



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:31 PM BST

PDB ID : 6CQJ
Title : Crystal structure of DR1 presenting the RQ13 peptide
Authors : Farenc, C.; Gras, S.; Rossjohn, J.
Deposited on : 2018-03-15
Resolution : 2.75 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

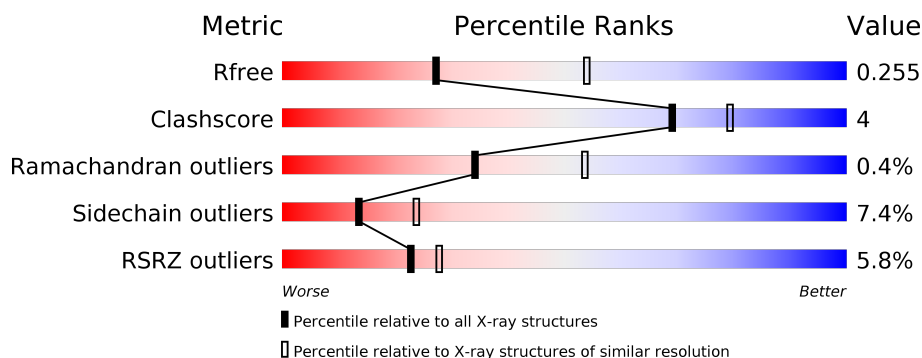
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



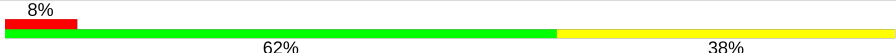
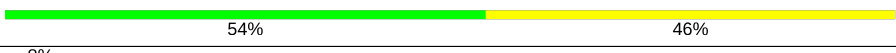
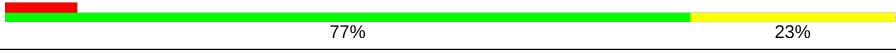
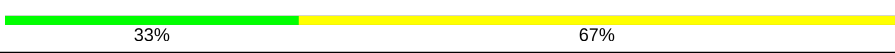
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	182	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>•</div> </div> </div>
1	D	182	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	G	182	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>••</div> </div> </div>
2	B	189	<div> <div>11%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>
2	E	189	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 5%</div> </div> </div>
2	H	189	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	C	13	
3	F	13	
3	I	13	
4	J	3	

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	J	2	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9642 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1480	958	240	277	5			
1	D	182	Total	C	N	O	S	0	1	0
			1503	974	243	281	5			
1	G	180	Total	C	N	O	S	0	1	0
			1491	964	244	278	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	ALA	conflict	UNP P01903
D	182	THR	ALA	conflict	UNP P01903
G	182	THR	ALA	conflict	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1492	940	265	281	6			
2	E	180	Total	C	N	O	S	0	0	0
			1477	932	263	276	6			
2	H	182	Total	C	N	O	S	0	0	0
			1492	940	265	281	6			

- Molecule 3 is a protein called Peptide from Capsid protein p24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			113	70	22	21			
3	F	13	Total	C	N	O	0	0	0
			113	70	22	21			

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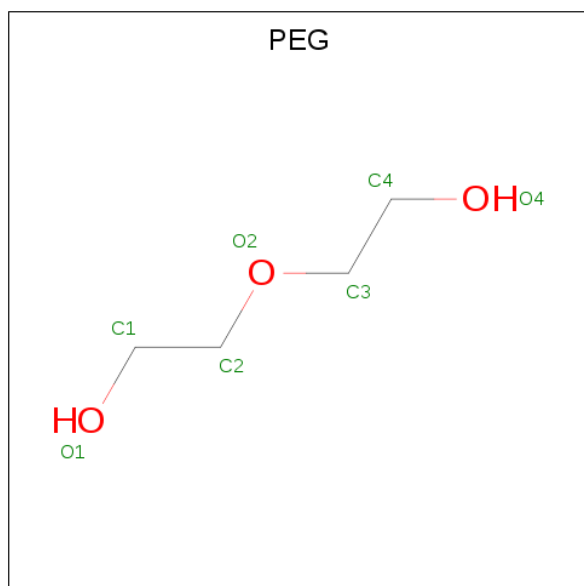
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	0	0	0
			113	70	22	21			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
4	J	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		

