



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:38 AM BST

PDB ID : 6DLD
Title : Crystal structure of IgLON5/NEGR1 heterodimer
Authors : Ranaivoson, F.M.; Turk, L.S.; Ozkan, E.; Montelione, G.T.; Comoletti, D.
Deposited on : 2018-06-01
Resolution : 3.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

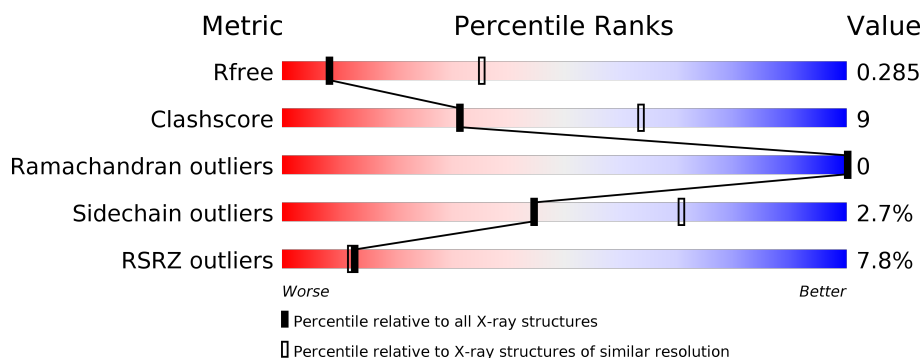
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 ≥ 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	303	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>10%</div> </div> </div>
1	C	303	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	304	<div> <div>12%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>19%</div> </div> </div>
2	D	304	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>12%</div> </div> </div>
3	E	4	<div> <div></div> <div> <div></div> <div>75%</div> <div>25%</div> </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
4	NAG	A	407	-	-	-	X
4	NAG	B	402	-	-	-	X
4	NAG	B	403	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7856 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 IgLON family member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2017	1252	355	400	10			
1	C	267	Total	C	N	O	S	0	0	0
			1937	1213	333	382	9			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASP	-	expression tag	UNP A6NGN9
A	21	TYR	-	expression tag	UNP A6NGN9
A	22	LYS	-	expression tag	UNP A6NGN9
A	23	ASP	-	expression tag	UNP A6NGN9
A	24	ASP	-	expression tag	UNP A6NGN9
A	25	ASP	-	expression tag	UNP A6NGN9
A	26	ASP	-	expression tag	UNP A6NGN9
A	27	LYS	-	expression tag	UNP A6NGN9
A	28	ALA	-	expression tag	UNP A6NGN9
A	29	ALA	-	expression tag	UNP A6NGN9
A	30	ALA	-	expression tag	UNP A6NGN9
A	317	LEU	-	expression tag	UNP A6NGN9
A	318	GLU	-	expression tag	UNP A6NGN9
A	319	VAL	-	expression tag	UNP A6NGN9
A	320	LEU	-	expression tag	UNP A6NGN9
A	321	PHE	-	expression tag	UNP A6NGN9
A	322	GLN	-	expression tag	UNP A6NGN9
C	20	ASP	-	expression tag	UNP A6NGN9
C	21	TYR	-	expression tag	UNP A6NGN9
C	22	LYS	-	expression tag	UNP A6NGN9
C	23	ASP	-	expression tag	UNP A6NGN9
C	24	ASP	-	expression tag	UNP A6NGN9
C	25	ASP	-	expression tag	UNP A6NGN9
C	26	ASP	-	expression tag	UNP A6NGN9
C	27	LYS	-	expression tag	UNP A6NGN9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	ALA	-	expression tag	UNP A6NGN9
C	29	ALA	-	expression tag	UNP A6NGN9
C	30	ALA	-	expression tag	UNP A6NGN9
C	317	LEU	-	expression tag	UNP A6NGN9
C	318	GLU	-	expression tag	UNP A6NGN9
C	319	VAL	-	expression tag	UNP A6NGN9
C	320	LEU	-	expression tag	UNP A6NGN9
C	321	PHE	-	expression tag	UNP A6NGN9
C	322	GLN	-	expression tag	UNP A6NGN9

- Molecule 2 is a protein called Neuronal growth regulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	S	0	0	0
			1719	1069	290	350	10			
2	D	269	Total	C	N	O	S	0	0	0
			1923	1203	329	382	9			

There are 34 discrepancies between the modelled and reference sequences:

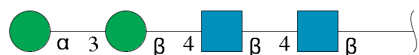
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	ASP	-	expression tag	UNP Q7Z3B1
B	28	TYR	-	expression tag	UNP Q7Z3B1
B	29	LYS	-	expression tag	UNP Q7Z3B1
B	30	ASP	-	expression tag	UNP Q7Z3B1
B	31	ASP	-	expression tag	UNP Q7Z3B1
B	32	ASP	-	expression tag	UNP Q7Z3B1
B	33	ASP	-	expression tag	UNP Q7Z3B1
B	34	LYS	-	expression tag	UNP Q7Z3B1
B	35	ALA	-	expression tag	UNP Q7Z3B1
B	36	ALA	-	expression tag	UNP Q7Z3B1
B	37	ALA	-	expression tag	UNP Q7Z3B1
B	325	LEU	-	expression tag	UNP Q7Z3B1
B	326	GLU	-	expression tag	UNP Q7Z3B1
B	327	VAL	-	expression tag	UNP Q7Z3B1
B	328	LEU	-	expression tag	UNP Q7Z3B1
B	329	PHE	-	expression tag	UNP Q7Z3B1
B	330	GLN	-	expression tag	UNP Q7Z3B1
D	27	ASP	-	expression tag	UNP Q7Z3B1
D	28	TYR	-	expression tag	UNP Q7Z3B1
D	29	LYS	-	expression tag	UNP Q7Z3B1
D	30	ASP	-	expression tag	UNP Q7Z3B1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	31	ASP	-	expression tag	UNP Q7Z3B1
D	32	ASP	-	expression tag	UNP Q7Z3B1
D	33	ASP	-	expression tag	UNP Q7Z3B1
D	34	LYS	-	expression tag	UNP Q7Z3B1
D	35	ALA	-	expression tag	UNP Q7Z3B1
D	36	ALA	-	expression tag	UNP Q7Z3B1
D	37	ALA	-	expression tag	UNP Q7Z3B1
D	325	LEU	-	expression tag	UNP Q7Z3B1
D	326	GLU	-	expression tag	UNP Q7Z3B1
D	327	VAL	-	expression tag	UNP Q7Z3B1
D	328	LEU	-	expression tag	UNP Q7Z3B1
D	329	PHE	-	expression tag	UNP Q7Z3B1
D	330	GLN	-	expression tag	UNP Q7Z3B1

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-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	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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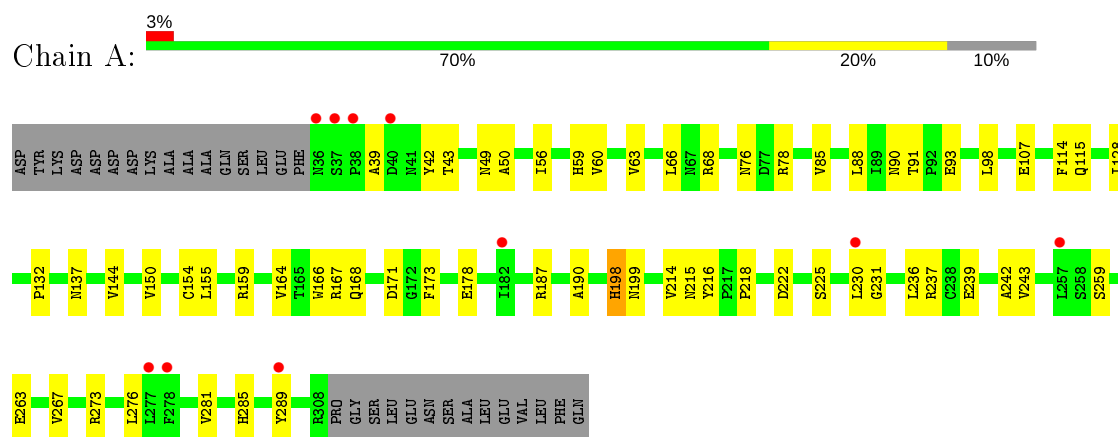
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

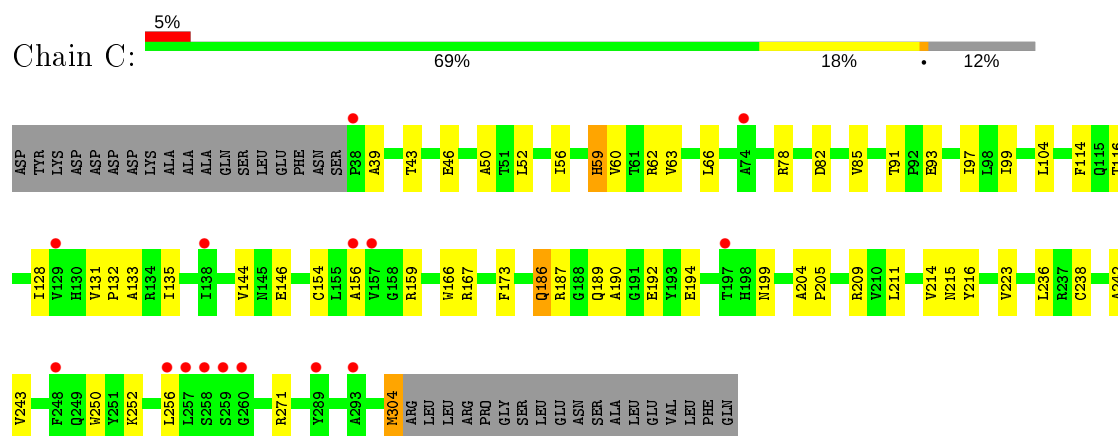
3 Residue-property plots [i](#)

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.

