B: 10% 84% 12% . .



- Molecule 3: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 33% 33% 33%



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

Chain F: 100%



- Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.21Å 124.24Å 186.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 36.05 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.20) 99.8 (36.05-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.237 , 0.275 0.238 , 0.277	Depositor DCC
$R_{free}$ test set	4589 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: MLI, 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	0.37	1/4097 (0.0%)	0.55	0/5558
1	C	0.36	0/4205	0.55	0/5699
2	B	0.40	0/471	0.48	0/640
2	D	0.40	0/464	0.57	1/631 (0.2%)
All	All	0.37	1/9237 (0.0%)	0.55	1/12528 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	CYS	CB-SG	-5.65	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	16	CYS	CA-CB-SG	-5.23	104.58	114.00

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	4007	0	3741	83	0
1	C	4109	0	3884	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	456	0	413	5	0
2	D	450	0	406	10	0
3	E	72	0	61	3	0
4	F	28	0	25	0	0
5	G	50	0	43	0	0
6	A	14	0	13	0	0
6	C	28	0	26	0	0
7	A	7	0	2	0	0
All	All	9221	0	8614	176	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 10.

All (176) 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:24:ARG:HH11	1:A:24:ARG:HG2	1.35	0.91
1:C:373:ASN:HB2	1:C:399:MET:HE3	1.58	0.85
1:A:194:ARG:HD3	1:A:210:GLY:O	1.77	0.83
1:C:333:GLN:NE2	2:D:47:GLU:HB2	1.92	0.83
1:A:194:ARG:O	1:A:204:CYS:HB2	1.77	0.83
1:A:15:ASN:CG	1:A:18:HIS:HD2	1.83	0.82
1:C:392:THR:HG22	1:C:423:GLN:HB3	1.64	0.78
1:A:73:VAL:HG12	1:A:108:GLU:HB2	1.65	0.78
1:A:163:HIS:HD2	1:A:165:SER:H	1.34	0.75
1:C:36:ASN:HD21	1:C:84:THR:HB	1.52	0.75
1:A:100:THR:HG22	1:A:123:HIS:HB3	1.71	0.72
1:C:374:ILE:HD13	1:C:384:LEU:HD21	1.71	0.72
1:C:330:ILE:HD11	1:C:381:PHE:CZ	2.24	0.72
1:A:204:CYS:O	1:C:201:ARG:NH2	2.25	0.69
1:C:101:TYR:HE2	2:D:27:ILE:HG22	1.59	0.68
1:C:333:GLN:HE22	2:D:47:GLU:HB2	1.58	0.67
1:A:484:TRP:HB2	1:A:490:GLN:HG3	1.75	0.67
1:A:214:GLY:H	1:A:219:ASP:HB3	1.59	0.66
1:A:327:ASN:ND2	1:A:370:GLY:HA3	2.11	0.65
1:C:371:TYR:CE1	1:C:399:MET:HE2	2.32	0.65
1:A:443:ILE:HG23	1:A:492:LEU:HD11	1.79	0.64
1:C:99:VAL:HG22	1:C:122:PHE:CD2	2.34	0.63
1:C:373:ASN:CB	1:C:399:MET:HE3	2.27	0.63
1:A:33:VAL:CG1	1:A:58:VAL:HG22	2.30	0.61
1:A:327:ASN:HD22	1:A:370:GLY:HA3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ASN:HB2	1:C:399:MET:CE	2.28	0.60
1:C:227:PHE:CZ	1:C:230:GLY:HA2	2.36	0.60
1:C:274:ASP:HB2	1:C:279:VAL:HG21	1.84	0.59
1:C:113:ARG:HH11	1:C:113:ARG:HG3	1.66	0.59
1:C:130:HIS:H	1:C:132:ARG:HH11	1.49	0.59
1:C:350[B]:ARG:NH1	1:C:350[B]:ARG:HB2	2.17	0.59
1:A:287:MET:HB2	1:A:296:CYS:HB3	1.85	0.59
1:C:228:ASP:HB2	1:C:263:CYS:HB2	1.86	0.58
1:C:398:LEU:HD23	1:C:403:PHE:HB3	1.85	0.58
1:A:444:ARG:HG2	1:A:481:ASP:HA	1.86	0.57
1:A:324:ILE:HD13	1:A:328:ILE:HD11	1.85	0.57
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.13	0.56
1:A:344:ASN:O	1:A:345:TYR:HB2	2.05	0.56
1:A:409:VAL:HG21	2:B:51:ILE:HG12	1.87	0.56
1:C:127:ASN:O	1:C:157:ARG:NH1	2.38	0.56
1:C:207:PHE:CE1	1:C:234:GLU:HB2	2.40	0.56
1:A:431:ILE:HG21	1:A:440:VAL:HG11	1.88	0.55
