



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:25 AM EDT

PDB ID : 7PDY / pdb_00007pdy
Title : A viral peptide from Marek's disease virus bound to chicken MHC-II molecule
Authors : Goryanin, A.; Cook, A.G.; Kaufman, J.; Halabi, S.
Deposited on : 2021-08-09
Resolution : 2.54 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

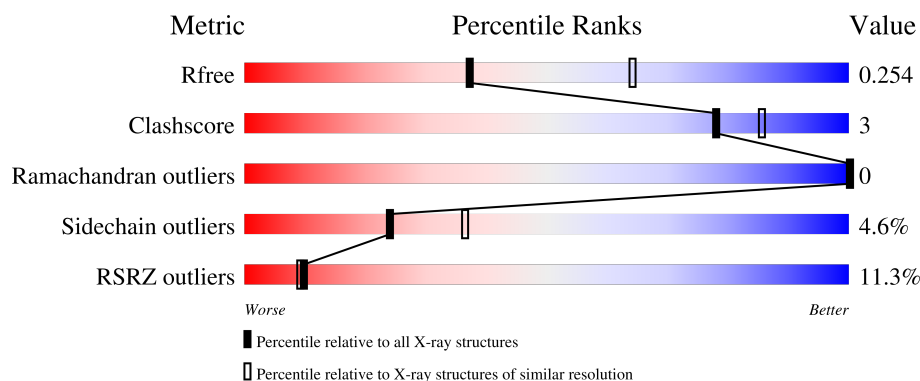
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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.



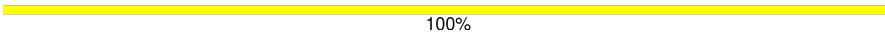
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	191	5% 92% 5% ..
1	C	191	12% 88% 7% ..
1	E	191	9% 83% 14% .
2	B	225	9% 79% 11% . 9%
2	D	225	15% 81% 7% . 10%

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Mol	Chain	Length	Quality of chain
2	F	225	
3	G	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	2	X	-	-	-
4	NAG	A	201	X	-	-	-
4	NAG	C	201	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9525 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 MHC class II alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	0
			1517	978	259	274	6			
1	C	184	Total	C	N	O	S	0	0	0
			1452	936	249	261	6			
1	E	184	Total	C	N	O	S	0	0	0
			1472	951	249	266	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	-	expression tag	UNP Q4U5Z6
A	3	ARG	-	expression tag	UNP Q4U5Z6
A	4	ARG	-	expression tag	UNP Q4U5Z6
C	2	ASP	-	expression tag	UNP Q4U5Z6
C	3	ARG	-	expression tag	UNP Q4U5Z6
C	4	ARG	-	expression tag	UNP Q4U5Z6
E	2	ASP	-	expression tag	UNP Q4U5Z6
E	3	ARG	-	expression tag	UNP Q4U5Z6
E	4	ARG	-	expression tag	UNP Q4U5Z6

- Molecule 2 is a protein called 38 kDa phosphoprotein,MHC class II beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1598	1012	274	305	7			
2	D	202	Total	C	N	O	S	0	0	0
			1579	1002	267	304	6			
2	F	204	Total	C	N	O	S	0	0	0
			1606	1017	277	305	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	ASP	-	expression tag	UNP P68348
B	-28	ARG	-	expression tag	UNP P68348
B	-27	PRO	-	expression tag	UNP P68348
B	-9	GLY	-	linker	UNP P68348
B	-8	GLY	-	linker	UNP P68348
B	-7	GLY	-	linker	UNP P68348
B	-6	GLY	-	linker	UNP P68348
B	-5	SER	-	linker	UNP P68348
B	-4	GLY	-	linker	UNP P68348
B	-3	GLY	-	linker	UNP P68348
B	-2	GLY	-	linker	UNP P68348
B	-1	GLY	-	linker	UNP P68348
B	0	SER	-	linker	UNP P68348
B	1	GLY	-	linker	UNP P68348
B	2	GLY	-	linker	UNP P68348
B	3	GLY	-	linker	UNP P68348
B	4	GLY	-	linker	UNP P68348
B	5	SER	-	linker	UNP P68348
D	-29	ASP	-	expression tag	UNP P68348
D	-28	ARG	-	expression tag	UNP P68348
D	-27	PRO	-	expression tag	UNP P68348
D	-9	GLY	-	linker	UNP P68348
D	-8	GLY	-	linker	UNP P68348
D	-7	GLY	-	linker	UNP P68348
D	-6	GLY	-	linker	UNP P68348
D	-5	SER	-	linker	UNP P68348
D	-4	GLY	-	linker	UNP P68348
D	-3	GLY	-	linker	UNP P68348
D	-2	GLY	-	linker	UNP P68348
D	-1	GLY	-	linker	UNP P68348
D	0	SER	-	linker	UNP P68348
D	1	GLY	-	linker	UNP P68348
D	2	GLY	-	linker	UNP P68348
D	3	GLY	-	linker	UNP P68348
D	4	GLY	-	linker	UNP P68348
D	5	SER	-	linker	UNP P68348
F	-29	ASP	-	expression tag	UNP P68348
F	-28	ARG	-	expression tag	UNP P68348
F	-27	PRO	-	expression tag	UNP P68348
F	-9	GLY	-	linker	UNP P68348
F	-8	GLY	-	linker	UNP P68348
F	-7	GLY	-	linker	UNP P68348
F	-6	GLY	-	linker	UNP P68348