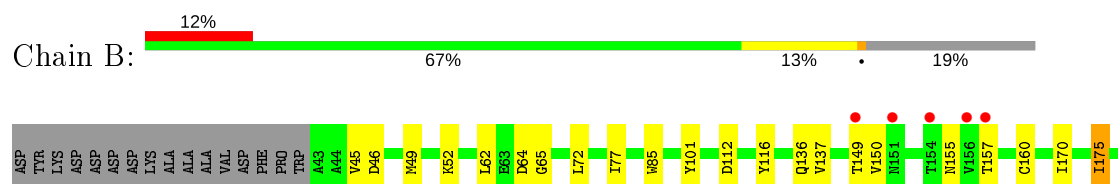
- Molecule 1: IgLON family member 5

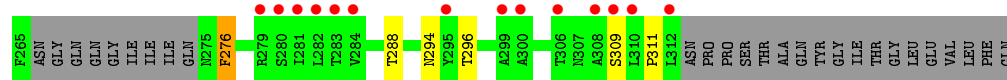
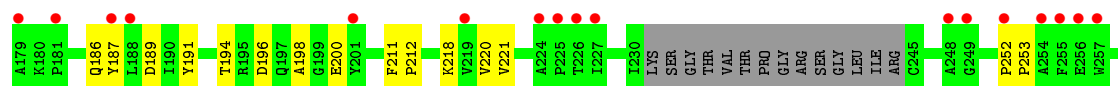


- Molecule 1: IgLON family member 5



- Molecule 2: Neuronal growth regulator 1





● Molecule 2: Neuronal growth regulator 1



● Molecule 3: alpha-D-mannopyranose-(1-3)-beta-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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.34Å 305.80Å 60.03Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	48.60 – 3.30 48.59 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.60-3.30) 99.1 (48.59-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.245 , 0.286 0.245 , 0.285	Depositor DCC
R_{free} test set	1586 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	120.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7856	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.24	0/2057	0.47	0/2821
1	C	0.25	0/1976	0.46	0/2712
2	B	0.25	0/1750	0.47	0/2409
2	D	0.26	0/1965	0.46	0/2695
All	All	0.25	0/7748	0.47	0/10637

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	2017	0	1857	35	0
1	C	1937	0	1765	41	0
2	B	1719	0	1515	25	0
2	D	1923	0	1686	36	0
3	E	50	0	43	0	0
4	A	56	0	52	2	0
4	B	42	0	39	1	0
4	C	70	0	65	3	0
4	D	42	0	39	1	0
All	All	7856	0	7061	134	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 9.