1:C:287:MET:HE2	1:C:296:CYS:HB3	1.88	0.55
1:A:33:VAL:HG13	1:A:58:VAL:HG22	1.88	0.55
1:C:36:ASN:HD22	1:C:60:GLY:HA3	1.71	0.55
1:C:444:ARG:NH1	1:C:447:ALA:HB2	2.22	0.55
1:A:228:ASP:HB3	1:A:233:LYS:HD3	1.87	0.54
1:C:514:TYR:CZ	1:C:534:ALA:HB2	2.41	0.54
1:A:432:GLN:HA	1:A:459:ASN:O	2.07	0.54
1:A:163:HIS:CD2	1:A:165:SER:H	2.20	0.54
1:C:306:GLY:N	1:C:325:ASP:O	2.39	0.54
1:C:42:LEU:HD23	1:C:49:LEU:HD11	1.88	0.54
1:C:65:SER:OG	1:C:66:HIS:HD2	1.91	0.54
1:C:432:GLN:HA	1:C:459:ASN:O	2.07	0.54
1:A:240:ARG:HB3	1:A:249:LEU:HD22	1.91	0.53
1:C:138:GLU:O	1:C:194:ARG:NH2	2.42	0.53
1:C:510:ILE:O	1:C:512:ASN:N	2.40	0.52
1:C:504:ILE:HG22	1:C:506:ASP:H	1.74	0.52
1:C:99:VAL:HG22	1:C:122:PHE:HD2	1.73	0.52
1:A:324:ILE:CD1	1:A:328:ILE:HD11	2.39	0.52
1:C:21:ARG:HG3	1:C:24:ARG:NH2	2.24	0.52
1:A:329:ARG:HD2	1:A:373:ASN:HB3	1.92	0.52
1:C:114:ASP:HB2	1:C:210:GLY:HA2	1.92	0.51
1:C:333:GLN:HE22	2:D:47:GLU:CB	2.22	0.51
1:A:413:LEU:HB3	1:A:437:LEU:HD22	1.93	0.51
1:C:279:VAL:HG12	1:C:281:SER:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:HG3	1:A:79:ILE:HB	1.91	0.51
1:A:15:ASN:CG	1:A:18:HIS:CD2	2.75	0.51
1:A:323:VAL:HG22	1:A:367:GLU:HB2	1.91	0.51
1:C:101:TYR:CE2	2:D:27:ILE:HG22	2.42	0.51
1:C:271:LEU:HD23	1:C:396:ARG:HG2	1.93	0.51
1:C:40:THR:HA	1:C:65:SER:O	2.11	0.51
1:C:333:GLN:HE21	2:D:47:GLU:HB2	1.75	0.50
1:C:456:VAL:HG23	2:D:58:LYS:HB2	1.94	0.50
1:A:190:CYS:HB2	1:C:201:ARG:NH1	2.26	0.50
1:A:448:ILE:HD11	1:A:484:TRP:CZ2	2.47	0.50
1:A:248:VAL:HA	1:C:279:VAL:HG13	1.93	0.50
1:C:340:ASP:HB3	1:C:349:PRO:HD2	1.94	0.49
1:A:18:HIS:CE1	2:B:52:ASP:HA	2.48	0.49
1:A:432:GLN:HE22	2:B:52:ASP:H	1.61	0.49
1:C:67:VAL:HG13	1:C:102:SER:OG	2.13	0.49
1:C:279:VAL:HG12	1:C:280:ARG:N	2.28	0.48
1:A:374:ILE:HD13	1:A:384:LEU:HD21	1.94	0.48
1:C:78:GLN:HA	1:C:112:LEU:HA	1.96	0.48
1:C:339:GLN:OE1	1:C:350[B]:ARG:NH2	2.47	0.48
1:C:64:ILE:HG23	1:C:67:VAL:HG11	1.94	0.48
1:C:327:ASN:HB3	1:C:371:TYR:H	1.79	0.48
1:A:437:LEU:HD13	1:A:438:CYS:H	1.77	0.48
1:C:200:PRO:O	1:C:201:ARG:CB	2.61	0.48
1:A:308:THR:O	1:A:329:ARG:HG3	2.13	0.48
1:A:288:ASP:OD2	1:A:396:ARG:NH2	2.46	0.48
1:C:189:GLN:OE1	1:C:200:PRO:HB3	2.14	0.48
1:C:228:ASP:OD2	1:C:233:LYS:HE3	2.14	0.48
1:A:451:GLU:HB3	1:A:453:GLU:OE2	2.13	0.48
1:C:24:ARG:O	1:C:28:THR:HB	2.14	0.48
1:C:217:GLN:HB2	1:C:231:VAL:HG23	1.96	0.48
1:C:33:VAL:CG1	1:C:58:VAL:HG22	2.44	0.48
1:C:33:VAL:HG13	1:C:58:VAL:HG22	1.95	0.48
1:C:504:ILE:HG22	1:C:505:ALA:N	2.28	0.47
1:A:327:ASN:ND2	1:A:371:TYR:H	2.12	0.47
1:A:475:SER:C	1:A:477:GLN:H	2.17	0.47
1:C:451:GLU:H	1:C:454:GLN:NE2	2.12	0.47
1:A:100:THR:HA	1:A:123:HIS:O	2.14	0.47
1:A:435:ARG:HH22	3:E:6:MAN:H2	1.79	0.47
1:C:373:ASN:CG	1:C:399:MET:CE	2.83	0.47
1:A:134:ILE:O	1:A:179:GLN:OE1	2.33	0.47
1:C:477:GLN:HE22	1:C:505:ALA:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:SER:HB3	1:A:94:LYS:HA	1.98	0.46
1:A:83:ARG:HH21	1:A:261:ALA:HB2	1.81	0.46
1:A:1:LYS:HG2	1:A:30:CYS:HA	1.96	0.46
1:A:274:ASP:HB2	1:A:293:CYS:HB2	1.97	0.46
1:A:410:LYS:HD2	1:A:433:HIS:HB3	1.97	0.46
1:A:429:VAL:HG13	1:A:456:VAL:HB	1.98	0.46
1:C:496:ASN:ND2	1:C:496:ASN:N	2.64	0.46
1:A:378:HIS:CD2	1:A:380:GLN:H	2.33	0.45
1:C:445:TRP:HB2	1:C:456:VAL:HG11	1.96	0.45
1:A:113:ARG:NH2	1:A:182:SER:OG	2.50	0.45
