



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:08 AM BST

PDB ID : 5U8Q  
Title : Structure of the ectodomain of the human Type 1 insulin-like growth factor receptor in complex with IGF-I  
Authors : Lawrence, M.; Xu, Y.  
Deposited on : 2016-12-14  
Resolution : 3.27 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

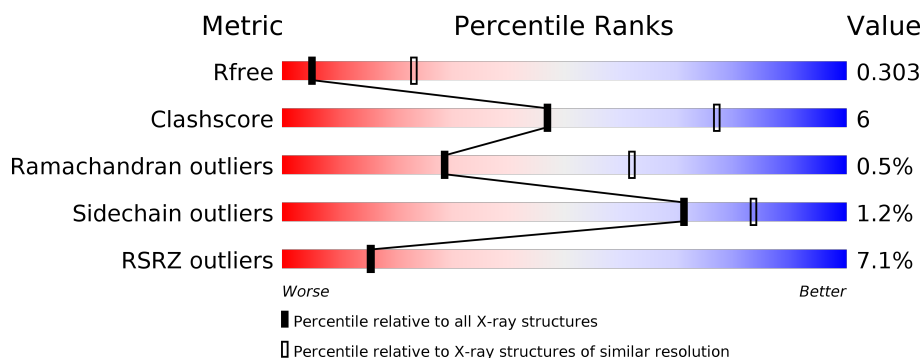
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.27 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	885	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>9%</div> </div> </div>
2	B	70	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>7%</div> <div>31%</div> </div> </div>
3	H	126	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
4	L	108	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>..</div> </div> </div>
5	C	2	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>
5	E	2	<div> <div></div> <div> <div></div> <div>100%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	D	4	<div><div></div><div>50%</div><div></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
5	NAG	C	2	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8704 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 Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6427	4066	1112	1202	47			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	MET	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	ARG	deletion	UNP P08069
A	?	-	SER	deletion	UNP P08069
A	?	-	ARG	deletion	UNP P08069
A	?	-	ASN	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	ALA	deletion	UNP P08069
A	?	-	ALA	deletion	UNP P08069
A	?	-	ASP	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	TYR	deletion	UNP P08069
A	?	-	ASN	deletion	UNP P08069
A	?	-	ILE	deletion	UNP P08069
A	?	-	THR	deletion	UNP P08069
A	?	-	ASP	deletion	UNP P08069
A	738	ALA	PRO	conflict	UNP P08069
A	739	GLY	GLU	conflict	UNP P08069
A	740	ASN	GLU	conflict	UNP P08069
A	741	ASN	LEU	conflict	UNP P08069

- Molecule 2 is a protein called Insulin-like growth factor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	48	Total	C	N	O	S	0	0	0
			375	235	63	70	7			

- Molecule 3 is a protein called Fv 24-60 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	118	Total	C	N	O	S	0	0	0
			915	581	150	181	3			

- Molecule 4 is a protein called Fv 24-60 light chain.

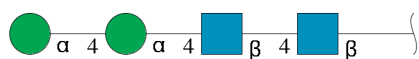
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	107	Total	C	N	O	S	0	0	0
			820	511	140	166	3			

- Molecule 5 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
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



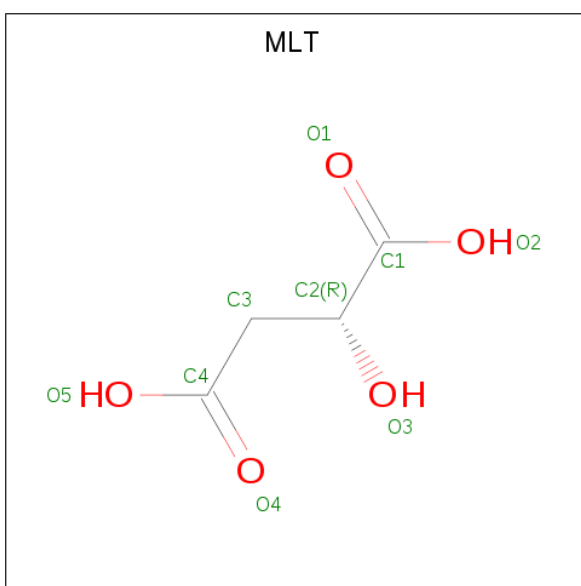
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