All (134) 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)
2:D:63:GLU:OE2	2:D:127:ARG:NH1	2.16	0.78
2:D:73:ASN:HB2	2:D:78:ILE:HD11	1.68	0.76
2:D:222:ASN:HB3	2:D:303:LEU:HD11	1.69	0.75
1:C:46:GLU:HB2	1:C:131:VAL:HG12	1.71	0.72
1:A:68:ARG:NH2	1:A:107:GLU:O	2.25	0.69
1:A:239:GLU:HG2	1:A:273:ARG:HG2	1.75	0.69
1:C:91:THR:HG22	1:C:93:GLU:H	1.56	0.68
2:D:233:GLY:N	2:D:242:LEU:O	2.26	0.68
1:C:186:GLN:HG2	1:C:189:GLN:HG3	1.74	0.68
1:A:76:ASN:OD1	1:A:90:ASN:ND2	2.29	0.66
1:C:167:ARG:NH2	1:C:194:GLU:OE1	2.24	0.66
1:A:132:PRO:HA	1:A:199:ASN:HD21	1.62	0.65
1:C:144:VAL:HG23	1:C:214:VAL:HG23	1.79	0.64
2:B:198:ALA:HB2	2:B:221:VAL:HG22	1.80	0.63
2:D:273:ILE:HG12	2:D:282:LEU:HD13	1.80	0.63
1:A:56:ILE:HB	1:A:60:VAL:HG21	1.81	0.63
4:C:405:NAG:H3	4:C:405:NAG:H83	1.81	0.62
1:C:63:VAL:HG23	1:C:114:PHE:HB3	1.81	0.62
1:A:259:SER:HB2	1:A:267:VAL:HG22	1.81	0.62
1:A:63:VAL:HG23	1:A:114:PHE:HB3	1.82	0.61
2:B:296:THR:HG21	4:B:402:NAG:H81	1.83	0.61
1:A:78:ARG:NH2	1:A:85:VAL:O	2.34	0.60
2:B:155:ASN:HB3	2:B:191:TYR:HA	1.83	0.60
1:A:49:ASN:HB3	1:A:98:LEU:HD11	1.82	0.60
2:B:294:ASN:HA	2:B:311:PRO:HA	1.83	0.59
1:C:167:ARG:HA	1:C:173:PHE:O	2.01	0.59
1:C:66:LEU:HD11	2:D:77:ILE:HD11	1.84	0.59
2:B:49:MET:SD	2:B:136:GLN:NE2	2.75	0.59
1:C:215:ASN:HA	1:C:243:VAL:HG23	1.83	0.59
4:A:407:NAG:H83	4:A:407:NAG:H3	1.85	0.58
2:D:230:ILE:HG12	2:D:310:LEU:HD22	1.85	0.58
2:B:52:LYS:HD2	2:B:137:VAL:HG22	1.86	0.58
2:D:39:ASP:OD1	2:D:40:PHE:N	2.34	0.58
2:B:72:LEU:HD23	2:B:77:ILE:HA	1.85	0.58
1:A:144:VAL:HG11	1:A:150:VAL:HG22	1.86	0.58
1:A:137:ASN:HB3	1:A:155:LEU:HB3	1.85	0.57
2:D:296:THR:HA	2:D:309:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASN:HA	1:A:243:VAL:HG23	1.87	0.57
1:A:236:LEU:HD12	1:A:276:LEU:HD23	1.86	0.57
1:C:194:GLU:HA	1:C:209:ARG:HA	1.87	0.55
1:C:56:ILE:HB	1:C:60:VAL:HG21	1.88	0.55
2:D:60:CYS:O	2:D:101:TYR:HB3	2.07	0.55
1:C:132:PRO:HA	1:C:199:ASN:HD22	1.72	0.54
2:B:175:ILE:HG22	2:B:200:GLU:O	2.09	0.53
2:D:189:ASP:OD1	2:D:189:ASP:N	2.41	0.53
1:A:88:LEU:HD11	1:A:98:LEU:HB2	1.91	0.53
2:B:189:ASP:N	2:B:189:ASP:OD1	2.42	0.52
2:D:71:TRP:CD1	2:D:101:TYR:HE1	2.28	0.52
1:A:187:ARG:HG2	1:A:216:TYR:CD2	2.44	0.52
2:D:139:PRO:HD3	2:D:207:ASN:HD22	1.74	0.52
1:C:50:ALA:HB3	1:C:99:ILE:HB	1.91	0.52
1:A:107:GLU:OE1	1:A:159:ARG:NH2	2.29	0.51
1:C:99:ILE:HD12	4:C:401:NAG:H81	1.92	0.51
1:A:43:THR:HG22	1:A:128:ILE:HB	1.91	0.51
1:C:236:LEU:HB3	1:C:304:MET:HE2	1.92	0.51
1:C:216:TYR:CE1	1:C:242:ALA:HA	2.46	0.51
1:C:271:ARG:H	1:C:271:ARG:HD2	1.76	0.51
1:A:154:CYS:HB2	1:A:166:TRP:CZ2	2.46	0.50
1:C:133:ALA:HB2	1:C:199:ASN:HB2	1.93	0.50
1:A:231:GLY:H	1:A:281:VAL:HG21	1.76	0.50
2:D:207:ASN:HD21	2:D:210:SER:HB3	1.75	0.50
1:C:250:TRP:HB3	1:C:256:LEU:HD23	1.94	0.50
1:A:115:GLN:HG3	2:B:85:TRP:HB3	1.93	0.50
2:B:211:PHE:N	2:B:212:PRO:HD2	2.26	0.50
2:D:73:ASN:HD22	4:D:401:NAG:H83	1.77	0.50
2:D:71:TRP:HD1	2:D:101:TYR:HE1	1.60	0.50
2:B:62:LEU:HD23	2:B:101:TYR:HB2	1.92	0.49
1:C:78:ARG:NH2	1:C:82:ASP:O	2.45	0.49
2:D:109:ASP:HB3	2:D:111:THR:HG22	1.94	0.48
2:D:186:GLN:HG3	2:D:187:TYR:CD1	2.49	0.48
1:C:131:VAL:HG22	1:C:159:ARG:H	1.79	0.47
2:B:194:THR:OG1	2:B:196:ASP:OD1	2.27	0.47
1:C:252:LYS:H	1:C:256:LEU:HB2	1.79	0.47
2:D:107:ASN:O	2:D:107:ASN:ND2	2.47	0.47
1:A:198:HIS:O	1:A:198:HIS:ND1	2.48	0.47
2:D:194:THR:OG1	2:D:196:ASP:OD1	2.26	0.47