1:C:109:ILE:HG22	1:C:112:LEU:HB2	1.98	0.45
1:C:70:LYS:HG3	1:C:105:TYR:CD1	2.52	0.45
1:C:369:THR:HA	1:C:394:HIS:HB2	1.99	0.45
1:A:405:ALA:HB2	1:A:427:GLY:HA3	1.99	0.45
2:B:16:CYS:HB3	2:B:20:ALA:HB3	1.98	0.45
1:C:36:ASN:ND2	1:C:60:GLY:HA3	2.30	0.45
1:C:445:TRP:N	1:C:446:PRO:HD2	2.32	0.45
1:C:496:ASN:H	1:C:496:ASN:ND2	2.15	0.45
1:C:88:LEU:HD21	2:D:27:ILE:HD11	1.99	0.45
1:A:416:LEU:HD21	1:A:440:VAL:CG1	2.47	0.45
1:C:12:VAL:CG1	1:C:41:TRP:CD1	3.00	0.45
1:C:132:ARG:HD3	1:C:132:ARG:H	1.82	0.45
1:C:373:ASN:CG	1:C:399:MET:HE3	2.38	0.45
1:C:200:PRO:O	1:C:201:ARG:HB2	2.17	0.44
1:C:342:TYR:CE1	1:C:348:GLY:HA2	2.52	0.44
1:A:339:GLN:NE2	1:A:348:GLY:O	2.50	0.44
2:D:8:PRO:HD2	2:D:33:TYR:CE2	2.53	0.44
1:A:114:ASP:HB2	1:A:210:GLY:HA2	1.99	0.44
1:A:433:HIS:CE1	3:E:4:MAN:H62	2.52	0.44
1:A:329:ARG:HD3	1:A:371:TYR:HE1	1.81	0.44
2:B:42:MET:HG2	2:B:50:GLU:HG3	1.99	0.44
1:C:40:THR:HG22	1:C:65:SER:HB3	2.00	0.44
1:C:53:ASP:HA	1:C:75:PRO:HD2	2.01	0.43
1:A:193:GLY:HA3	1:C:201:ARG:NH1	2.33	0.43
1:A:24:ARG:NH1	1:A:24:ARG:HG2	2.15	0.43
1:C:110:PRO:O	1:C:111:ASP:CB	2.66	0.43
1:A:433:HIS:HE1	3:E:4:MAN:H62	1.83	0.43
1:A:44:ASN:HD21	1:A:46:ASN:HB2	1.82	0.43
1:C:373:ASN:CB	1:C:399:MET:CE	2.94	0.43
1:C:433:HIS:CE1	1:C:460:GLU:HG3	2.53	0.42
1:A:211:GLY:HA3	1:A:221:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:O	1:A:75:PRO:HD3	2.19	0.42
1:C:274:ASP:O	1:C:275:ASN:C	2.57	0.42
1:C:126:TYR:O	1:C:155:PRO:O	2.38	0.42
1:A:116:LEU:HA	1:A:141:SER:HB3	2.01	0.42
1:A:329:ARG:HD3	1:A:371:TYR:CE1	2.54	0.42
1:A:378:HIS:HD2	1:A:380:GLN:H	1.67	0.42
1:A:409:VAL:HG12	1:A:410:LYS:HD3	2.02	0.42
1:A:44:ASN:HB3	1:A:47:LEU:HG	2.02	0.42
1:A:71:LYS:HE2	1:A:71:LYS:HB3	1.91	0.42
1:C:172:GLY:H	1:C:177:ASN:HB3	1.85	0.42
1:C:319:ARG:HA	1:C:361:VAL:HG13	2.02	0.42
1:A:416:LEU:HD21	1:A:440:VAL:HG12	2.01	0.42
1:A:154:ALA:HA	1:A:155:PRO:HD3	1.86	0.41
1:C:273:ARG:HD3	1:C:292:GLU:OE2	2.20	0.41
1:C:64:ILE:O	1:C:99:VAL:HA	2.20	0.41
1:A:407:ALA:HA	1:A:430:VAL:O	2.20	0.41
1:C:423:GLN:HA	1:C:448:ILE:O	2.20	0.41
1:A:237:PRO:HA	1:A:238:PRO:HD3	1.92	0.41
2:D:16:CYS:HB3	2:D:20:ALA:HB3	2.02	0.41
1:A:327:ASN:HD22	1:A:371:TYR:H	1.69	0.41
1:A:16:LYS:HG2	1:A:43:PRO:HG3	2.03	0.41
1:C:113:ARG:NH1	1:C:113:ARG:HG3	2.34	0.41
1:C:62:ILE:CD1	1:C:77:LEU:HD11	2.51	0.41
1:A:71:LYS:HG2	1:A:106:THR:CG2	2.51	0.40
1:A:74:PHE:HB2	1:A:109:ILE:HG23	2.03	0.40
1:C:80:ILE:HB	1:C:115:VAL:HG22	2.03	0.40
1:A:356:PRO:HG3	1:A:381:PHE:HB2	2.03	0.40
1:A:489:ASP:HB3	1:A:502:THR:HG22	2.04	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	514/601 (86%)	473 (92%)	38 (7%)	3 (1%)	25	64
1	C	528/601 (88%)	492 (93%)	31 (6%)	5 (1%)	17	56
2	B	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
2	D	55/58 (95%)	52 (94%)	3 (6%)	0	100	100
All	All	1152/1318 (87%)	1068 (93%)	76 (7%)	8 (1%)	22	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	CYS
1	C	511	SER
1	A	0	HIS
1	A	476	ASP
1	C	212	CYS
1	C	275	ASN
1	C	260	GLY
1	C	526	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	438/531 (82%)	419 (96%)	19 (4%)	29	64
1	C	452/531 (85%)	417 (92%)	35 (8%)	13	44
2	B	48/51 (94%)	45 (94%)	3 (6%)	18	52
2	D	47/51 (92%)	44 (94%)	3 (6%)	17	52
All	All	985/1164 (85%)	925 (94%)	60 (6%)	18	54

