



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:43 AM UTC

PDB ID : 6CQJ / pdb_00006cqj
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

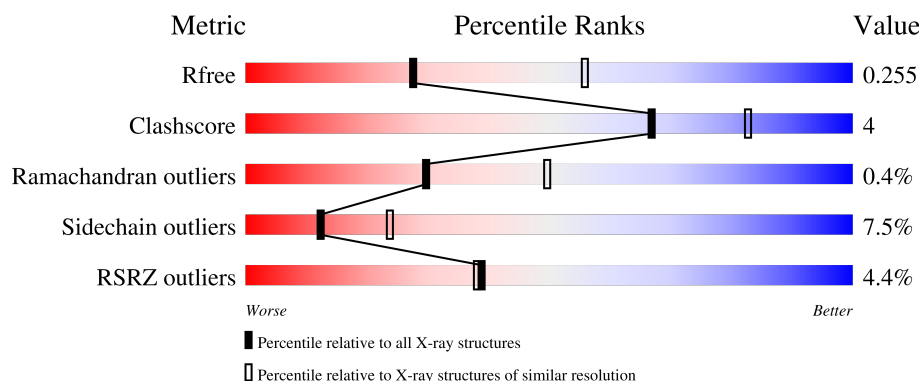
1 Overall quality at a glance i

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	0% 88% 9% ..
1	D	182	2% 87% 12% .
1	G	182	3% 80% 15% ..
2	B	189	11% 74% 23% .
2	E	189	5% 75% 17% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	189	5% 77% 19%
3	C	13	62% 38%
3	F	13	62% 38%
3	I	13	85% 15%
4	J	3	33% 67%

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.

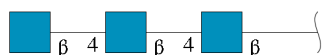
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			113	70	22	21			
3	F	13	Total	C	N	O	0	0	0
			113	70	22	21			

Continued on next page...

Continued from previous page...

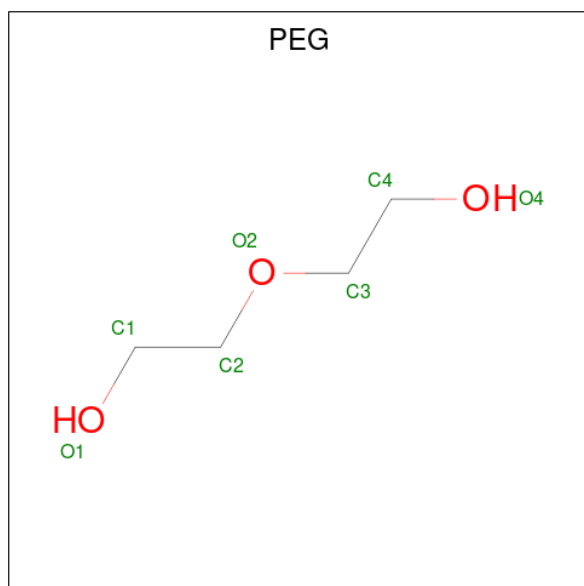
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	0	0	0
			113	70	22	21			

- 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 (CCD ID: 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 (CCD ID: 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 (CCD ID: NA) (formula: Na).

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

Continued on next page...

Continued from previous page...

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

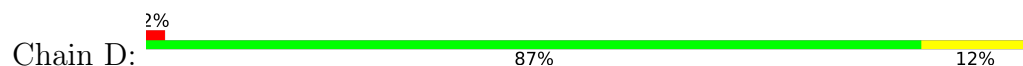
3 Residue-property plots [i](#)

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.