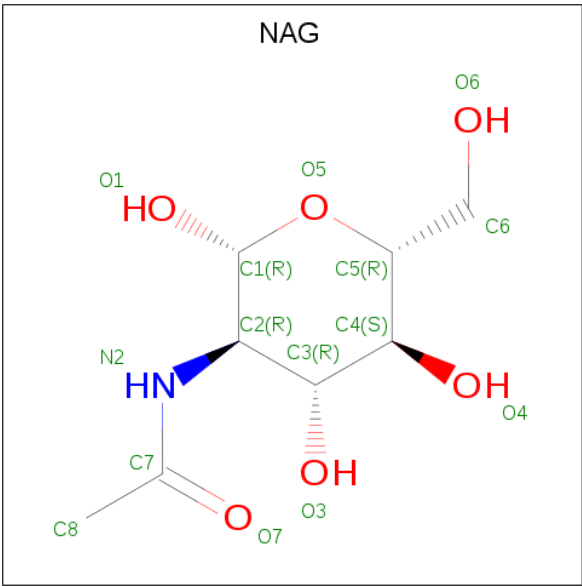
- Molecule 8 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

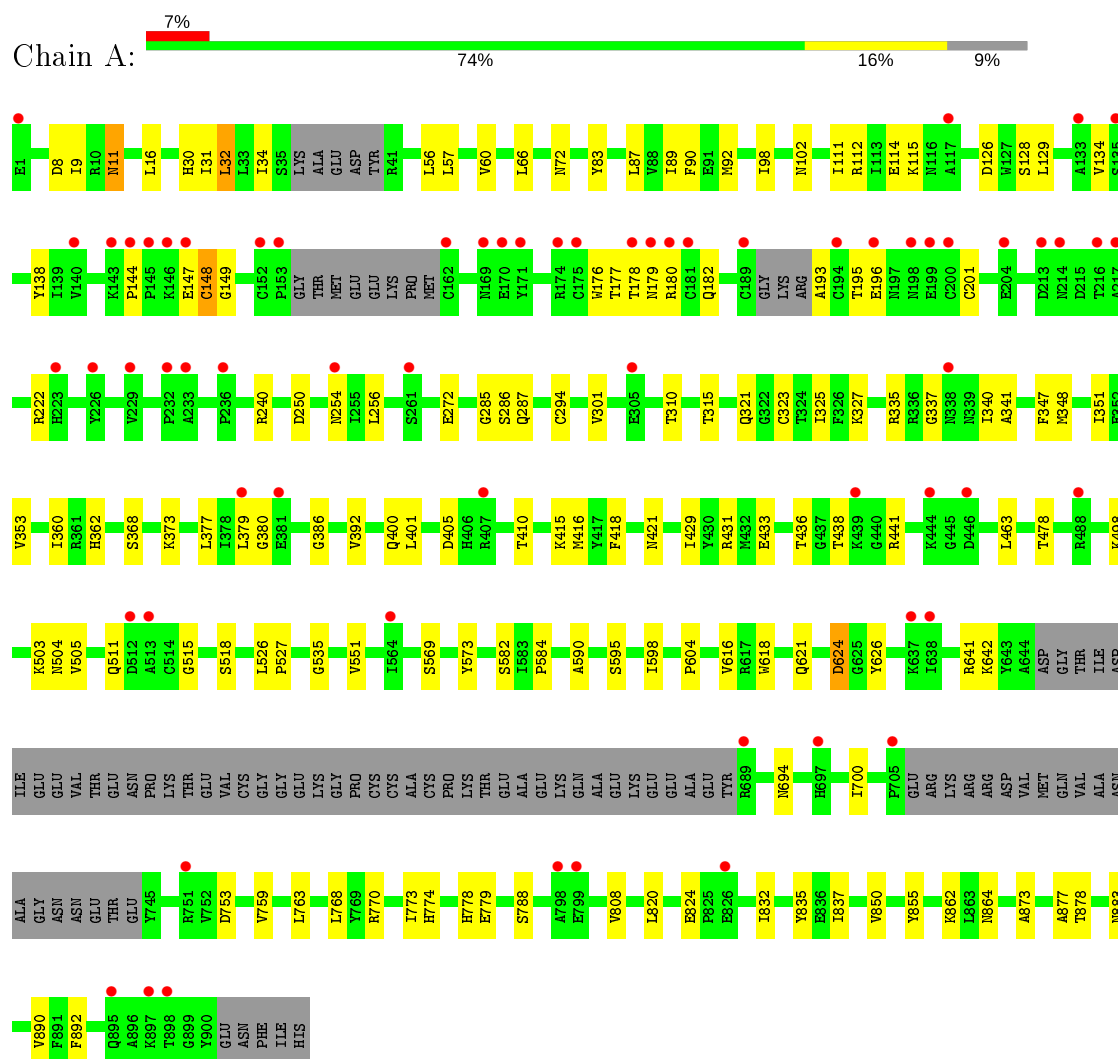


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

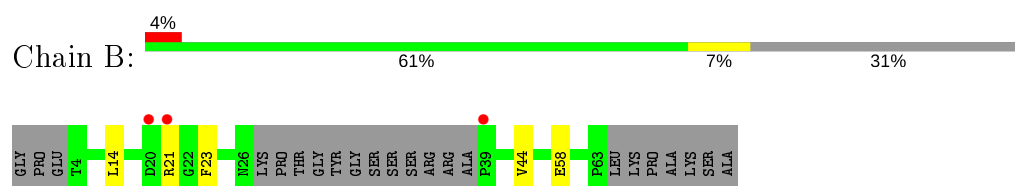
### 3 Residue-property plots [i](#)

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.