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	24	ARG
1	A	33	VAL

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Mol	Chain	Res	Type
1	A	104	MET
1	A	128	LEU
1	A	167	THR
1	A	185	THR
1	A	233	LYS
1	A	249	LEU
1	A	267	CYS
1	A	287	MET
1	A	300	CYS
1	A	375	GLU
1	A	416	LEU
1	A	429	VAL
1	A	437	LEU
1	A	453	GLU
1	A	456	VAL
1	A	463	ARG
1	C	12	VAL
1	C	33	VAL
1	C	47	LEU
1	C	52	LEU
1	C	67	VAL
1	C	77	LEU
1	C	84	THR
1	C	99	VAL
1	C	102	SER
1	C	104	MET
1	C	107	LEU
1	C	125	ASN
1	C	128	LEU
1	C	132	ARG
1	C	137	SER
1	C	156	GLU
1	C	185	THR
1	C	201	ARG
1	C	223	CYS
1	C	231	VAL
1	C	265	LYS
1	C	296	CYS
1	C	300	CYS
1	C	304	CYS
1	C	308	THR
1	C	322	THR

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Mol	Chain	Res	Type
1	C	327	ASN
1	C	330	ILE
1	C	331	LEU
1	C	354	LEU
1	C	406	LEU
1	C	462	LEU
1	C	465	ASP
1	C	496	ASN
1	C	537	ASP
2	D	4	THR
2	D	27	ILE
2	D	42	MET
2	B	7	CYS
2	B	42	MET
2	B	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	163	HIS
1	A	177	ASN
1	A	275	ASN
1	A	327	ASN
1	A	378	HIS
1	A	394	HIS
1	A	420	ASN
1	A	449	GLN
1	A	454	GLN
1	C	36	ASN
1	C	54	ASN
1	C	66	HIS
1	C	177	ASN
1	C	205	HIS
1	C	327	ASN
1	C	333	GLN
1	C	373	ASN
1	C	394	HIS
1	C	420	ASN
1	C	433	HIS
1	C	454	GLN
1	C	496	ASN

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Mol	Chain	Res	Type
1	C	498	ASN
2	D	44	GLN

### 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 ⓘ

12 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	E	1	1,3	14,14,15	0.64	0	17,19,21	1.54	2 (11%)
3	NAG	E	2	3	14,14,15	0.62	0	17,19,21	0.79	0
3	MAN	E	3	3	11,11,12	0.72	0	15,15,17	1.73	4 (26%)
3	MAN	E	4	3	11,11,12	0.89	0	15,15,17	2.59	8 (53%)
3	MAN	E	5	3	11,11,12	0.69	0	15,15,17	0.65	0
3	MAN	E	6	3	11,11,12	0.69	0	15,15,17	1.30	3 (20%)
4	NAG	F	1	1,4	14,14,15	0.63	0	17,19,21	1.17	1 (5%)
4	NAG	F	2	4	14,14,15	0.48	0	17,19,21	1.18	2 (11%)
5	NAG	G	1	1,5	14,14,15	0.50	0	17,19,21	1.36	3 (17%)
5	NAG	G	2	5	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
5	MAN	G	3	5	11,11,12	0.72	0	15,15,17	1.32	1 (6%)
5	MAN	G	4	5	11,11,12	0.71	0	15,15,17	1.56	4 (26%)

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	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	MAN	E	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	E	4	3	1/1/4/5	2/2/19/22	0/1/1/1
3	MAN	E	5	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	E	6	3	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	MAN	G	4	5	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	-5.57	104.64	112.19
3	E	1	NAG	C2-N2-C7	4.98	130.00	122.90
3	E	4	MAN	C2-C3-C4	3.66	117.23	110.89
3	E	4	MAN	O5-C5-C6	3.36	112.47	107.20
3	E	4	MAN	C3-C4-C5	3.28	116.09	110.24
3	E	3	MAN	C1-C2-C3	3.27	113.69	109.67
3	E	3	MAN	O5-C5-C6	3.19	112.20	107.20
5	G	1	NAG	C2-N2-C7	3.09	127.30	122.90
3	E	4	MAN	O4-C4-C5	-3.03	101.76	109.30
4	F	2	NAG	C1-O5-C5	2.97	116.21	112.19
4	F	1	NAG	C4-C3-C2	2.90	115.27	111.02
5	G	4	MAN	C1-O5-C5	-2.87	108.31	112.19
3	E	4	MAN	O5-C1-C2	-2.86	106.35	110.77
3	E	1	NAG	O7-C7-N2	2.68	126.88	121.95
5	G	4	MAN	C3-C4-C5	2.66	114.98	110.24
3	E	6	MAN	C3-C4-C5	2.65	114.97	110.24
3	E	3	MAN	O3-C3-C2	-2.64	104.93	109.99
5	G	2	NAG	C1-O5-C5	2.62	115.74	112.19
3	E	4	MAN	O4-C4-C3	2.59	116.34	110.35
5	G	3	MAN	O3-C3-C2	2.58	114.94	109.99
5	G	4	MAN	C2-C3-C4	2.55	115.31	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C1-O5-C5	2.53	115.62	112.19
3	E	6	MAN	C2-C3-C4	2.45	115.13	110.89
3	E	3	MAN	O3-C3-C4	-2.43	104.72	110.35
5	G	4	MAN	O5-C5-C6	2.31	110.82	107.20
3	E	6	MAN	O5-C5-C6	2.26	110.75	107.20
4	F	2	NAG	C3-C4-C5	2.11	114.01	110.24
3	E	4	MAN	C1-C2-C3	-2.04	107.16	109.67
5	G	1	NAG	O5-C5-C6	2.02	110.38	107.20

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	4	MAN	C1
5	G	3	MAN	C1
3	E	3	MAN	C1
3	E	6	MAN	C1
3	E	5	MAN	C1
3	E	4	MAN	C1

All (12) torsion outliers are listed below:

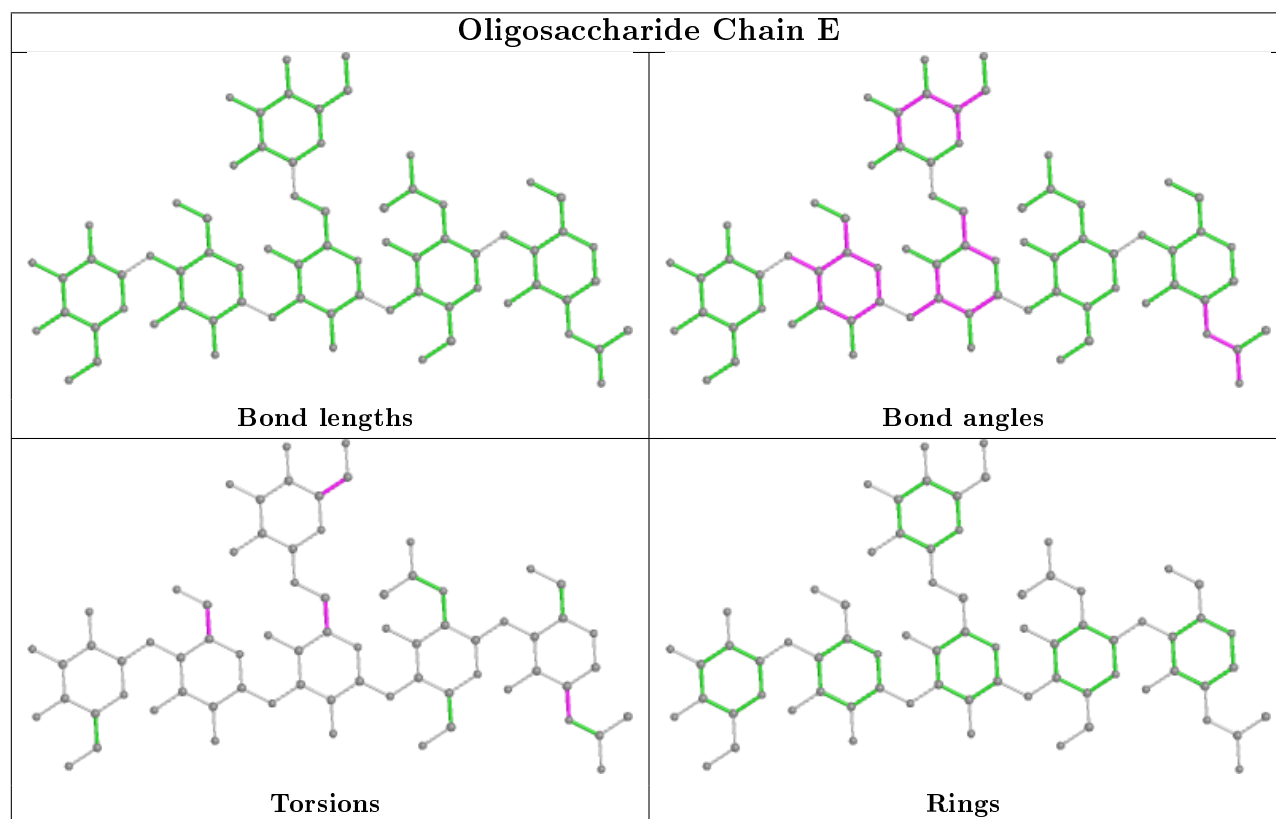
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
4	F	2	NAG	O5-C5-C6-O6
5	G	3	MAN	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
5	G	3	MAN	O5-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
3	E	3	MAN	C4-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7