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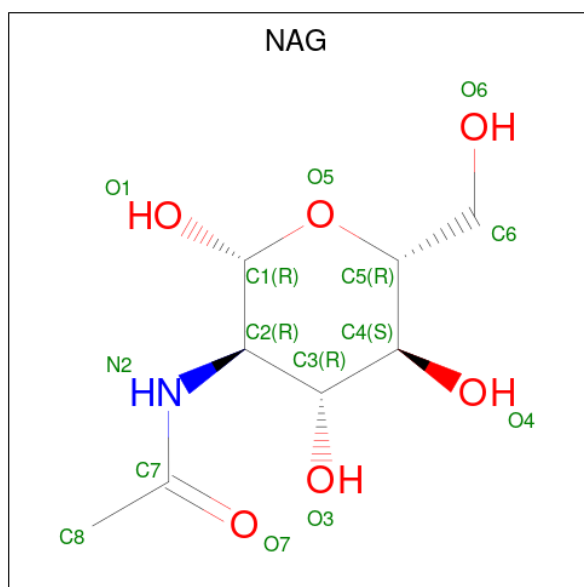
Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	SER	-	linker	UNP P68348
F	-4	GLY	-	linker	UNP P68348
F	-3	GLY	-	linker	UNP P68348
F	-2	GLY	-	linker	UNP P68348
F	-1	GLY	-	linker	UNP P68348
F	0	SER	-	linker	UNP P68348
F	1	GLY	-	linker	UNP P68348
F	2	GLY	-	linker	UNP P68348
F	3	GLY	-	linker	UNP P68348
F	4	GLY	-	linker	UNP P68348
F	5	SER	-	linker	UNP P68348

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



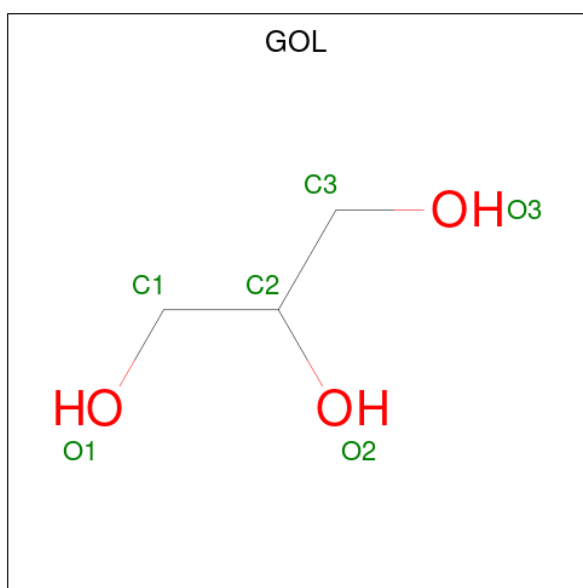
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	0
			44	44		
8	B	32	Total	O	0	0
			32	32		
8	C	21	Total	O	0	0
			21	21		
8	D	9	Total	O	0	0
			9	9		
8	E	21	Total	O	0	0
			21	21		
8	F	20	Total	O	0	0
			20	20		

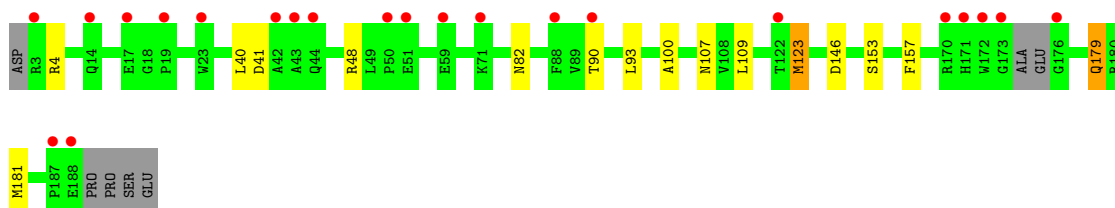
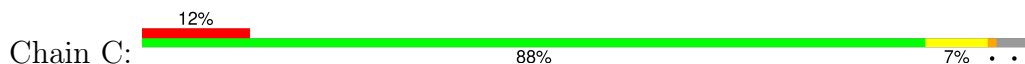
3 Residue-property plots [i](#)

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.