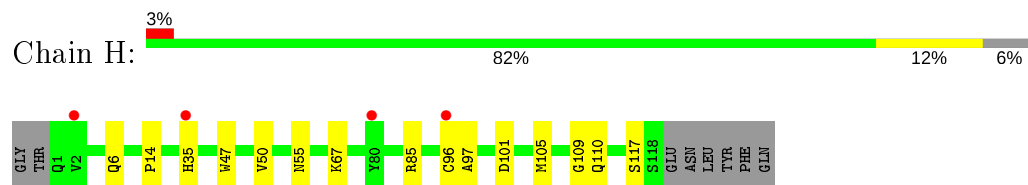
- Molecule 1: Insulin-like growth factor 1 receptor



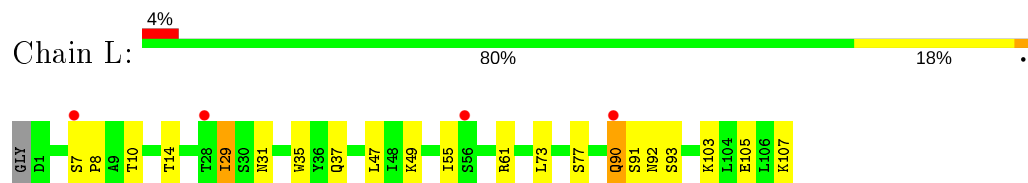
- Molecule 2: Insulin-like growth factor I



- Molecule 3: Fv 24-60 heavy chain



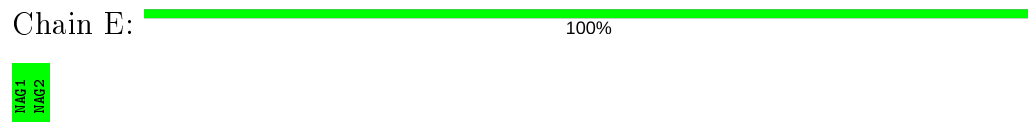
- Molecule 4: Fv 24-60 light chain



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.69 Å 197.66 Å 117.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.17 – 3.27 22.17 – 3.27	Depositor EDS
% Data completeness (in resolution range)	98.6 (22.17-3.27) 99.1 (22.17-3.27)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.30 Å)	Xtriage
Refinement program	phenix.refine 1.11.1-2575_1692, PHENIX 1.11.1-2575_1692	Depositor
R, $R_{free}$	0.260 , 0.303 0.260 , 0.303	Depositor DCC
$R_{free}$ test set	1524 reflections (4.72%)	wwPDB-V
Wilson B-factor (Å <sup>2</sup> )	111.0	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 97.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8704	wwPDB-V
Average B, all atoms (Å <sup>2</sup> )	177.0	wwPDB-V

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: SO4, NAG, MLT, 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	0.24	0/6582	0.44	0/8931
2	B	0.24	0/381	0.39	0/511
3	H	0.24	0/936	0.44	0/1270
4	L	0.25	0/838	0.47	0/1136
All	All	0.24	0/8737	0.44	0/11848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	6427	0	6220	81	0
2	B	375	0	347	5	0
3	H	915	0	888	10	0
4	L	820	0	792	13	0
5	C	28	0	25	1	0
5	E	28	0	25	0	0
6	D	50	0	43	0	0
7	A	10	0	0	0	0
8	A	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	42	0	39	0	0
All	All	8704	0	8383	106	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 6.