- 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	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Na	0	0
			1	1		
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	42	Total	O	0	0
			42	42		
8	B	51	Total	O	0	0
			51	51		
8	C	6	Total	O	0	0
			6	6		
8	D	32	Total	O	0	0
			32	32		

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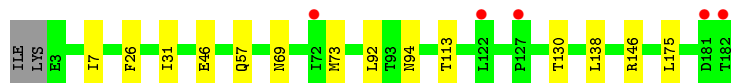
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	41	Total 41	O 41	0	0
8	F	6	Total 6	O 6	0	0
8	G	41	Total 41	O 41	0	0
8	H	39	Total 39	O 39	0	0
8	I	10	Total 10	O 10	0	0

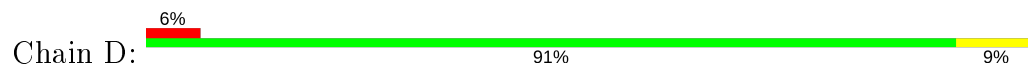
3 Residue-property plots [i](#)

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.

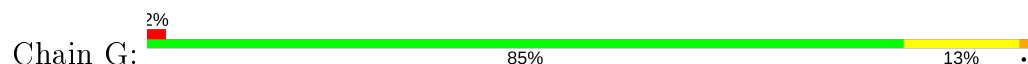
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



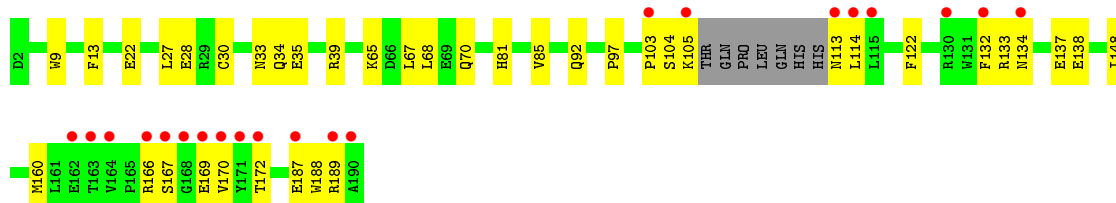
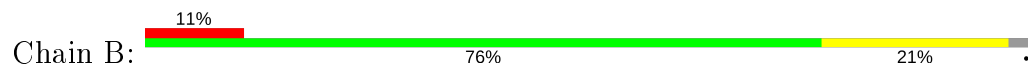
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



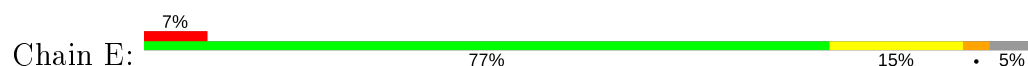
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

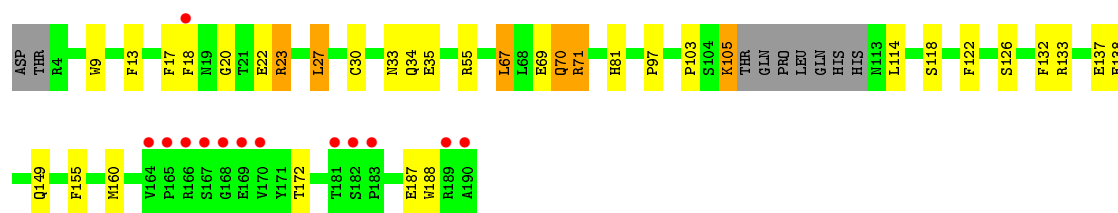


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

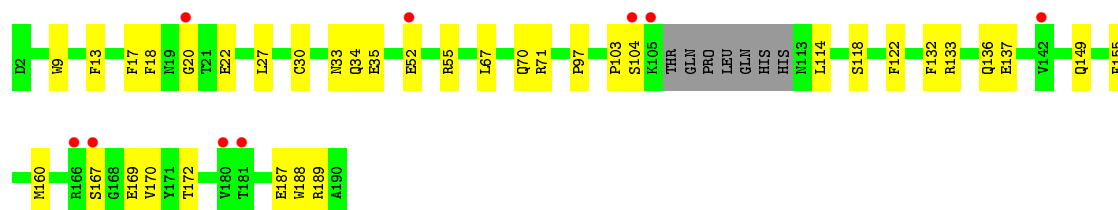
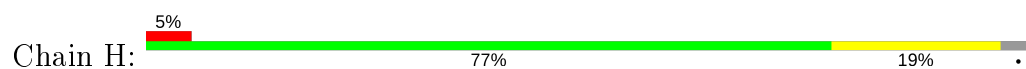