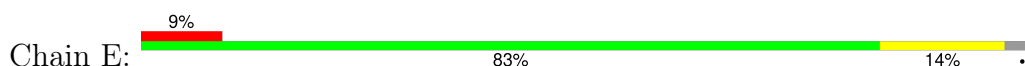
- Molecule 1: MHC class II alpha chain



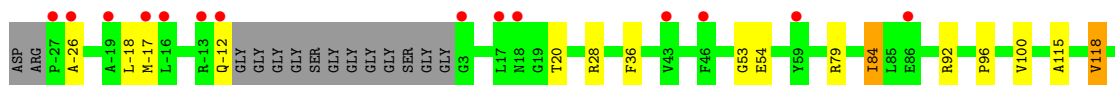
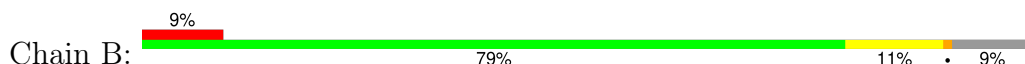
- Molecule 1: MHC class II alpha chain



- Molecule 1: MHC class II alpha chain

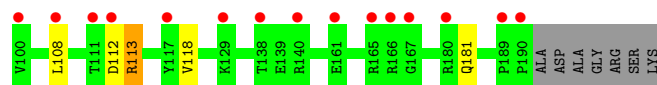
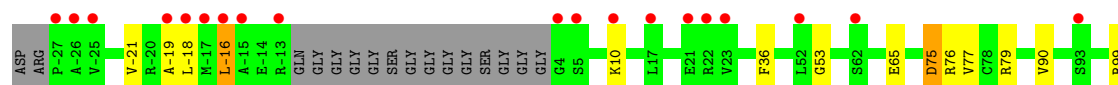
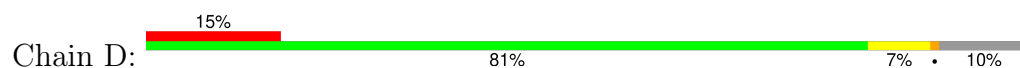


- Molecule 2: 38 kDa phosphoprotein, MHC class II beta chain

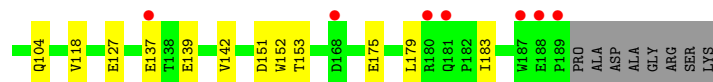
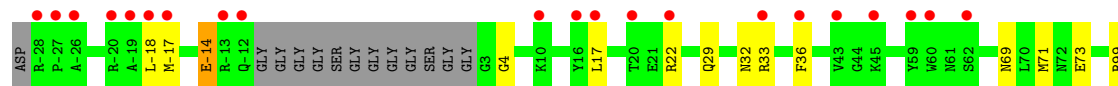
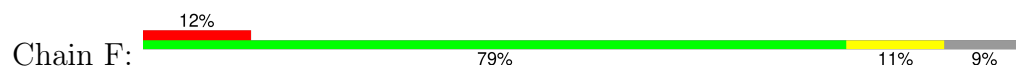




- Molecule 2: 38 kDa phosphoprotein,MHC class II beta chain



- Molecule 2: 38 kDa phosphoprotein,MHC class II beta chain



- Molecule 3: 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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.54Å 238.54Å 76.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	206.58 – 2.54 206.58 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.0 (206.58-2.54) 99.0 (206.58-2.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.216 , 0.252 0.217 , 0.254	Depositor DCC
R_{free} test set	4205 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9525	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: ACT, GOL, NAG, 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	0.95	0/1567	1.28	4/2134 (0.2%)
1	C	1.00	0/1497	1.29	4/2040 (0.2%)
1	E	0.95	0/1518	1.29	2/2066 (0.1%)
2	B	1.00	0/1638	1.25	0/2233
2	D	1.00	0/1619	1.24	2/2210 (0.1%)
2	F	0.98	0/1645	1.22	0/2241
All	All	0.98	0/9484	1.26	12/12924 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	LEU	CB-CA-C	-11.66	92.35	111.36
1	A	19	PRO	N-CA-C	-8.20	95.58	112.47
1	C	41	ASP	N-CA-C	-7.66	104.55	114.04
1	A	19	PRO	CB-CA-C	6.70	122.61	111.56
1	A	183	GLU	CB-CA-C	6.61	119.35	109.63
1	E	19	PRO	N-CA-C	-5.44	102.14	110.95
1	E	12	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	112	TYR	CB-CA-C	5.40	119.68	109.37
1	C	90	THR	CB-CA-C	5.21	117.80	109.62
1	C	82	ASN	CB-CA-C	5.03	118.60	111.86
2	D	-16	LEU	CA-C-N	5.01	127.97	120.95
2	D	-16	LEU	C-N-CA	5.01	127.97	120.95