All (106) 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:511:GLN:H	1:A:515:GLY:HA3	1.58	0.69
1:A:114:GLU:HG2	1:A:115:LYS:HG3	1.75	0.68
1:A:433:GLU:HA	1:A:436:THR:HB	1.75	0.67
1:A:337:GLY:HA3	1:A:340:ILE:HD11	1.78	0.66
1:A:144:PRO:HG2	1:A:147:GLU:HB2	1.78	0.64
1:A:348:MET:HA	1:A:351:ILE:HD13	1.81	0.63
1:A:9:ILE:HD13	1:A:16:LEU:HA	1.81	0.62
1:A:240:ARG:HD2	1:A:272:GLU:HG2	1.82	0.61
1:A:256:LEU:O	3:H:55:ASN:ND2	2.34	0.61
1:A:360:ILE:HB	1:A:392:VAL:HG12	1.83	0.60
3:H:67:LYS:NZ	3:H:85:ARG:O	2.33	0.60
1:A:808:VAL:HB	1:A:890:VAL:HG11	1.83	0.60
1:A:87:LEU:HB3	1:A:111:ILE:HD12	1.86	0.58
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.85	0.58
3:H:47:TRP:HZ2	3:H:50:VAL:HG23	1.69	0.58
1:A:193:ALA:HB1	1:A:201:CYS:HB2	1.87	0.57
1:A:112:ARG:NH1	1:A:114:GLU:OE1	2.38	0.57
1:A:148:CYS:SG	1:A:149:GLY:N	2.78	0.56
4:L:10:THR:HG22	4:L:103:LYS:HB3	1.86	0.56
1:A:340:ILE:HB	1:A:511:GLN:HG3	1.86	0.56
1:A:129:LEU:HD11	1:A:182:GLN:HE21	1.71	0.56
1:A:598:ILE:HG22	1:A:759:VAL:HG22	1.88	0.56
4:L:90:GLN:OE1	4:L:92:ASN:ND2	2.39	0.55
2:B:21:ARG:NH1	2:B:58:GLU:OE1	2.34	0.55
1:A:878:THR:HA	1:A:883:ASN:HA	1.89	0.54
3:H:97:ALA:HB1	3:H:105:MET:HB3	1.90	0.54
4:L:7:SER:HB2	4:L:8:PRO:HD3	1.90	0.54
1:A:112:ARG:HG3	1:A:138:TYR:HB3	1.90	0.53
1:A:31:ILE:HB	1:A:57:LEU:HD23	1.90	0.53
1:A:66:LEU:HD12	1:A:98:ILE:HG23	1.91	0.53
1:A:301:VAL:HG11	1:A:327:LYS:HE3	1.91	0.53
4:L:49:LYS:HG3	4:L:55:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:VAL:HG22	1:A:377:LEU:HB2	1.91	0.52
1:A:503:LYS:O	1:A:573:TYR:OH	2.22	0.52
4:L:29:ILE:HG13	4:L:31:ASN:O	2.10	0.51
1:A:526:LEU:HD12	1:A:527:PRO:HD2	1.92	0.51
1:A:778:HIS:CD2	1:A:779:GLU:HG2	2.46	0.51
1:A:503:LYS:O	1:A:505:VAL:N	2.42	0.51
3:H:47:TRP:CZ2	3:H:50:VAL:HG23	2.45	0.51
1:A:89:ILE:HG23	1:A:92:MET:HG3	1.93	0.51
1:A:595:SER:HA	1:A:763:LEU:HB2	1.92	0.51
1:A:753:ASP:OD1	1:A:753:ASP:N	2.40	0.50
1:A:582:SER:HB3	1:A:604:PRO:HB2	1.93	0.50
1:A:584:PRO:HG2	1:A:773:ILE:HG22	1.92	0.50
1:A:285:GLY:O	1:A:287:GLN:N	2.45	0.49
1:A:392:VAL:HG23	1:A:421:ASN:HD21	1.78	0.49
2:B:14:LEU:HB3	2:B:23:PHE:HE2	1.78	0.49
1:A:774:HIS:CE1	1:A:788:SER:HB3	2.48	0.49
1:A:90:PHE:HD1	1:A:114:GLU:HB3	1.78	0.48
1:A:694:ASN:HA	2:B:44:VAL:HG21	1.96	0.48
1:A:34:ILE:HB	1:A:60:VAL:HG13	1.95	0.47
1:A:32:LEU:HD11	1:A:56:LEU:HD22	1.96	0.47