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain





- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



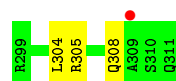
- Molecule 3: Peptide from Capsid protein p24



- Molecule 3: Peptide from Capsid protein p24



- Molecule 3: Peptide from Capsid protein p24



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(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 1	Depositor
Cell constants a, b, c, α , β , γ	68.68Å 82.02Å 83.05Å 61.56° 88.20° 86.47°	Depositor
Resolution (Å)	47.96 – 2.75 36.51 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.96-2.75) 98.6 (36.51-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.197 , 0.249 0.204 , 0.255	Depositor DCC
R_{free} test set	1929 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9642	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PEG, NAG

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	0.52	0/1525	0.77	0/2080
1	D	0.53	0/1551	0.73	0/2115
1	G	0.53	0/1536	0.76	0/2094
2	B	0.51	0/1528	0.71	0/2073
2	E	0.52	0/1513	0.73	0/2052
2	H	0.50	0/1528	0.73	0/2073
3	C	0.54	0/114	0.83	0/149
3	F	0.55	0/114	0.80	0/149
3	I	0.52	0/114	0.74	0/149
All	All	0.52	0/9523	0.74	0/12934

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

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	1480	0	1413	4	0
1	D	1503	0	1446	6	0
1	G	1491	0	1425	13	0
2	B	1492	0	1426	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1477	0	1415	19	0
2	H	1492	0	1426	13	0
3	C	113	0	111	3	0
3	F	113	0	111	5	0
3	I	113	0	111	1	0
4	J	42	0	37	0	0
5	A	7	0	10	1	0
5	B	7	0	10	0	0
5	E	7	0	10	2	0
5	G	7	0	10	0	0
6	A	14	0	13	0	0
6	D	14	0	13	1	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
8	A	42	0	0	0	0
8	B	51	0	0	0	0
8	C	6	0	0	0	0
8	D	32	0	0	1	0
8	E	41	0	0	1	0
8	F	6	0	0	0	0
8	G	41	0	0	1	0
8	H	39	0	0	0	0
8	I	10	0	0	0	0
All	All	9642	0	8987	68	0