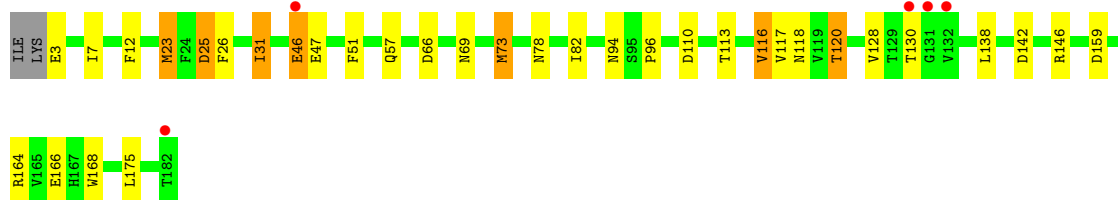
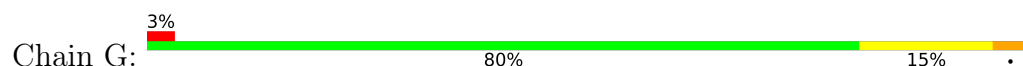
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



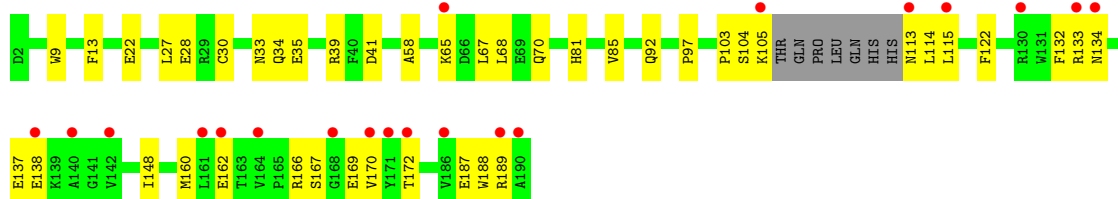
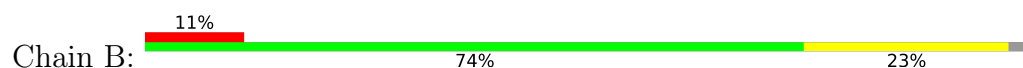
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



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

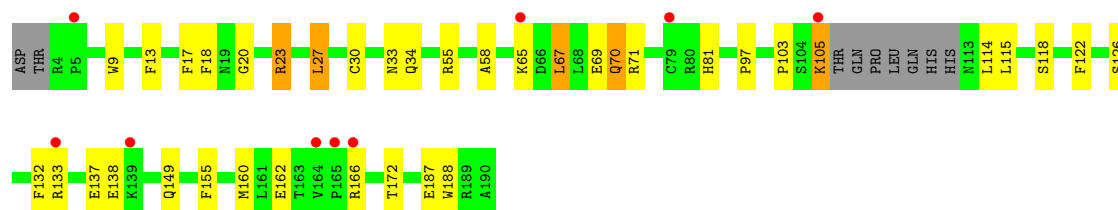


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



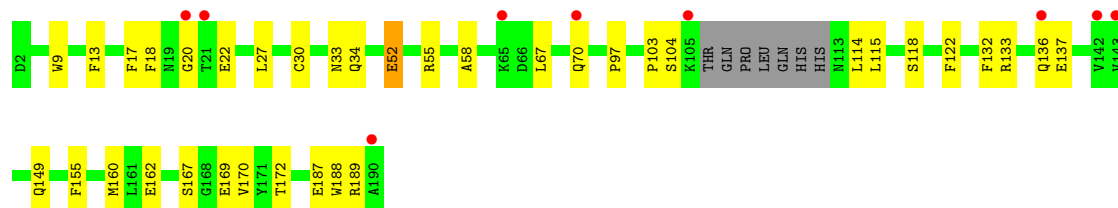
- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

Chain E: 



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

Chain H: 



- Molecule 3: Peptide from Capsid protein p24

Chain C: 



- Molecule 3: Peptide from Capsid protein p24

Chain F: 



- Molecule 3: Peptide from Capsid protein p24

Chain I: 



- 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

Chain J: 



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 47.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.96-2.75) 98.6 (47.96-2.75)	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)	0.33 , 63.0	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	0.93	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: NAG, NA, PEG