3:H:6:GLN:H	3:H:110:GLN:HE22	1.60	0.47
1:A:405:ASP:OD1	1:A:431:ARG:NE	2.48	0.47
1:A:250:ASP:O	1:A:254:ASN:ND2	2.42	0.47
1:A:478:THR:HG22	1:A:535:GLY:HA3	1.97	0.47
1:A:72:ASN:HA	1:A:102:ASN:HD22	1.80	0.47
3:H:35:HIS:NE2	3:H:101:ASP:O	2.45	0.47
1:A:126:ASP:OD1	1:A:128:SER:OG	2.26	0.46
1:A:335:ARG:HH11	1:A:362:HIS:HB3	1.80	0.46
1:A:624:ASP:OD1	1:A:641:ARG:NH1	2.48	0.46
1:A:401:LEU:HD11	1:A:429:ILE:HG22	1.98	0.46
1:A:8:ASP:HA	1:A:30:HIS:HB2	1.97	0.46
3:H:35:HIS:HB2	3:H:97:ALA:HB3	1.98	0.46
1:A:177:THR:HG23	1:A:180:ARG:H	1.81	0.45
1:A:11:ASN:CG	2:B:23:PHE:H	2.19	0.45
1:A:325:ILE:HG23	1:A:353:VAL:HB	1.98	0.45
1:A:222:ARG:HH11	5:C:2:NAG:H82	1.81	0.45
1:A:590:ALA:HB3	1:A:598:ILE:HD11	1.98	0.45
1:A:177:THR:HG23	1:A:179:ASN:H	1.81	0.45
4:L:14:THR:HG23	4:L:107:LYS:HB3	1.97	0.45
3:H:96:CYS:O	3:H:109:GLY:N	2.45	0.45
1:A:438:THR:HG22	1:A:441:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:HB3	2:B:23:PHE:CE2	2.51	0.45
1:A:618:TRP:HA	1:A:770:ARG:O	2.17	0.45
1:A:551:VAL:N	1:A:569:SER:OG	2.42	0.44
4:L:91:SER:OG	4:L:91:SER:O	2.33	0.44
1:A:177:THR:OG1	1:A:178:THR:N	2.50	0.44
1:A:368:SER:HA	1:A:400:GLN:O	2.18	0.44
1:A:377:LEU:HD23	1:A:410:THR:HB	1.98	0.44
4:L:92:ASN:OD1	4:L:93:SER:N	2.51	0.44
1:A:128:SER:HA	1:A:134:VAL:HG21	2.00	0.44
1:A:873:ALA:HB2	1:A:892:PHE:HE1	1.82	0.44
1:A:835:TYR:HB2	1:A:850:VAL:HB	2.00	0.43
1:A:498:LYS:HD2	1:A:518:SER:HB2	1.99	0.43
1:A:323:CYS:HB2	1:A:351:ILE:HD11	2.00	0.43
1:A:176:TRP:CD1	1:A:182:GLN:HA	2.54	0.43
1:A:820:LEU:HD12	1:A:837:ILE:HD13	2.00	0.43
1:A:195:THR:OG1	1:A:196:GLU:N	2.51	0.43
1:A:341:ALA:HB2	1:A:511:GLN:HE21	1.84	0.43
1:A:824:GLU:HB2	1:A:855:TYR:CE1	2.54	0.43
1:A:32:LEU:HD23	1:A:700:ILE:HG23	2.01	0.42
1:A:832:ILE:HD12	1:A:877:ALA:HB1	2.02	0.42
4:L:49:LYS:HE2	4:L:55:ILE:HG13	2.01	0.41
1:A:321:GLN:HB2	1:A:347:PHE:HD1	1.85	0.41
1:A:386:GLY:O	1:A:415:LYS:NZ	2.41	0.41
3:H:14:PRO:HD3	3:H:117:SER:O	2.20	0.41
4:L:61:ARG:HD2	4:L:77:SER:O	2.20	0.41
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.56	0.41
1:A:621:GLN:HB2	1:A:768:LEU:HB3	2.03	0.41
1:A:416:MET:HB3	1:A:418:PHE:HE1	1.85	0.41
1:A:616:VAL:HG12	1:A:773:ILE:HG12	2.03	0.41
1:A:642:LYS:HE2	1:A:642:LYS:HB3	1.86	0.41
1:A:463:LEU:HB2	1:A:569:SER:HB3	2.02	0.41
1:A:862:LYS:HE3	1:A:864:ASN:HB3	2.02	0.41
4:L:103:LYS:NZ	4:L:105:GLU:HB3	2.36	0.40