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

All (68) 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:B:170:VAL:HB	2:B:189:ARG:HE	1.46	0.80
2:E:105:LYS:HD2	2:E:105:LYS:H	1.53	0.74
2:E:70:GLN:HE21	2:E:71:ARG:HH11	1.36	0.73
2:E:114:LEU:HD22	2:E:160:MET:HB3	1.74	0.70
1:G:120:THR:HG23	1:G:164:ARG:HB3	1.75	0.69
1:D:168:TRP:CD1	6:D:202:NAG:H82	2.29	0.68
2:B:114:LEU:HD22	2:B:160:MET:HB3	1.76	0.67
1:G:118:ASN:HB2	1:G:166:GLU:HB2	1.77	0.66
1:D:118:ASN:HB2	1:D:166:GLU:HB2	1.79	0.65
1:G:120:THR:HG22	8:G:311:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASP:HB2	8:E:301:HOH:O	1.99	0.61
2:E:70:GLN:NE2	2:E:71:ARG:HH11	1.99	0.60
2:H:149:GLN:HB3	2:H:155:PHE:CE1	2.37	0.59
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.86	0.58
2:E:97:PRO:HB3	2:E:122:PHE:HB3	1.87	0.57
2:H:52:GLU:HA	2:H:55:ARG:HE	1.69	0.57
2:H:97:PRO:HB3	2:H:122:PHE:HB3	1.87	0.57
1:G:47:GLU:HG3	1:G:51:PHE:HE2	1.72	0.55
2:H:13:PHE:CD2	3:I:304:LEU:HD23	2.42	0.55
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.43	0.54
2:H:114:LEU:HD13	2:H:160:MET:HG2	1.90	0.53
2:E:9:TRP:CH2	2:E:30:CYS:HB3	2.44	0.52
1:G:47:GLU:HG3	1:G:51:PHE:CE2	2.45	0.52
2:H:132:PHE:HB2	2:H:172:THR:HB	1.90	0.52
2:E:132:PHE:HB2	2:E:172:THR:HB	1.92	0.52
2:B:132:PHE:HB2	2:B:172:THR:HB	1.92	0.52
2:H:17:PHE:HB3	2:H:20:GLY:O	2.11	0.51
2:B:85:VAL:HG22	3:C:299:ARG:HB3	1.92	0.50
2:H:114:LEU:HD22	2:H:160:MET:HB3	1.94	0.50
2:H:9:TRP:CH2	2:H:30:CYS:HB3	2.47	0.50
2:E:149:GLN:HB3	2:E:155:PHE:CE2	2.47	0.49
1:D:96:PRO:HD3	2:E:118:SER:OG	2.13	0.49
2:E:103:PRO:HG3	2:E:188:TRP:CZ2	2.47	0.48
2:B:166:ARG:O	2:B:169:GLU:HB2	2.13	0.48
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.95	0.48
2:E:55:ARG:HE	5:E:201:PEG:H12	1.78	0.48
1:D:69:ASN:O	1:D:73:MET:HG2	2.14	0.47
2:H:103:PRO:HG3	2:H:188:TRP:CZ2	2.50	0.47
2:B:103:PRO:HG3	2:B:188:TRP:CZ2	2.49	0.47
1:A:138:LEU:HB2	1:A:146:ARG:HG2	1.97	0.47
1:A:69:ASN:O	1:A:73:MET:HG2	2.16	0.46
2:B:13:PHE:CD2	3:C:304:LEU:HD23	2.51	0.46
5:A:201:PEG:H31	2:B:148:ILE:HG23	1.97	0.46
1:A:7:ILE:HG12	1:A:26:PHE:HD1	1.80	0.45
2:B:134:ASN:HD21	2:B:169:GLU:HG2	1.80	0.45
1:D:138:LEU:HB2	1:D:146:ARG:HG2	1.97	0.45
1:G:69:ASN:O	1:G:73:MET:HG2	2.18	0.44
2:H:170:VAL:HG12	2:H:189:ARG:HG2	2.00	0.43
2:E:17:PHE:HB3	2:E:20:GLY:O	2.18	0.43
3:F:304:LEU:HD12	3:F:304:LEU:HA	1.90	0.43
1:G:3:GLU:HB3	2:H:18:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:PHE:CD2	3:F:304:LEU:HD23	2.54	0.42
2:E:27:LEU:HA	2:E:27:LEU:HD23	1.91	0.42
2:E:67:LEU:HD11	3:F:307:GLU:HG2	2.00	0.42
2:E:18:PHE:HB2	2:E:23:ARG:HB3	2.02	0.42
2:B:81:HIS:CD2	3:C:302:LYS:HG3	2.55	0.42
1:G:138:LEU:HB2	1:G:146[B]:ARG:HG3	2.02	0.41
1:G:116:VAL:CG1	1:G:168:TRP:CZ3	3.03	0.41
2:B:104:SER:O	2:B:114:LEU:HB2	2.20	0.41
1:G:26:PHE:HB2	1:G:31:ILE:HD11	2.01	0.41
1:G:96:PRO:HD3	2:H:118:SER:OG	2.20	0.41
8:D:301:HOH:O	3:F:299:ARG:HB2	2.21	0.41
2:B:28:GLU:O	2:B:39:ARG:HA	2.21	0.41
1:G:116:VAL:HG13	1:G:168:TRP:CZ3	2.56	0.41
1:G:7:ILE:HG12	1:G:26:PHE:HD1	1.86	0.41
2:E:81:HIS:CD2	3:F:302:LYS:HG3	2.56	0.41
2:E:103:PRO:HG3	2:E:188:TRP:HZ2	1.85	0.40
2:E:55:ARG:HH11	5:E:201:PEG:H12	1.86	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	178/182 (98%)	174 (98%)	4 (2%)	0	100	100
1	D	181/182 (100%)	178 (98%)	3 (2%)	0	100	100
1	G	179/182 (98%)	176 (98%)	3 (2%)	0	100	100
2	B	178/189 (94%)	171 (96%)	6 (3%)	1 (1%)	25	42
2	E	176/189 (93%)	170 (97%)	5 (3%)	1 (1%)	25	42
2	H	178/189 (94%)	171 (96%)	5 (3%)	2 (1%)	14	25
3	C	11/13 (85%)	11 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	11/13 (85%)	11 (100%)	0	0	100	100
3	I	11/13 (85%)	11 (100%)	0	0	100	100
All	All	1103/1152 (96%)	1073 (97%)	26 (2%)	4 (0%)	34	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	33	ASN
2	E	33	ASN
2	H	33	ASN
2	H	169	GLU