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	0.89	2/1525 (0.1%)	1.34	6/2080 (0.3%)
1	D	0.90	0/1551	1.31	7/2115 (0.3%)
1	G	0.93	3/1536 (0.2%)	1.35	13/2094 (0.6%)
2	B	0.86	0/1528	1.20	4/2073 (0.2%)
2	E	0.90	0/1513	1.25	4/2052 (0.2%)
2	H	0.85	0/1528	1.22	3/2073 (0.1%)
3	C	0.77	0/114	1.35	0/149
3	F	0.84	0/114	1.41	0/149
3	I	0.81	0/114	1.18	0/149
All	All	0.88	5/9523 (0.1%)	1.28	37/12934 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	73	MET	SD-CE	-7.14	1.61	1.79
1	A	73	MET	SD-CE	-5.97	1.64	1.79
1	G	23	MET	SD-CE	-5.75	1.65	1.79
1	A	23	MET	SD-CE	-5.54	1.65	1.79
1	G	82	ILE	CA-CB	5.26	1.60	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25	ASP	CA-CB-CG	11.62	124.22	112.60
1	A	25	ASP	CA-CB-CG	10.01	122.61	112.60
1	D	25	ASP	CA-CB-CG	7.40	120.00	112.60
1	G	142	ASP	CA-CB-CG	6.25	118.85	112.60
2	E	166	ARG	CA-C-N	5.86	128.72	120.28
2	E	166	ARG	C-N-CA	5.86	128.72	120.28
2	B	58	ALA	CA-C-N	5.86	128.05	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	ALA	C-N-CA	5.86	128.05	120.44
1	G	66	ASP	CA-CB-CG	5.83	118.43	112.60
1	D	159	ASP	CA-CB-CG	5.73	118.33	112.60
2	H	52	GLU	CB-CG-CD	5.57	122.07	112.60
2	H	58	ALA	CA-C-N	5.45	127.85	120.44
2	H	58	ALA	C-N-CA	5.45	127.85	120.44
1	G	12	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	142	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	31	ILE	N-CA-C	-5.32	105.66	110.82
1	A	66	ASP	CA-CB-CG	5.30	117.90	112.60
2	E	58	ALA	CA-C-N	5.25	127.26	120.44
2	E	58	ALA	C-N-CA	5.25	127.26	120.44
1	D	78	ASN	CA-C-N	5.24	129.58	122.19
1	D	78	ASN	C-N-CA	5.24	129.58	122.19
1	G	78	ASN	CA-C-N	5.23	129.57	122.19
1	G	78	ASN	C-N-CA	5.23	129.57	122.19
1	D	66	ASP	CA-C-N	5.17	127.47	120.44
1	D	66	ASP	C-N-CA	5.17	127.47	120.44
1	G	57	GLN	CA-C-N	5.16	125.71	119.98
1	G	57	GLN	C-N-CA	5.16	125.71	119.98
1	G	159	ASP	CA-CB-CG	5.15	117.75	112.60
1	G	31	ILE	N-CA-C	-5.11	106.09	110.74
1	A	78	ASN	CA-C-N	5.09	129.42	122.34
1	A	78	ASN	C-N-CA	5.09	129.42	122.34
1	G	46	GLU	CA-C-N	5.08	127.34	120.38
1	G	46	GLU	C-N-CA	5.08	127.34	120.38
1	G	110	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	31	ILE	N-CA-C	-5.03	105.95	110.82
2	B	41	ASP	CA-CB-CG	5.02	117.62	112.60
2	B	35	GLU	CB-CG-CD	5.00	121.10	112.60

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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:9:TRP:CH2	2:H:30:CYS:HB3	2.47	0.50
2:H:114:LEU:HD22	2:H:160:MET:HB3	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:13:PHE:CD2	3:F:304:LEU:HD23	2.54	0.42
2:E:27:LEU:HD23	2:E:27:LEU:HA	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
2:E:81:HIS:CD2	3:F:302:LYS:HG3	2.56	0.41
1:G:7:ILE:HG12	1:G:26:PHE:HD1	1.86	0.41
1:G:116:VAL:HG13	1:G:168:TRP:CZ3	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	21	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	176/189 (93%)	170 (97%)	5 (3%)	1 (1%)	21	38
2	H	178/189 (94%)	171 (96%)	5 (3%)	2 (1%)	11	22
3	C	11/13 (85%)	11 (100%)	0	0	100	100
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%)	30	50