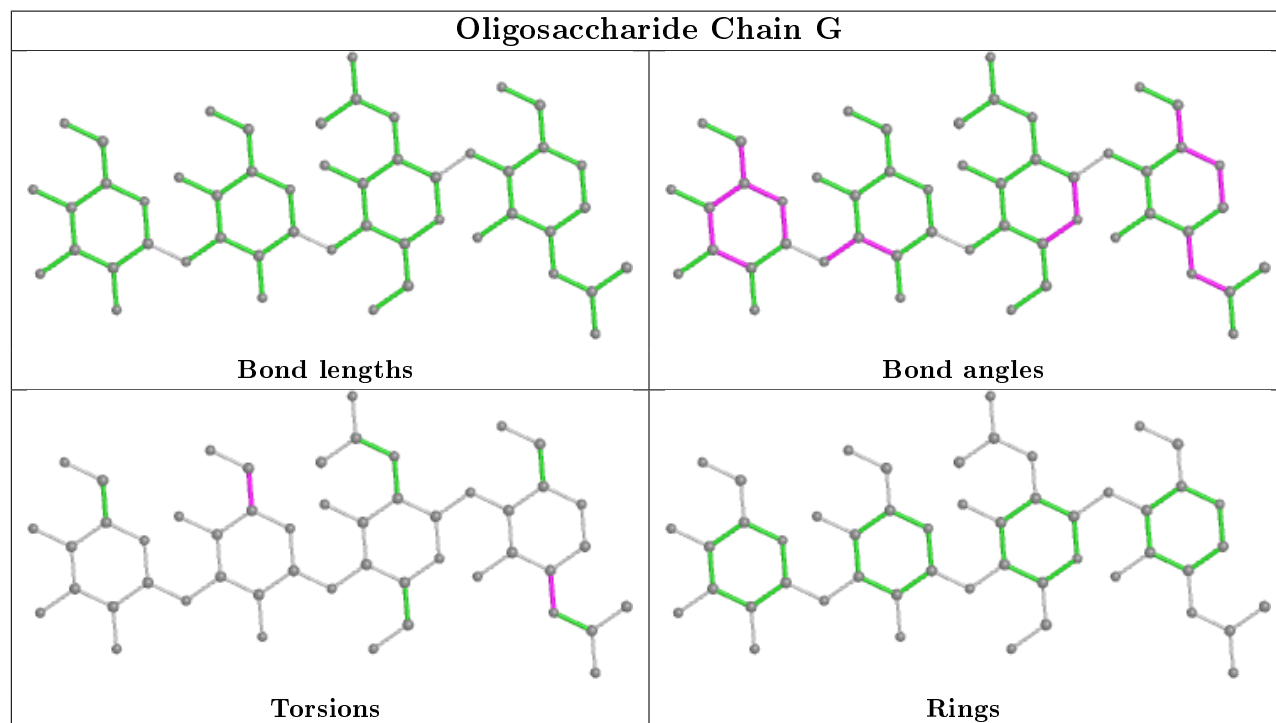
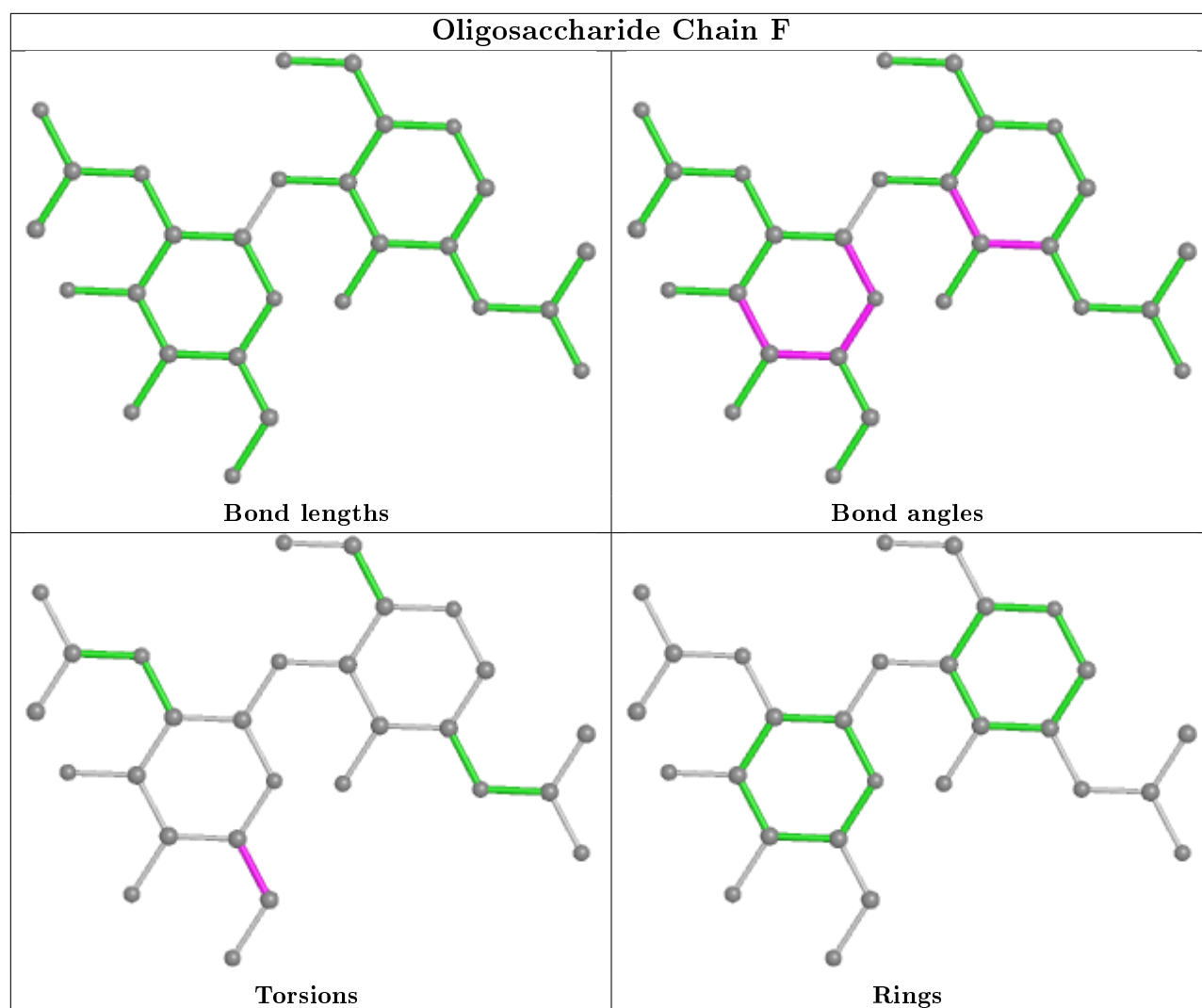
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	MAN	2	0
3	E	6	MAN	1	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

4 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
7	MLI	A	596	-	0,6,6	0.00	-	0,7,7	0.00	-
6	NAG	A	3830	1	14,14,15	0.48	0	17,19,21	0.91	1 (5%)
6	NAG	C	3440	1	14,14,15	0.64	0	17,19,21	1.00	1 (5%)
6	NAG	C	596	1	14,14,15	0.65	0	17,19,21	0.98	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MLI	A	596	-	-	0/0/4/4	-
6	NAG	A	3830	1	-	2/6/23/26	0/1/1/1
6	NAG	C	3440	1	-	0/6/23/26	0/1/1/1
6	NAG	C	596	1	1/1/5/7	0/6/23/26	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(°)
6	A	3830	NAG	C1-O5-C5	3.09	116.39	112.19
6	C	596	NAG	C4-C3-C2	2.07	114.05	111.02
6	C	3440	NAG	C1-O5-C5	2.05	114.97	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	596	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3830	NAG	C4-C5-C6-O6
6	A	3830	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	522/601 (86%)	0.11	25 (4%) 30 18	58, 81, 119, 169	0
1	C	531/601 (88%)	0.15	16 (3%) 50 34	52, 74, 121, 166	0
2	B	57/58 (98%)	0.24	6 (10%) 6 3	70, 103, 136, 144	0
2	D	57/58 (98%)	-0.11	0 100 100	58, 72, 95, 112	0
All	All	1167/1318 (88%)	0.12	47 (4%) 38 25	52, 78, 124, 169	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	507	CYS	6.3
1	C	299	PRO	4.8
1	A	506	ASP	4.8
1	A	508	GLY	3.9
1	A	518	ASN	3.7
2	B	14	TRP	3.5
1	A	521	CYS	3.5
1	C	526	PRO	3.4
1	C	296	CYS	3.3
1	A	499	PHE	3.1
1	A	510	ILE	3.0
1	A	505	ALA	3.0
2	B	2	PHE	2.9
1	A	168	HIS	2.9
1	C	158	GLU	2.8
1	A	175	PRO	2.8
1	C	153	THR	2.8
1	C	532	ASN	2.8
1	A	498	ASN	2.8
1	C	297	ASN	2.7
1	A	524	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	509	TYR	2.7
1	C	518	ASN	2.7
1	A	154	ALA	2.7
2	B	21	HIS	2.6
1	A	192	GLY	2.5
1	C	536	ALA	2.5
1	A	164	GLU	2.5
1	A	495	LYS	2.5
1	A	502	THR	2.5
1	A	496	ASN	2.4
2	B	28	ALA	2.4
1	A	520	THR	2.4
1	A	497	PHE	2.4
1	C	301	PRO	2.4
1	C	510	ILE	2.3
2	B	27	ILE	2.3
2	B	29	ASP	2.3
1	C	525	HIS	2.3
1	C	509	TYR	2.2
1	C	298	GLY	2.2
1	A	517	ASP	2.2
1	A	488	THR	2.2
1	C	295	PRO	2.2
1	A	504	ILE	2.2
1	A	514	TYR	2.0
1	C	275	ASN	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.