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	165/167 (99%)	158 (96%)	7 (4%)	30	49
1	D	168/167 (101%)	160 (95%)	8 (5%)	25	44
1	G	166/167 (99%)	156 (94%)	10 (6%)	19	33
2	B	164/171 (96%)	148 (90%)	16 (10%)	8	13
2	E	162/171 (95%)	147 (91%)	15 (9%)	9	15
2	H	164/171 (96%)	151 (92%)	13 (8%)	12	22
3	C	11/11 (100%)	9 (82%)	2 (18%)	1	2
3	F	11/11 (100%)	9 (82%)	2 (18%)	1	2
3	I	11/11 (100%)	9 (82%)	2 (18%)	1	2
All	All	1022/1047 (98%)	947 (93%)	75 (7%)	13	25

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	92	LEU
1	A	94	ASN
1	A	113	THR
1	A	130	THR
1	A	175	LEU
2	B	22	GLU
2	B	27	LEU
2	B	34	GLN
2	B	35	GLU
2	B	65	LYS
2	B	67	LEU
2	B	68	LEU
2	B	70	GLN
2	B	92	GLN
2	B	105	LYS
2	B	113	ASN
2	B	133	ARG
2	B	137	GLU
2	B	138	GLU
2	B	167	SER
2	B	187	GLU
3	C	305	ARG
3	C	308	GLN
1	D	25	ASP
1	D	46	GLU
1	D	57	GLN
1	D	92	LEU
1	D	94	ASN
1	D	130	THR
1	D	156	SER
1	D	175	LEU
2	E	22	GLU
2	E	23	ARG
2	E	27	LEU
2	E	34	GLN
2	E	35	GLU
2	E	67	LEU
2	E	69	GLU
2	E	70	GLN
2	E	71	ARG
2	E	105	LYS
2	E	126	SER

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Mol	Chain	Res	Type
2	E	133	ARG
2	E	137	GLU
2	E	138	GLU
2	E	187	GLU
3	F	308	GLN
3	F	311	GLN
1	G	25	ASP
1	G	46	GLU
1	G	92	LEU
1	G	94	ASN
1	G	116	VAL
1	G	117	VAL
1	G	120	THR
1	G	130	THR
1	G	156	SER
1	G	175	LEU
2	H	22	GLU
2	H	27	LEU
2	H	34	GLN
2	H	35	GLU
2	H	67	LEU
2	H	70	GLN
2	H	71	ARG
2	H	104	SER
2	H	133	ARG
2	H	136	GLN
2	H	137	GLU
2	H	167	SER
2	H	187	GLU
3	I	305	ARG
3	I	308	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	149	GLN
2	E	70	GLN
2	E	149	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 ⓘ

3 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$
4	NAG	J	1	1,4	14,14,15	0.33	0	17,19,21	0.67	0
4	NAG	J	2	4	14,14,15	0.41	0	17,19,21	1.94	2 (11%)
4	NAG	J	3	4	14,14,15	0.41	0	17,19,21	1.05	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	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	NAG	J	3	4	-	1/6/23/26	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	J	2	NAG	C1-O5-C5	6.66	121.21	112.19
4	J	3	NAG	C1-O5-C5	3.71	117.22	112.19
4	J	2	NAG	C3-C4-C5	2.39	114.50	110.24

There are no chirality outliers.