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%)	26	49
1	D	168/167 (101%)	158 (94%)	10 (6%)	17	32
1	G	166/167 (99%)	155 (93%)	11 (7%)	15	29
2	B	164/171 (96%)	147 (90%)	17 (10%)	7	13
2	E	162/171 (95%)	147 (91%)	15 (9%)	8	16
2	H	164/171 (96%)	151 (92%)	13 (8%)	11	21
3	C	11/11 (100%)	9 (82%)	2 (18%)	2	3
3	F	11/11 (100%)	10 (91%)	1 (9%)	9	17
3	I	11/11 (100%)	10 (91%)	1 (9%)	9	17
All	All	1022/1047 (98%)	945 (92%)	77 (8%)	12	24

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	46	GLU
1	A	94	ASN
1	A	113	THR
1	A	128	VAL
1	A	130	THR
1	A	175	LEU
2	B	22	GLU
2	B	27	LEU
2	B	34	GLN
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	115	LEU
2	B	133	ARG
2	B	137	GLU
2	B	138	GLU
2	B	162	GLU
2	B	167	SER
2	B	187	GLU
3	C	305	ARG
3	C	308	GLN
1	D	1	ILE
1	D	25	ASP
1	D	46	GLU
1	D	57	GLN
1	D	94	ASN
1	D	113	THR
1	D	128	VAL
1	D	130	THR
1	D	156	SER
1	D	175	LEU
2	E	23	ARG
2	E	27	LEU
2	E	34	GLN
2	E	65	LYS
2	E	67	LEU
2	E	69	GLU
2	E	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	105	LYS
2	E	115	LEU
2	E	126	SER
2	E	133	ARG
2	E	137	GLU
2	E	138	GLU
2	E	162	GLU
2	E	187	GLU
3	F	308	GLN
1	G	23	MET
1	G	25	ASP
1	G	46	GLU
1	G	94	ASN
1	G	113	THR
1	G	116	VAL
1	G	117	VAL
1	G	120	THR
1	G	128	VAL
1	G	130	THR
1	G	175	LEU
2	H	22	GLU
2	H	27	LEU
2	H	34	GLN
2	H	67	LEU
2	H	70	GLN
2	H	104	SER
2	H	115	LEU
2	H	133	ARG
2	H	136	GLN
2	H	137	GLU
2	H	162	GLU
2	H	167	SER
2	H	187	GLU
3	I	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
2	B	10	GLN
2	B	149	GLN
2	E	10	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	34	GLN
2	E	70	GLN
2	E	150	ASN
2	E	156	GLN
2	H	10	GLN
2	H	70	GLN
2	H	113	ASN
2	H	150	ASN
2	H	156	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	0.34	0	17,19,21	0.68	0
4	NAG	J	2	4	14,14,15	0.43	0	17,19,21	1.95	2 (11%)
4	NAG	J	3	4	14,14,15	0.43	0	17,19,21	1.08	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	6.73	121.21	112.19
4	J	3	NAG	C1-O5-C5	3.76	117.22	112.19
4	J	2	NAG	C3-C4-C5	2.35	114.50	110.23

There are no chirality outliers.