1:A:164:VAL:HG21	1:A:178:GLU:HG2	1.97	0.46
1:C:204:ALA:N	1:C:205:PRO:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:HIS:O	2:D:295:TYR:OH	2.18	0.46
1:C:43:THR:HA	1:C:128:ILE:O	2.16	0.46
2:B:150:VAL:O	2:B:221:VAL:HA	2.16	0.46
1:C:52:LEU:HD12	1:C:97:ILE:HD11	1.97	0.46
2:B:296:THR:HA	2:B:309:SER:HA	1.97	0.45
1:C:187:ARG:HA	1:C:214:VAL:HG11	1.98	0.45
2:D:42:TRP:O	2:D:61:TYR:OH	2.23	0.45
2:D:206:GLU:HB3	2:D:212:PRO:HB3	1.99	0.45
1:C:39:ALA:HB3	4:C:405:NAG:H81	1.98	0.45
2:D:78:ILE:HG22	2:D:79:PHE:CD2	2.51	0.45
1:A:263:GLU:O	1:A:285:HIS:NE2	2.43	0.45
2:B:252:PRO:HA	2:B:253:PRO:HD3	1.88	0.45
1:C:82:ASP:O	1:C:85:VAL:HG12	2.16	0.45
1:C:62:ARG:HB3	2:D:85:TRP:CE2	2.52	0.44
1:A:66:LEU:HD11	2:B:77:ILE:HD11	1.99	0.44
1:C:135:ILE:HD13	1:C:156:ALA:HB2	2.00	0.44
2:B:112:ASP:O	2:B:116:TYR:OH	2.21	0.44
1:A:230:LEU:HA	1:A:281:VAL:HG11	1.98	0.44
1:A:218:PRO:HB3	1:A:242:ALA:HB2	2.00	0.44
2:B:64:ASP:OD1	2:B:65:GLY:N	2.51	0.43
2:D:211:PHE:HD1	2:D:212:PRO:HD2	1.82	0.43
1:C:104:LEU:HD11	1:C:159:ARG:HG3	2.01	0.43
2:D:157:THR:HA	2:D:189:ASP:HA	2.00	0.43
1:C:144:VAL:O	1:C:215:ASN:N	2.45	0.43
1:A:91:THR:HG22	1:A:93:GLU:H	1.84	0.43
1:A:222:ASP:OD2	1:A:237:ARG:NH2	2.52	0.43
2:B:200:GLU:HA	2:B:218:LYS:HA	2.01	0.42
2:B:149:THR:HG22	2:B:220:VAL:HB	2.01	0.42
1:C:192:GLU:HG3	1:C:211:LEU:HD13	2.00	0.42
2:D:139:PRO:HB3	2:D:168:PRO:HB3	2.01	0.42
2:B:186:GLN:HG3	2:B:187:TYR:CD1	2.54	0.42
1:C:146:GLU:N	1:C:215:ASN:O	2.46	0.42
1:C:250:TRP:O	1:C:256:LEU:HB3	2.20	0.42
1:C:59:HIS:O	1:C:116:THR:HG23	2.20	0.42
2:D:67:SER:HB3	2:D:121:GLN:O	2.19	0.42
1:A:167:ARG:HA	1:A:173:PHE:O	2.19	0.42
1:C:154:CYS:HB2	1:C:166:TRP:CZ2	2.54	0.42
2:D:68:LYS:HG3	2:D:68:LYS:H	1.59	0.41
2:D:80:ALA:HB3	2:D:85:TRP:CZ3	2.55	0.41
1:A:42:TYR:HE2	1:A:50:ALA:HB1	1.86	0.41
1:C:62:ARG:NH2	2:D:83:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:THR:HG22	2:D:189:ASP:HB3	2.02	0.41
2:D:228:GLN:N	2:D:246:GLU:O	2.51	0.41
2:B:157:THR:HG22	2:B:189:ASP:HB3	2.02	0.41
1:C:190:ALA:HB2	1:C:214:VAL:HG12	2.03	0.41
1:A:285:HIS:O	1:A:289:TYR:OH	2.19	0.41
2:D:257:TRP:HD1	2:D:273:ILE:HD13	1.85	0.41
1:C:216:TYR:CE2	1:C:243:VAL:HG22	2.55	0.41
1:A:39:ALA:O	4:A:407:NAG:N2	2.37	0.41
2:B:276:PHE:HA	2:B:276:PHE:HD1	1.75	0.41
1:A:236:LEU:O	1:A:276:LEU:N	2.40	0.41
2:B:160:CYS:O	2:B:170:ILE:HD13	2.21	0.40
1:A:168:GLN:NE2	1:A:171:ASP:HB3	2.36	0.40
1:C:223:VAL:HG22	1:C:238:CYS:SG	2.61	0.40
2:D:160:CYS:HB2	2:D:172:TRP:CZ2	2.57	0.40
1:A:190:ALA:HB2	1:A:214:VAL:HG22	2.04	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	271/303 (89%)	260 (96%)	11 (4%)	0	100	100
1	C	265/303 (88%)	257 (97%)	8 (3%)	0	100	100
2	B	241/304 (79%)	226 (94%)	15 (6%)	0	100	100
2	D	265/304 (87%)	257 (97%)	8 (3%)	0	100	100
All	All	1042/1214 (86%)	1000 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/258 (80%)	203 (98%)	3 (2%)	65	81
1	C	191/258 (74%)	188 (98%)	3 (2%)	62	79
2	B	168/261 (64%)	163 (97%)	5 (3%)	41	68
2	D	184/261 (70%)	175 (95%)	9 (5%)	25	56
All	All	749/1038 (72%)	729 (97%)	20 (3%)	44	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	198	HIS
1	A	225	SER
2	B	45	VAL
2	B	46	ASP
2	B	175	ILE
2	B	276	PHE
2	B	288	THR
1	C	59	HIS
1	C	186	GLN
1	C	304	MET
2	D	62	LEU
2	D	68	LYS
2	D	83	ASP
2	D	146	ASN
2	D	174	HIS
2	D	182	PHE
2	D	211	PHE
2	D	216	LYS
2	D	258	TYR