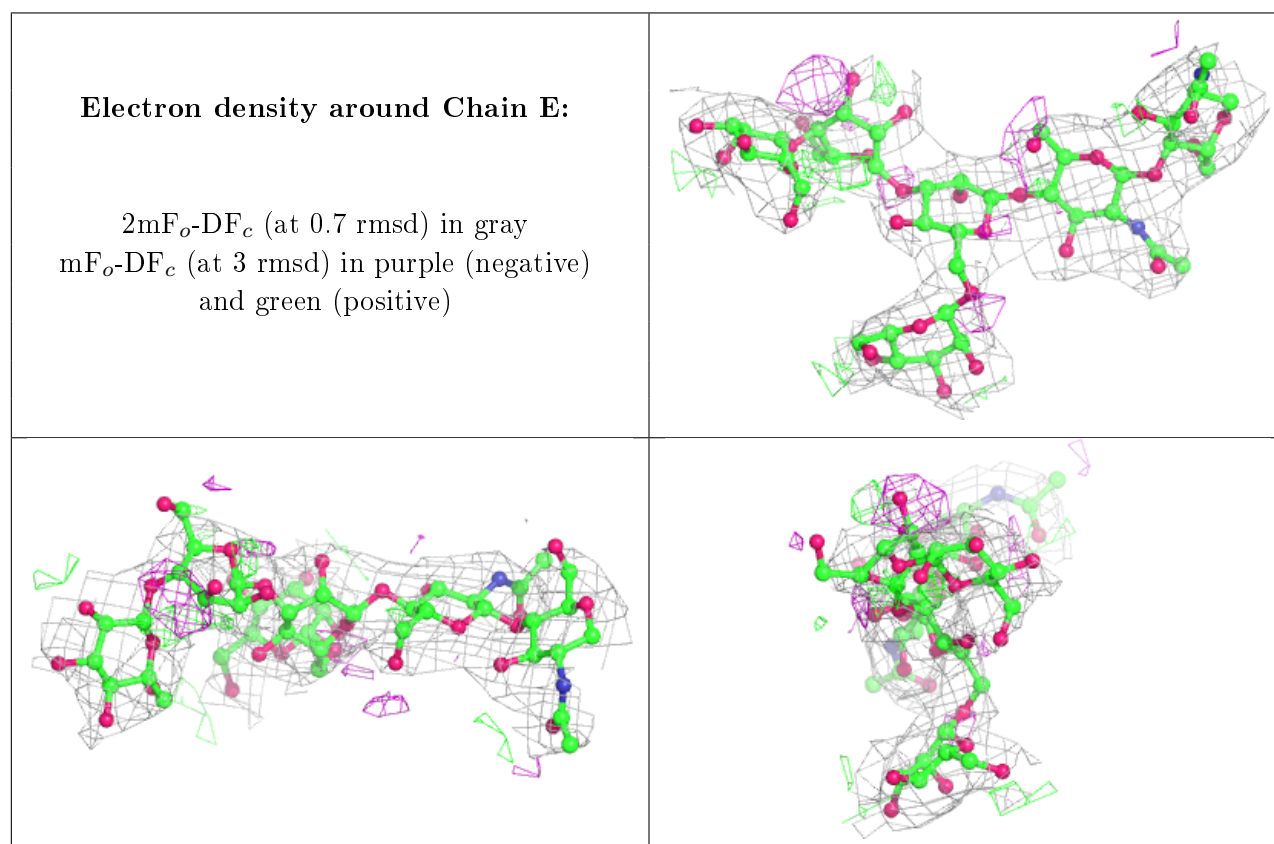
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	E	6	11/12	0.73	0.40	94,95,95,96	0
3	MAN	E	4	11/12	0.82	0.31	88,90,91,91	0