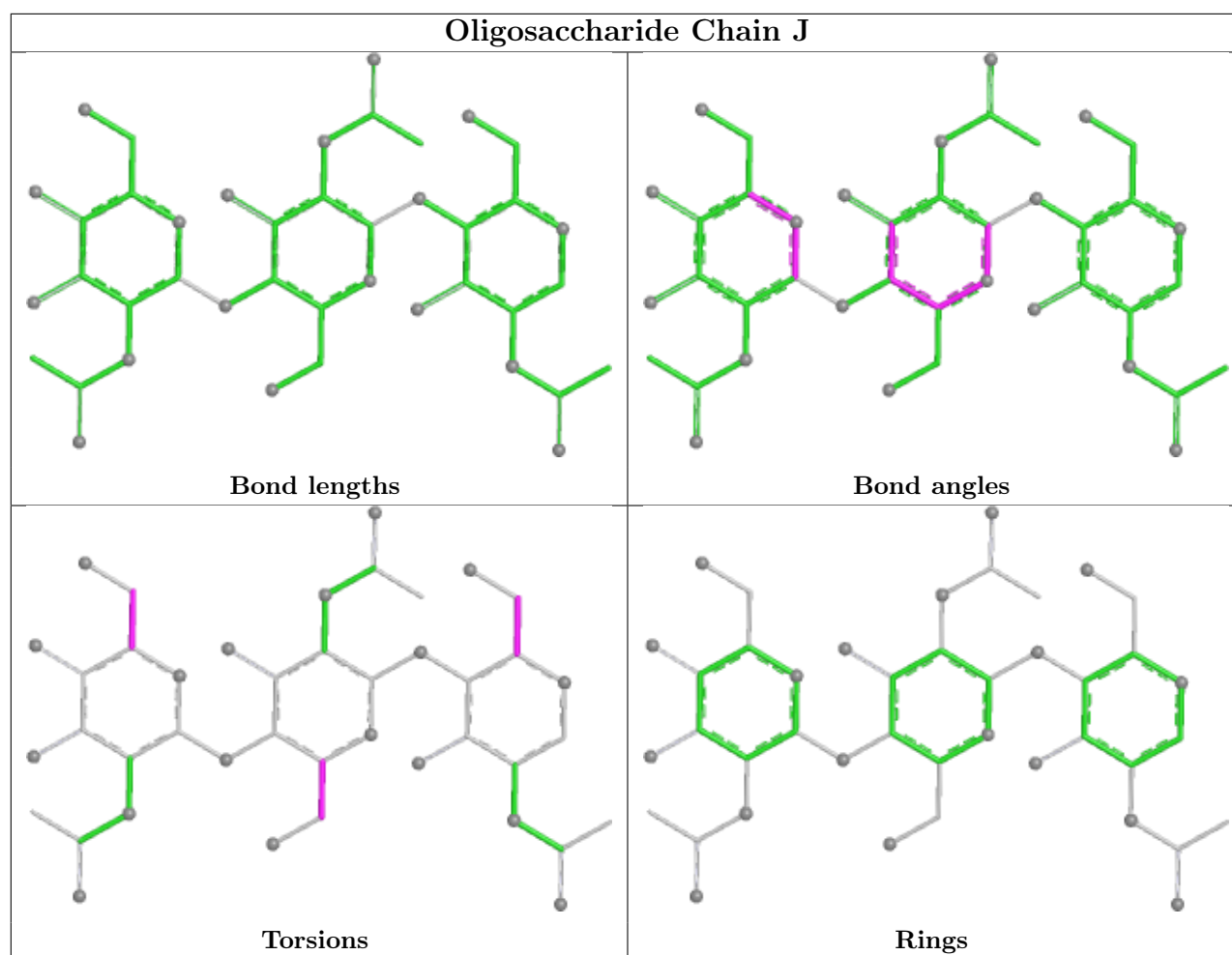
All (4) torsion outliers are listed below:

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	A	201	-	6,6,6	0.25	0	5,5,5	0.27	0
5	PEG	G	201	-	6,6,6	0.42	0	5,5,5	0.32	0
5	PEG	B	201	-	6,6,6	0.19	0	5,5,5	0.13	0
6	NAG	A	202	1	14,14,15	0.44	0	17,19,21	1.35	1 (5%)
5	PEG	E	201	-	6,6,6	0.42	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	202	1	14,14,15	0.41	0	17,19,21	1.59	3 (17%)