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

Mol	Chain	Res	Type
1	A	90	ASN
1	A	199	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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.15	0	17,19,21	0.53	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	E	3	3	11,11,12	0.57	0	15,15,17	0.69	0
3	MAN	E	4	3	11,11,12	0.68	0	15,15,17	0.89	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	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	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	E	4	MAN	O2-C2-C3	-2.20	105.74	110.14

There are no chirality outliers.

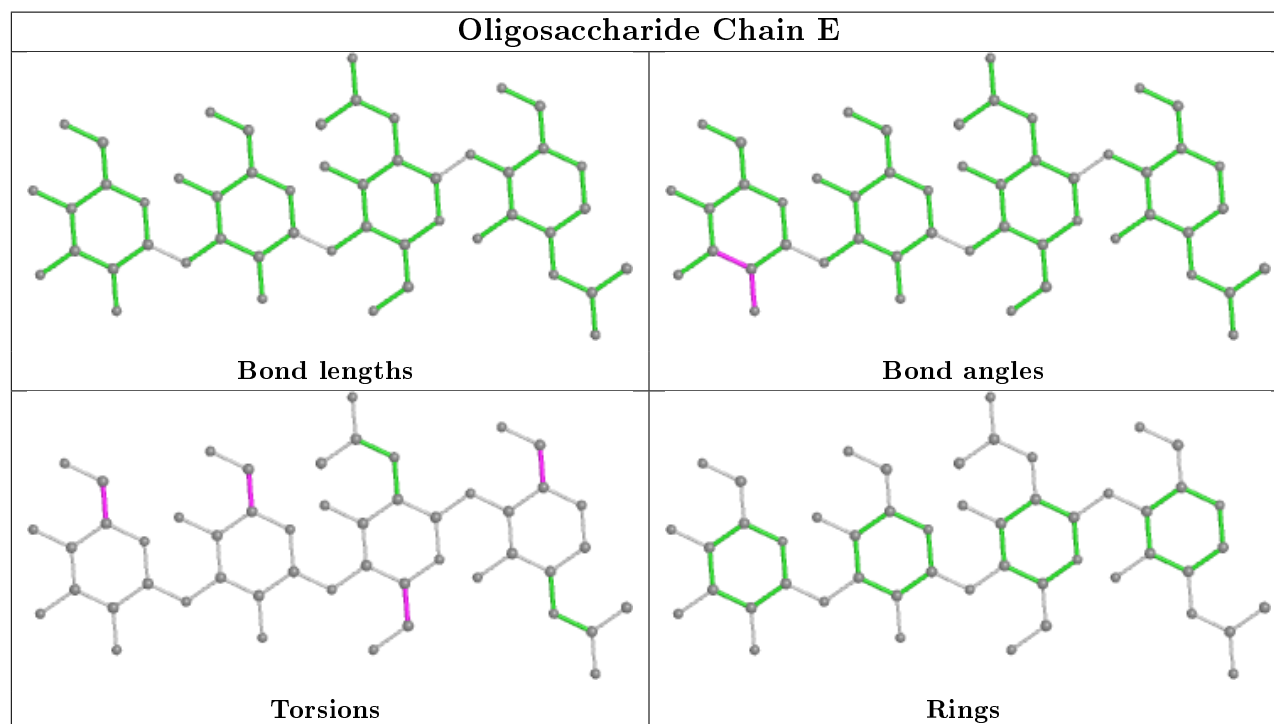
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

15 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	C	403	1	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	D	403	2	14,14,15	0.28	0	17,19,21	0.34	0
4	NAG	D	402	2	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	B	402	2	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	B	403	2	14,14,15	0.60	0	17,19,21	0.87	1 (5%)
4	NAG	C	404	1	14,14,15	0.32	0	17,19,21	0.54	0
4	NAG	C	405	1	14,14,15	0.56	0	17,19,21	1.16	1 (5%)
4	NAG	B	401	2	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	D	401	2	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	A	405	1	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	C	402	1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	C	401	1	14,14,15	0.18	0	17,19,21	0.58	0
4	NAG	A	406	1	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	A	408	1	14,14,15	0.37	0	17,19,21	0.40	0
4	NAG	A	407	1	14,14,15	0.53	0	17,19,21	1.31	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
4	NAG	C	403	1	-	1/6/23/26	0/1/1/1
4	NAG	D	403	2	-	2/6/23/26	0/1/1/1
4	NAG	D	402	2	-	2/6/23/26	0/1/1/1
4	NAG	B	402	2	-	0/6/23/26	0/1/1/1
4	NAG	B	403	2	-	2/6/23/26	0/1/1/1
4	NAG	C	404	1	-	3/6/23/26	0/1/1/1
4	NAG	C	405	1	-	4/6/23/26	0/1/1/1
4	NAG	B	401	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	401	2	-	2/6/23/26	0/1/1/1
4	NAG	A	405	1	-	2/6/23/26	0/1/1/1
4	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	401	1	-	4/6/23/26	0/1/1/1
4	NAG	A	406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	408	1	-	3/6/23/26	0/1/1/1
4	NAG	A	407	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	407	NAG	C2-N2-C7	4.30	129.03	122.90
4	C	405	NAG	C2-N2-C7	4.08	128.72	122.90
4	B	403	NAG	C2-N2-C7	2.01	125.77	122.90