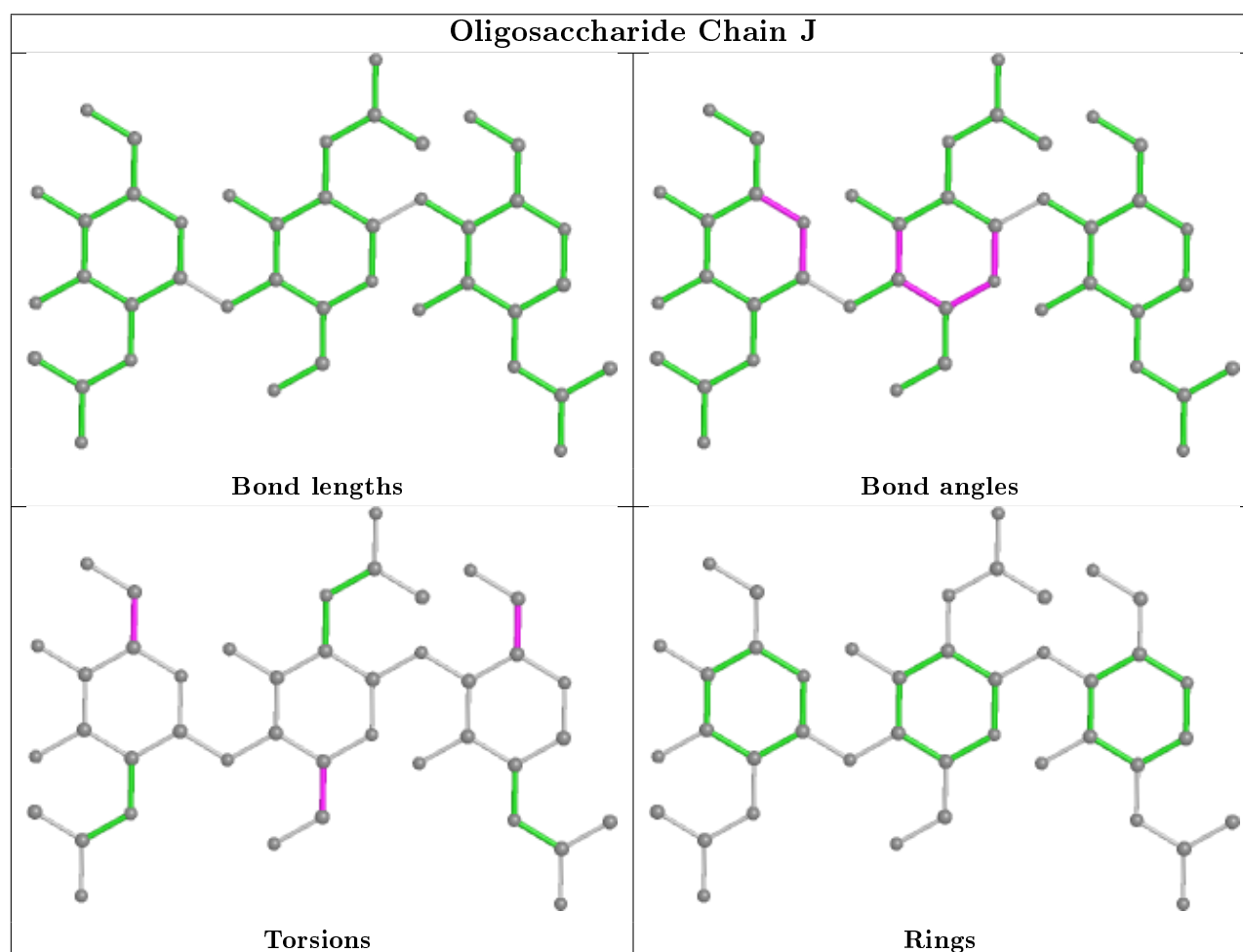
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	J	3	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	J	2	NAG	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 [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PEG	G	201	-	6,6,6	0.41	0	5,5,5	0.33	0
6	NAG	D	202	1	14,14,15	0.39	0	17,19,21	1.52	3 (17%)
5	PEG	A	201	-	6,6,6	0.25	0	5,5,5	0.27	0
5	PEG	E	201	-	6,6,6	0.41	0	5,5,5	0.22	0
6	NAG	A	202	1	14,14,15	0.42	0	17,19,21	1.32	1 (5%)
5	PEG	B	201	-	6,6,6	0.19	0	5,5,5	0.12	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	PEG	G	201	-	-	1/4/4/4	-
6	NAG	D	202	1	-	2/6/23/26	0/1/1/1
5	PEG	A	201	-	-	3/4/4/4	-
5	PEG	E	201	-	-	3/4/4/4	-
6	NAG	A	202	1	-	1/6/23/26	0/1/1/1
5	PEG	B	201	-	-	1/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	202	NAG	C1-O5-C5	4.69	118.55	112.19
6	D	202	NAG	O5-C1-C2	-3.79	105.30	111.29
6	D	202	NAG	C1-O5-C5	3.52	116.96	112.19
6	D	202	NAG	C1-C2-N2	3.45	116.38	110.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	202	NAG	C8-C7-N2-C2
6	D	202	NAG	O7-C7-N2-C2
5	E	201	PEG	O1-C1-C2-O2
5	E	201	PEG	O2-C3-C4-O4
5	A	201	PEG	O2-C3-C4-O4
6	A	202	NAG	O5-C5-C6-O6
5	E	201	PEG	C1-C2-O2-C3
5	A	201	PEG	C1-C2-O2-C3
5	G	201	PEG	C4-C3-O2-C2
5	B	201	PEG	O2-C3-C4-O4
5	A	201	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	202	NAG	1	0
5	A	201	PEG	1	0
5	E	201	PEG	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	180/182 (98%)	0.06	5 (2%) 53 62	26, 44, 72, 104	1 (0%)
1	D	182/182 (100%)	0.41	11 (6%) 21 26	36, 54, 77, 98	1 (0%)
1	G	180/182 (98%)	0.14	4 (2%) 62 70	30, 45, 73, 118	1 (0%)