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	A	201	-	-	3/4/4/4	-
5	PEG	G	201	-	-	1/4/4/4	-
5	PEG	B	201	-	-	1/4/4/4	-
6	NAG	A	202	1	-	1/6/23/26	0/1/1/1
5	PEG	E	201	-	-	3/4/4/4	-
6	NAG	D	202	1	-	2/6/23/26	0/1/1/1

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	4.75	118.55	112.19
6	D	202	NAG	O5-C1-C2	-3.87	105.30	111.29
6	D	202	NAG	C1-C2-N2	3.77	116.38	110.43
6	D	202	NAG	C1-O5-C5	3.56	116.96	112.19

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
5	A	201	PEG	1	0
5	E	201	PEG	2	0
6	D	202	NAG	1	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%)	0.22	2 (1%) 78 77	26, 44, 71, 104	1 (0%)
1	D	182/182 (100%)	0.54	4 (2%) 62 60	36, 54, 76, 98	2 (1%)
1	G	180/182 (98%)	0.28	5 (2%) 55 53	16, 45, 73, 118	2 (1%)
2	B	182/189 (96%)	0.48	20 (10%) 10 9	25, 47, 103, 124	0
2	E	180/189 (95%)	0.39	9 (5%) 34 34	32, 49, 87, 120	0
2	H	182/189 (96%)	0.46	9 (4%) 35 34	32, 50, 83, 101	0
3	C	13/13 (100%)	0.12	0 100 100	27, 41, 62, 75	0
3	F	13/13 (100%)	0.28	0 100 100	37, 43, 82, 94	0
3	I	13/13 (100%)	0.30	0 100 100	35, 45, 67, 78	0
All	All	1125/1152 (97%)	0.39	49 (4%) 39 38	16, 48, 84, 124	5 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ILE	4.1
2	B	190	ALA	3.8
1	A	182	THR	3.8
1	G	182	THR	3.8
2	E	164	VAL	3.8
2	B	172	THR	3.2
2	B	105	LYS	3.2
2	B	189	ARG	3.1
1	G	132	VAL	3.0
2	E	165	PRO	2.9
2	B	186	VAL	2.8
2	H	142	VAL	2.8
2	E	105	LYS	2.7
1	A	126	LYS	2.7
2	B	134	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	126	LYS	2.6
2	E	5	PRO	2.6
2	H	136	GLN	2.6
2	H	143	VAL	2.5
2	E	133	ARG	2.5
2	B	170	VAL	2.5
2	H	190	ALA	2.5
2	B	171	TYR	2.4
1	G	130	THR	2.4
2	H	20	GLY	2.4
2	H	105	LYS	2.4
2	B	161	LEU	2.4
2	B	130	ARG	2.4
2	B	162	GLU	2.3
2	H	65	LYS	2.3
2	H	70	GLN	2.3
1	D	94	ASN	2.3
1	G	46	GLU	2.3
2	B	133	ARG	2.3
1	D	182	THR	2.3
2	H	21	THR	2.3
2	B	115	LEU	2.3
2	B	164	VAL	2.3
2	E	166	ARG	2.2
2	B	168	GLY	2.2
2	B	113	ASN	2.1
2	E	65	LYS	2.1
2	B	65	LYS	2.1
2	B	138	GLU	2.1
2	E	79	CYS	2.1
2	B	140	ALA	2.0
2	E	139	LYS	2.0
1	G	131	GLY	2.0
2	B	142	VAL	2.0