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	789/885 (89%)	723 (92%)	61 (8%)	5 (1%)	25	58
2	B	44/70 (63%)	40 (91%)	4 (9%)	0	100	100
3	H	116/126 (92%)	111 (96%)	5 (4%)	0	100	100
4	L	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
All	All	1054/1189 (89%)	973 (92%)	76 (7%)	5 (0%)	29	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	SER
1	A	11	ASN
1	A	379	LEU
1	A	380	GLY
1	A	504	ASN

### 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	715/787 (91%)	706 (99%)	9 (1%)	69	82
2	B	41/57 (72%)	41 (100%)	0	100	100
3	H	100/107 (94%)	100 (100%)	0	100	100
4	L	95/95 (100%)	93 (98%)	2 (2%)	53	75
All	All	951/1046 (91%)	940 (99%)	11 (1%)	71	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	83	TYR
1	A	148	CYS
1	A	294	CYS
1	A	310	THR
1	A	315	THR
1	A	373	LYS
1	A	624	ASP
1	A	626	TYR
4	L	29	ILE
4	L	90	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	L	90	GLN
4	L	92	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 ⓘ

8 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
5	NAG	C	1	1,5	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	C	2	5	14,14,15	0.27	0	17,19,21	0.52	0
6	NAG	D	1	1,6	14,14,15	0.46	0	17,19,21	0.38	0
6	NAG	D	2	6	14,14,15	0.29	0	17,19,21	0.45	0
6	MAN	D	3	6	11,11,12	0.95	0	15,15,17	1.17	2 (13%)
6	MAN	D	4	6	11,11,12	0.72	1 (9%)	15,15,17	1.21	2 (13%)
5	NAG	E	1	1,5	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	E	2	5	14,14,15	0.23	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	MAN	D	3	6	-	0/2/19/22	0/1/1/1
6	MAN	D	4	6	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	4	MAN	C1-C2	2.07	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	4	MAN	C1-O5-C5	3.57	117.03	112.19
6	D	3	MAN	C1-O5-C5	2.69	115.84	112.19
6	D	3	MAN	O2-C2-C3	-2.25	105.62	110.14
6	D	4	MAN	O2-C2-C3	-2.17	105.78	110.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

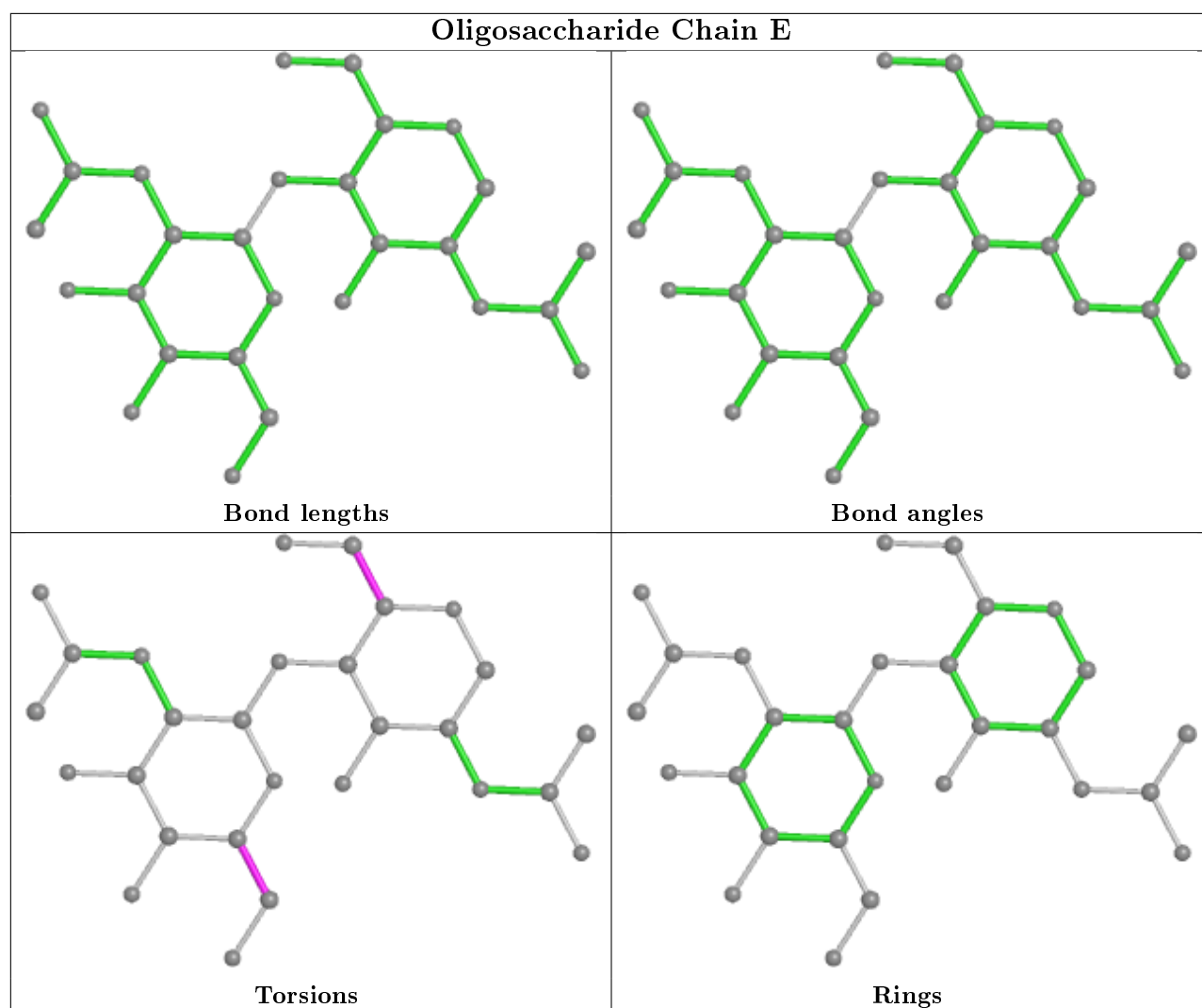
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
6	D	4	MAN	O5-C5-C6-O6
6	D	4	MAN	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	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 ⓘ