2	B	182/189 (96%)	0.47	21 (11%) 4 5	25, 47, 103, 124	0
2	E	180/189 (95%)	0.25	13 (7%) 15 18	32, 49, 87, 120	0
2	H	182/189 (96%)	0.21	9 (4%) 29 36	32, 50, 83, 101	0
3	C	13/13 (100%)	0.18	1 (7%) 13 16	27, 41, 62, 75	0
3	F	13/13 (100%)	0.22	0 100 100	37, 43, 82, 94	0
3	I	13/13 (100%)	0.38	1 (7%) 13 16	35, 45, 67, 78	0
All	All	1125/1152 (97%)	0.26	65 (5%) 23 28	25, 48, 84, 124	3 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	167	SER	6.1
1	D	1	ILE	5.9
2	E	166	ARG	5.9
2	B	190	ALA	5.5
2	B	168	GLY	4.7
2	B	170	VAL	4.4
2	B	162	GLU	4.3
1	G	46	GLU	4.3
2	B	172	THR	4.3
2	E	168	GLY	4.3
2	B	189	ARG	4.2
1	D	172[A]	GLU	4.1
2	E	165	PRO	4.0
2	B	105	LYS	4.0
1	G	132	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	164	VAL	3.8
1	G	182	THR	3.8
1	D	2	LYS	3.8
2	B	167	SER	3.8
2	E	182	SER	3.7
2	B	169	GLU	3.6
2	B	171	TYR	3.5
2	B	134	ASN	3.5
1	A	182	THR	3.5
2	E	189	ARG	3.4
1	D	128	VAL	3.3
2	H	167	SER	3.2
2	H	52	GLU	3.0
2	B	114	LEU	3.0
1	A	122	LEU	2.9
1	D	175	LEU	2.9
2	B	113	ASN	2.9
2	B	163	THR	2.9
2	H	104	SER	2.9
2	E	170	VAL	2.8
1	D	123	ARG	2.8
2	E	169	GLU	2.8
2	B	164	VAL	2.8
2	B	130	ARG	2.7
2	H	166	ARG	2.7
1	A	127	PRO	2.7
3	I	309	ALA	2.7
1	D	57	GLN	2.7
2	E	183	PRO	2.7
2	E	190	ALA	2.6
3	C	311	GLN	2.6
1	D	86	PRO	2.6
2	H	180	VAL	2.5
1	A	72	ILE	2.5
2	B	166	ARG	2.5
2	B	187	GLU	2.5
1	G	131	GLY	2.5
2	B	103	PRO	2.4
2	H	181	THR	2.4
2	E	18	PHE	2.3
2	H	20	GLY	2.3
2	E	181	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	181	ASP	2.2
1	D	127	PRO	2.1
1	D	171	ASP	2.1
2	H	105	LYS	2.1
2	B	132	PHE	2.1
1	D	78	ASN	2.1
2	B	115	LEU	2.0
2	H	142	VAL	2.0