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

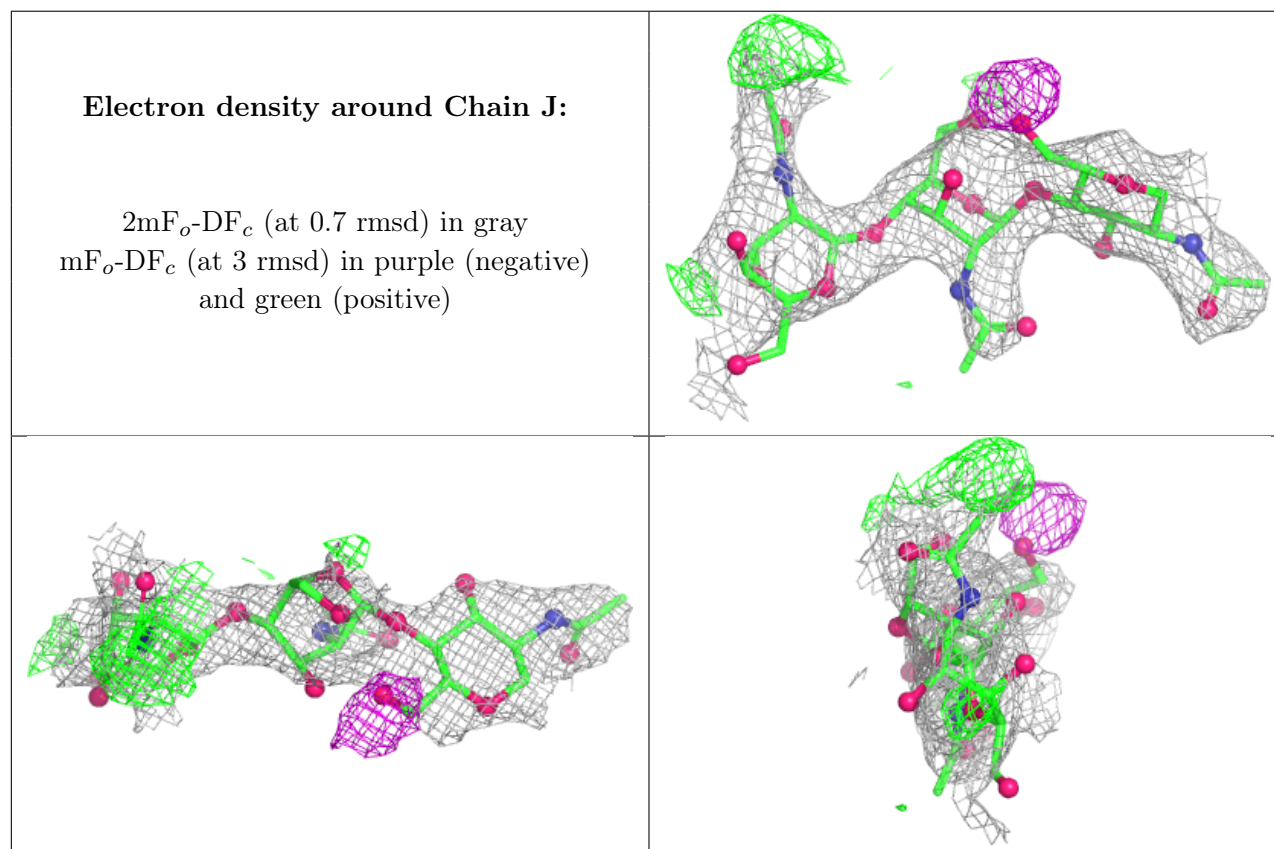
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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
4	NAG	J	3	14/15	0.23	0.24	110,120,124,124	0
4	NAG	J	2	14/15	0.58	0.18	107,111,114,114	0
4	NAG	J	1	14/15	0.83	0.15	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($\text{\AA}^2$)	Q<0.9
6	NAG	D	202	14/15	0.72	0.16	86,94,97,98	0
6	NAG	A	202	14/15	0.81	0.13	42,77,85,86	0
5	PEG	B	201	7/7	0.87	0.15	72,74,76,76	0
7	NA	D	201	1/1	0.89	0.19	58,58,58,58	0
5	PEG	E	201	7/7	0.90	0.13	36,37,45,49	0
7	NA	G	202	1/1	0.91	0.32	59,59,59,59	0
5	PEG	A	201	7/7	0.92	0.12	37,41,52,54	0
5	PEG	G	201	7/7	0.95	0.09	37,39,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.