6 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	$\# Z  > 2$
9	NAG	A	1004	1	14,14,15	0.25	0	17,19,21	0.54	0
7	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.05	0
7	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.05	0
9	NAG	A	1007	1	14,14,15	0.40	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MLT	A	1003	-	2,8,8	0.50	0	3,10,10	0.86	0
9	NAG	A	1012	1	14,14,15	0.31	0	17,19,21	0.56	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
9	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1004	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1012	1	-	1/6/23/26	0/1/1/1
8	MLT	A	1003	-	-	2/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1003	MLT	C1-C2-C3-C4
8	A	1003	MLT	O3-C2-C3-C4
9	A	1004	NAG	C3-C2-N2-C7
9	A	1012	NAG	C3-C2-N2-C7

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	801/885 (90%)	0.42	65 (8%) 12 11	119, 174, 259, 316	0
2	B	48/70 (68%)	0.27	3 (6%) 20 20	140, 171, 205, 214	0
3	H	118/126 (93%)	0.16	4 (3%) 45 43	109, 147, 196, 222	0
4	L	107/108 (99%)	0.23	4 (3%) 41 39	102, 157, 202, 242	0
All	All	1074/1189 (90%)	0.37	76 (7%) 16 16	102, 170, 251, 316	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	TYR	7.1
1	A	233	ALA	6.4
1	A	146	LYS	5.8
1	A	799	GLU	5.6
1	A	512	ASP	5.4
1	A	178	THR	5.1
1	A	169	ASN	4.8
1	A	444	LYS	4.6
1	A	174	ARG	4.3
1	A	179	ASN	4.3
1	A	147	GLU	4.3
2	B	20	ASP	4.1
1	A	638	ILE	4.0
1	A	216	THR	3.8
1	A	826	GLU	3.7
1	A	379	LEU	3.7
1	A	895	GLN	3.6
1	A	897	LYS	3.6
1	A	439	LYS	3.6
2	B	21	ARG	3.5
1	A	153	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	751	ARG	3.5
1	A	133	ALA	3.5
1	A	689	ARG	3.5
1	A	798	ALA	3.5
1	A	140	VAL	3.4
1	A	217	ALA	3.4
1	A	144	PRO	3.4
1	A	407	ARG	3.2
1	A	446	ASP	3.2
1	A	170	GLU	3.1
1	A	162	CYS	3.0
3	H	96	CYS	2.9
1	A	226	TYR	2.9
1	A	117	ALA	2.8
1	A	175	CYS	2.8
1	A	135	SER	2.8
1	A	261	SER	2.8
1	A	198	ASN	2.8
3	H	35	HIS	2.7
4	L	7	SER	2.7
1	A	196	GLU	2.7
1	A	189	CYS	2.7
1	A	213	ASP	2.6
1	A	637	LYS	2.6
1	A	145	PRO	2.5
1	A	194	CYS	2.4
3	H	80	TYR	2.4
3	H	2	VAL	2.4
1	A	214	ASN	2.4
1	A	181	CYS	2.4
1	A	305	GLU	2.4
1	A	232	PRO	2.3
4	L	90	GLN	2.3
1	A	705	PRO	2.3
1	A	229	VAL	2.3
4	L	28	THR	2.3
1	A	143	LYS	2.3
1	A	223	HIS	2.3
1	A	564	ILE	2.3
1	A	488	ARG	2.3
1	A	1	GLU	2.3
1	A	204	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	180	ARG	2.2
1	A	199	GLU	2.2
1	A	898	THR	2.1
1	A	200	CYS	2.1
2	B	39	PRO	2.1
1	A	697	HIS	2.1
1	A	236	PRO	2.1
1	A	152	CYS	2.1
1	A	513	ALA	2.1
4	L	56	SER	2.0
1	A	381	GLU	2.0
1	A	254	ASN	2.0
1	A	338	ASN	2.0