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

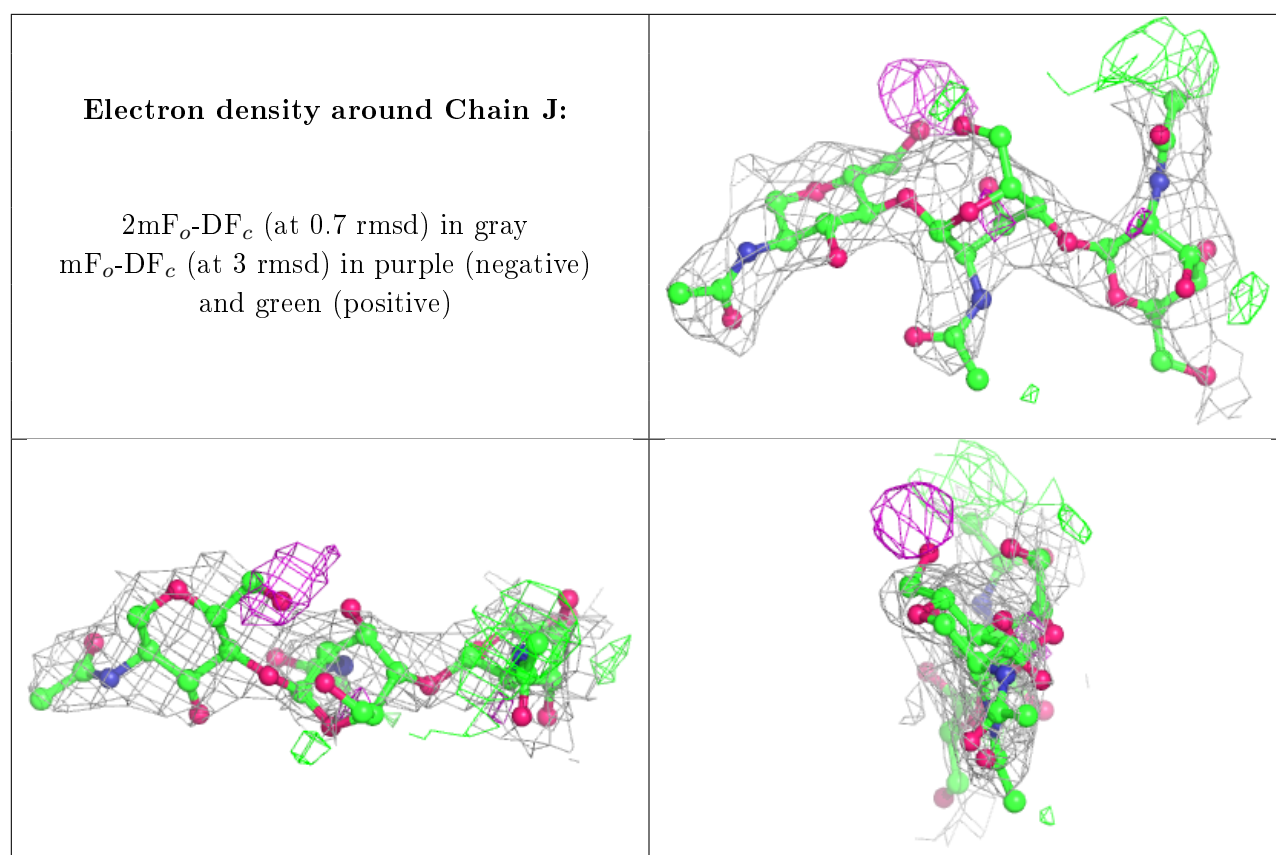
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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(\AA^2)	Q<0.9
4	NAG	J	3	14/15	0.55	0.37	110,120,124,124	0
4	NAG	J	2	14/15	0.77	0.42	107,111,114,114	0
4	NAG	J	1	14/15	0.84	0.31	71,86,97,101	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, 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(\AA^2)	Q<0.9
7	NA	D	201	1/1	0.73	0.15	58,58,58,58	0
6	NAG	D	202	14/15	0.79	0.22	86,94,97,98	0
6	NAG	A	202	14/15	0.82	0.18	42,77,85,86	0
7	NA	G	202	1/1	0.87	0.38	59,59,59,59	0
5	PEG	B	201	7/7	0.90	0.18	72,74,76,76	0
5	PEG	A	201	7/7	0.93	0.20	37,41,52,54	0
5	PEG	E	201	7/7	0.94	0.13	36,37,45,49	0
5	PEG	G	201	7/7	0.97	0.12	37,39,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.