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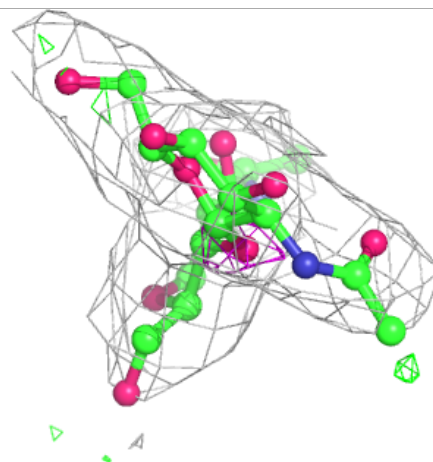
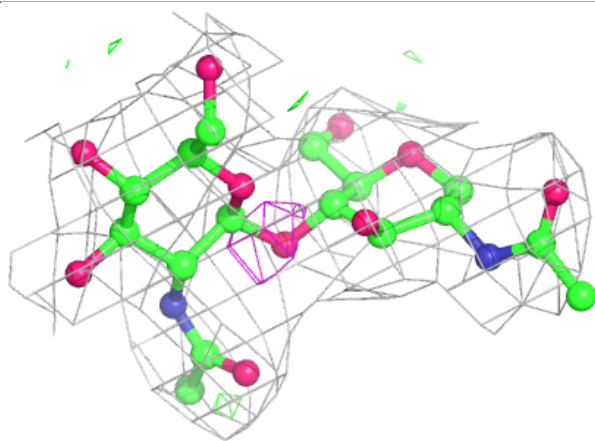
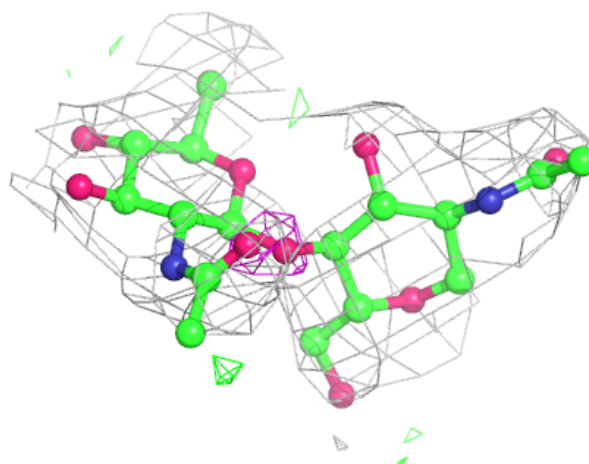
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	G	4	11/12	0.84	0.25	70,72,73,73	0
3	MAN	E	3	11/12	0.87	0.28	82,85,89,92	0
3	MAN	E	5	11/12	0.88	0.30	90,91,91,91	0
4	NAG	F	1	14/15	0.90	0.18	73,78,80,83	0
5	MAN	G	3	11/12	0.90	0.24	69,70,71,71	0
4	NAG	F	2	14/15	0.92	0.21	85,87,87,88	0
3	NAG	E	1	14/15	0.94	0.23	66,69,71,71	0
3	NAG	E	2	14/15	0.95	0.23	73,74,76,79	0
5	NAG	G	2	14/15	0.96	0.28	65,66,67,68	0
5	NAG	G	1	14/15	0.97	0.28	59,61,63,64	0

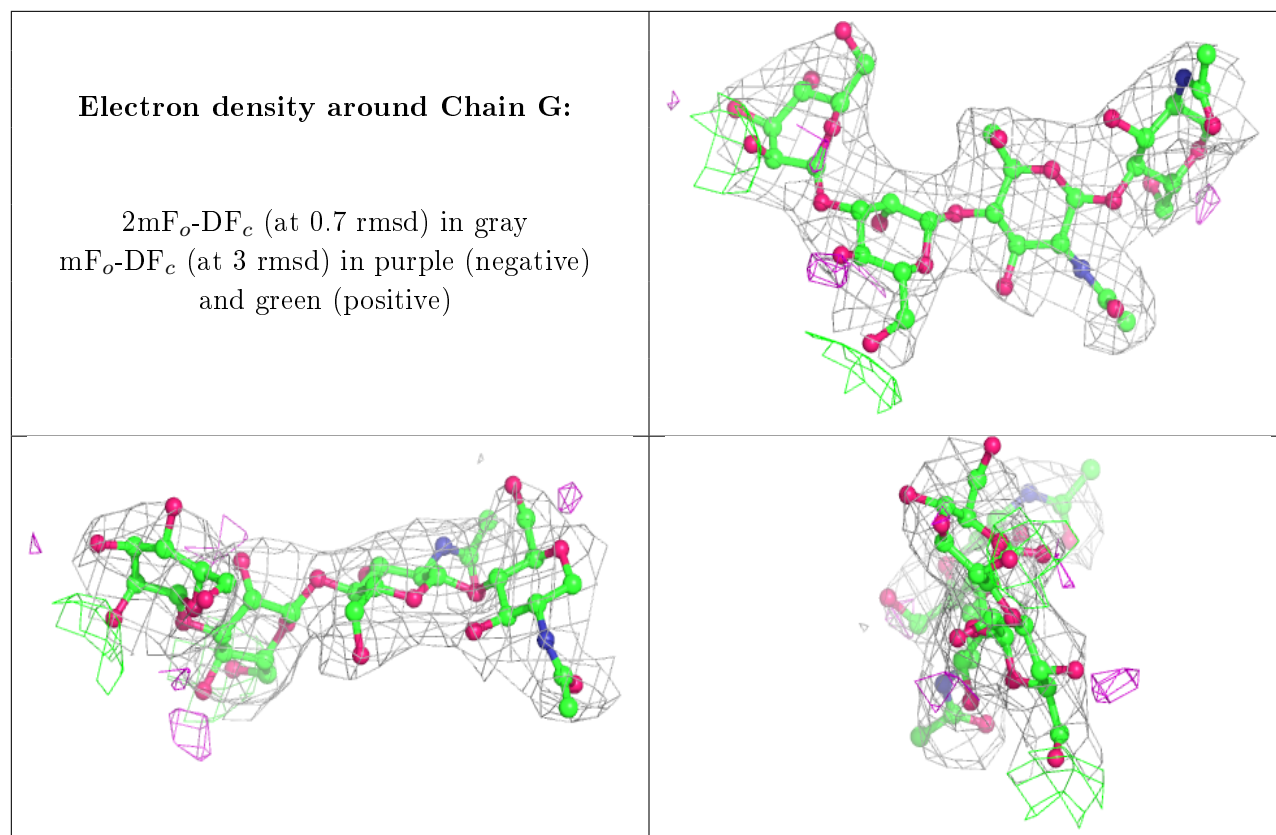
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain F:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MLI	A	596	7/7	0.76	0.41	69,70,70,71	0
6	NAG	C	3440	14/15	0.82	0.30	87,90,92,93	0
6	NAG	A	3830	14/15	0.88	0.21	76,79,80,80	0
6	NAG	C	596	14/15	0.88	0.40	81,84,85,85	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.