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	NAG	C3-C2-N2-C7
4	A	408	NAG	C4-C5-C6-O6
4	D	402	NAG	O5-C5-C6-O6
4	A	405	NAG	O5-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6
4	C	401	NAG	O5-C5-C6-O6
4	A	408	NAG	O5-C5-C6-O6
4	D	403	NAG	C4-C5-C6-O6
4	C	401	NAG	C4-C5-C6-O6
4	C	405	NAG	C8-C7-N2-C2
4	C	405	NAG	O7-C7-N2-C2
4	D	401	NAG	C8-C7-N2-C2
4	D	401	NAG	O7-C7-N2-C2
4	A	407	NAG	C8-C7-N2-C2
4	A	407	NAG	O7-C7-N2-C2
4	A	405	NAG	C4-C5-C6-O6
4	D	402	NAG	C4-C5-C6-O6
4	D	403	NAG	O5-C5-C6-O6
4	C	402	NAG	C4-C5-C6-O6
4	C	403	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	405	NAG	O5-C5-C6-O6
4	A	407	NAG	O5-C5-C6-O6
4	B	403	NAG	C4-C5-C6-O6
4	C	404	NAG	C3-C2-N2-C7
4	A	408	NAG	C3-C2-N2-C7
4	C	404	NAG	C4-C5-C6-O6
4	C	404	NAG	O5-C5-C6-O6
4	C	405	NAG	C3-C2-N2-C7
4	C	401	NAG	C3-C2-N2-C7
4	A	407	NAG	C3-C2-N2-C7
4	C	401	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	NAG	1	0
4	C	405	NAG	2	0
4	D	401	NAG	1	0
4	C	401	NAG	1	0
4	A	407	NAG	2	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, 95th 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 ²)	Q<0.9
1	A	273/303 (90%)	0.22	10 (3%) 41 38	59, 104, 169, 210	0
1	C	267/303 (88%)	0.28	15 (5%) 24 23	73, 116, 191, 255	0
2	B	247/304 (81%)	0.69	36 (14%) 2 2	68, 135, 214, 266	0
2	D	269/304 (88%)	0.41	21 (7%) 13 12	64, 132, 203, 221	0
All	All	1056/1214 (86%)	0.39	82 (7%) 13 12	59, 117, 201, 266	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	ALA	5.7
2	B	224	ALA	5.4
2	B	156	VAL	5.3
1	A	36	ASN	5.2
1	C	38	PRO	4.8
2	D	156	VAL	4.7
2	B	254	ALA	4.7
2	D	201	TYR	4.3
1	C	259	SER	4.3
2	B	201	TYR	4.2
2	B	284	VAL	4.2
2	B	249	GLY	4.1
1	A	278	PHE	4.0
2	B	227	ILE	4.0
1	C	258	SER	3.9
2	B	257	TRP	3.9
2	B	226	THR	3.7
2	B	188	LEU	3.6
1	A	257	LEU	3.6
1	C	289	TYR	3.6
1	A	37	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	225	PRO	3.4
2	B	181	PRO	3.4
2	B	306	THR	3.3
2	B	299	ALA	3.2
2	B	151	ASN	3.1
2	B	310	LEU	3.1
2	D	248	ALA	3.0
2	B	252	PRO	3.0
1	C	197	THR	3.0
1	A	230	LEU	3.0
2	D	299	ALA	2.9
2	B	309	SER	2.8
2	D	300	ALA	2.8
2	D	271	ILE	2.8
1	C	129	VAL	2.8
2	D	305	THR	2.8
2	D	63	GLU	2.8
2	D	280	SER	2.8
2	D	187	TYR	2.7
2	D	254	ALA	2.7
2	B	312	LEU	2.7
2	D	288	THR	2.7
2	B	282	LEU	2.7
1	C	156	ALA	2.6
1	C	138	ILE	2.6
2	B	280	SER	2.6
2	D	158	LEU	2.6
2	B	281	ILE	2.6
2	B	149	THR	2.6
1	C	248	PHE	2.5
2	B	255	PHE	2.5
1	C	293	ALA	2.5
1	A	277	LEU	2.5
1	C	157	VAL	2.5
2	B	300	ALA	2.5
2	D	193	ILE	2.5
2	D	291	HIS	2.5
2	D	62	LEU	2.4
1	A	289	TYR	2.4
2	B	256	GLU	2.4
1	A	38	PRO	2.4
1	A	40	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	283	THR	2.3
2	B	157	THR	2.3
2	B	308	ALA	2.3
1	C	257	LEU	2.3
1	C	260	GLY	2.2
2	B	179	ALA	2.2
1	A	182	ILE	2.2
2	D	121	GLN	2.2
2	B	187	TYR	2.2
2	D	257	TRP	2.2
2	D	295	TYR	2.2
1	C	256	LEU	2.1
2	B	295	TYR	2.1
2	B	154	THR	2.1
2	B	279	ARG	2.1
2	D	296	THR	2.1
2	B	219	VAL	2.1
1	C	74	ALA	2.0
2	D	230	ILE	2.0