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

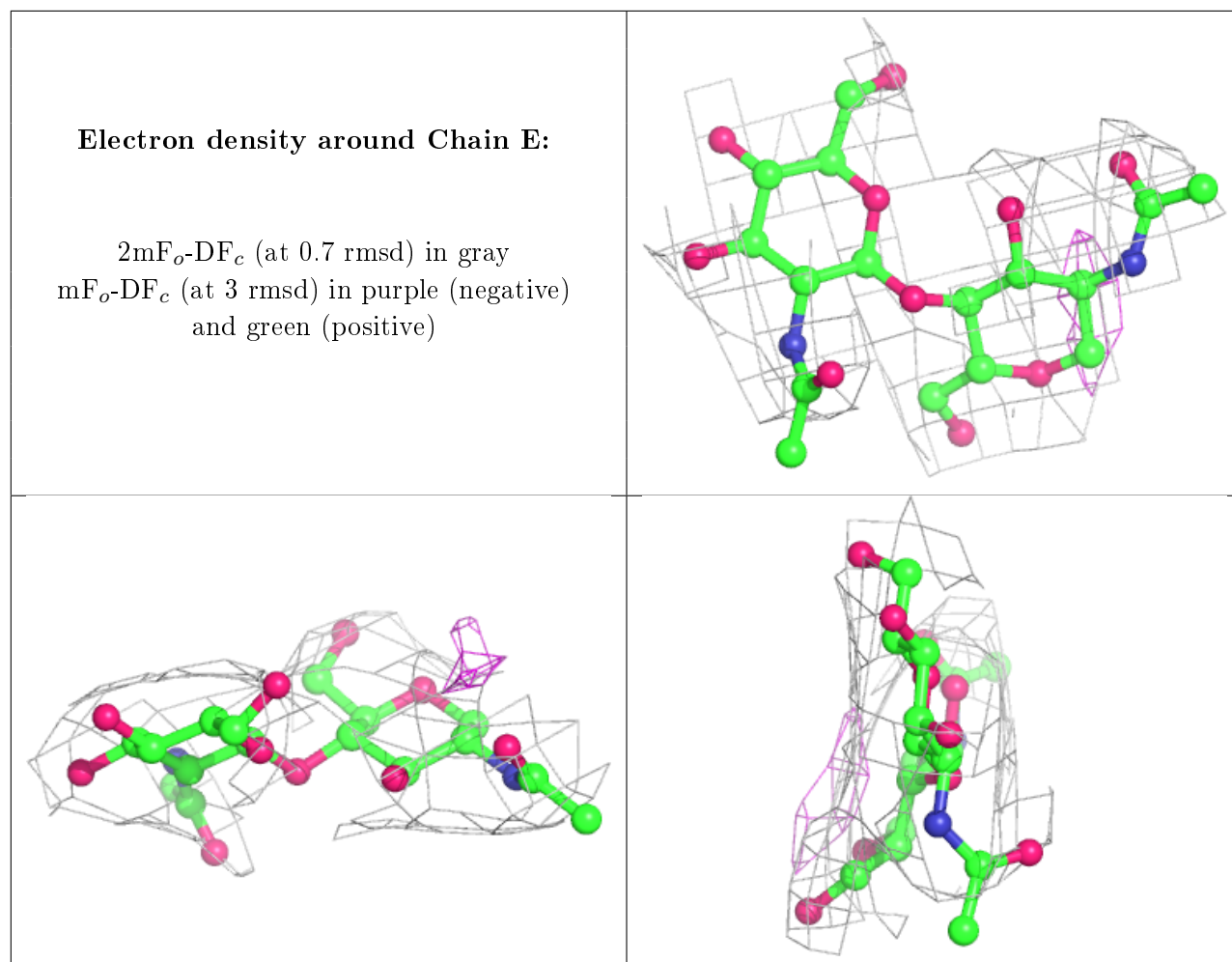
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	C	2	14/15	0.77	0.47	161,231,239,242	0
6	MAN	D	4	11/12	0.81	0.59	189,225,236,236	0
6	MAN	D	3	11/12	0.83	0.45	219,242,253,261	0
6	NAG	D	1	14/15	0.84	0.18	136,164,184,214	0
5	NAG	C	1	14/15	0.87	0.20	177,211,224,225	0
6	NAG	D	2	14/15	0.87	0.34	168,202,218,239	0
5	NAG	E	1	14/15	0.90	0.27	119,153,169,179	0
5	NAG	E	2	14/15	0.91	0.37	150,177,196,200	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( $\text{\AA}^2$ )	Q<0.9
9	NAG	A	1007	14/15	0.64	0.33	188,239,290,327	0
7	SO4	A	1002	5/5	0.74	0.36	172,185,208,221	0
9	NAG	A	1012	14/15	0.74	0.39	159,188,214,215	0
9	NAG	A	1004	14/15	0.81	0.61	172,207,225,227	0
7	SO4	A	1001	5/5	0.82	0.27	163,205,216,216	0
8	MLT	A	1003	9/9	0.83	0.31	137,153,160,161	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.