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

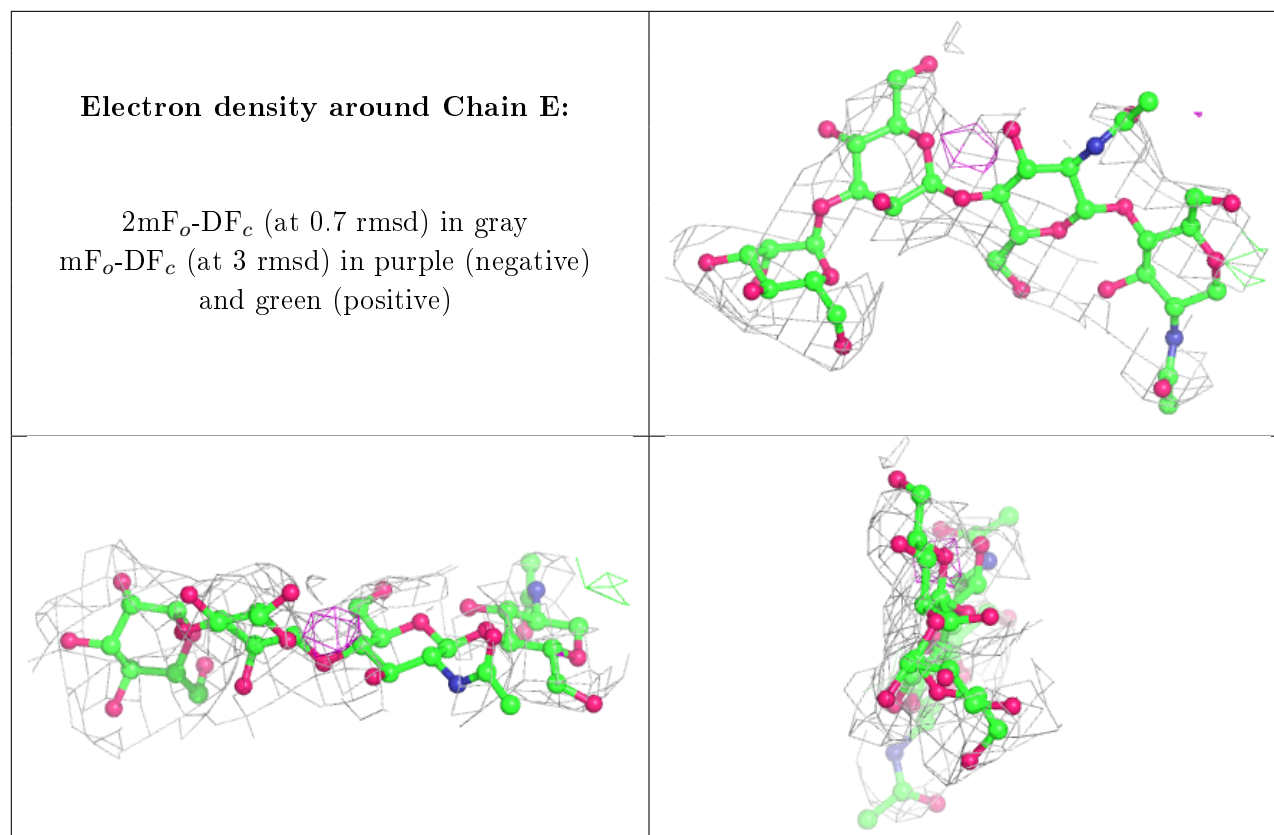
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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 ²)	Q<0.9
3	BMA	E	3	11/12	0.85	0.23	147,177,183,184	0
3	MAN	E	4	11/12	0.87	0.13	174,182,191,193	0
3	NAG	E	2	14/15	0.92	0.24	111,133,157,177	0
3	NAG	E	1	14/15	0.97	0.26	68,90,105,110	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 ⓘ

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, 95th 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 ²)	Q<0.9
4	NAG	A	407	14/15	0.66	0.43	151,186,200,201	0
4	NAG	B	402	14/15	0.76	0.47	169,200,219,220	0
4	NAG	C	403	14/15	0.76	0.36	190,201,220,222	0
4	NAG	B	403	14/15	0.80	0.47	84,124,177,186	0
4	NAG	D	403	14/15	0.80	0.23	156,173,191,195	0
4	NAG	C	401	14/15	0.84	0.27	71,89,100,106	0
4	NAG	A	408	14/15	0.85	0.28	137,166,180,187	0
4	NAG	A	406	14/15	0.85	0.26	109,139,177,182	0
4	NAG	C	404	14/15	0.88	0.16	134,147,164,164	0
4	NAG	C	405	14/15	0.88	0.29	134,153,157,159	0
4	NAG	B	401	14/15	0.89	0.18	115,154,171,172	0
4	NAG	D	402	14/15	0.91	0.10	105,127,140,147	0
4	NAG	D	401	14/15	0.93	0.30	87,98,135,154	0
4	NAG	A	405	14/15	0.94	0.15	77,105,122,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	C	402	14/15	0.94	0.16	86,107,123,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.