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	1517	0	1423	2	1
1	C	1452	0	1338	7	0
1	E	1472	0	1372	11	1
2	B	1598	0	1483	11	1
2	D	1579	0	1457	11	0
2	F	1606	0	1499	15	0
3	G	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
5	E	6	0	8	0	0
6	A	4	0	3	0	0
6	B	8	0	6	0	0
6	C	8	0	6	1	0
6	D	4	0	3	0	0
6	F	4	0	3	0	0
7	A	7	0	10	0	0
7	B	5	0	5	0	1
8	A	44	0	0	0	0
8	B	32	0	0	2	0
8	C	21	0	0	1	0
8	D	9	0	0	0	0
8	E	21	0	0	0	0
8	F	20	0	0	2	0
All	All	9525	0	8725	50	3

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 3.

All (50) 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:112:ASP:OD2	1:E:183:GLU:CD	2.45	0.60
1:C:123:MET:HG3	1:C:153:SER:HB2	1.88	0.56
1:C:48:ARG:HH12	6:C:203:ACT:H2	1.74	0.51
5:C:204:GOL:C3	8:C:309:HOH:O	2.58	0.51
2:F:17:LEU:HB3	8:F:314:HOH:O	2.10	0.50
1:E:86:GLN:CG	2:F:32:ASN:HB3	2.42	0.49
2:B:36:PHE:O	2:B:53:GLY:HA3	2.13	0.49
1:E:107:ASN:HB3	1:E:157:PHE:CE1	2.48	0.49
1:C:100:ALA:HB1	2:D:99:ARG:CZ	2.43	0.49
1:C:179:GLN:HB2	2:F:142:VAL:HG13	1.94	0.49
2:B:100:VAL:HG21	2:B:187:TRP:HB2	1.94	0.48
2:B:92:ARG:O	8:B:301:HOH:O	2.20	0.48
1:E:86:GLN:HG3	2:F:32:ASN:HB3	1.95	0.47
2:D:-19:ALA:HA	2:D:10:LYS:NZ	2.30	0.47
1:C:146:ASP:CG	2:F:33:ARG:HH12	2.23	0.47
2:B:115:ALA:HB1	2:B:157:LEU:HD11	1.95	0.47
2:F:17:LEU:HB2	2:F:22:ARG:HB3	1.95	0.47
2:B:151:ASP:O	2:B:152:TRP:HB2	2.15	0.46
2:B:20:THR:O	2:B:79:ARG:NH1	2.42	0.46
2:D:36:PHE:O	2:D:53:GLY:HA3	2.16	0.46
2:D:112:ASP:OD2	1:E:183:GLU:OE1	2.33	0.46
2:D:-19:ALA:HA	2:D:10:LYS:HZ3	1.81	0.46
2:F:151:ASP:O	2:F:152:TRP:HB2	2.16	0.45
2:B:100:VAL:HA	2:B:115:ALA:O	2.17	0.45
1:E:91:PRO:HB3	1:E:116:PHE:HB3	1.99	0.44
2:D:112:ASP:HB3	2:D:113:ARG:HG3	2.00	0.44
2:B:28:ARG:HD3	8:B:313:HOH:O	2.18	0.44
2:F:-18:LEU:HD23	2:F:-18:LEU:N	2.33	0.44
2:B:96:PRO:HB3	2:B:118:VAL:HG12	2.00	0.43
2:D:75:ASP:HA	2:D:79:ARG:HB2	1.99	0.43
2:B:-26:ALA:HB3	2:B:84:ILE:HG23	2.00	0.43
1:E:136:VAL:HA	1:E:154:TYR:O	2.18	0.43
2:D:-21:VAL:HG22	2:D:77:VAL:HG21	2.01	0.43
1:E:13:TYR:CE1	1:E:67:MET:HA	2.54	0.42
1:C:93:LEU:HD12	1:C:93:LEU:HA	1.91	0.42
1:E:85:GLN:NE2	2:F:4:GLY:HA2	2.34	0.42
2:F:71:MET:HE3	2:F:71:MET:HB3	1.94	0.42
1:A:19:PRO:O	1:A:19:PRO:HD2	2.19	0.42
2:F:29:GLN:HB3	2:F:36:PHE:CZ	2.55	0.41
2:B:133:ASN:HA	2:B:169:SER:HG	1.84	0.41
2:D:181:GLN:N	2:D:181:GLN:OE1	2.54	0.41
1:E:11:GLU:HA	1:E:25:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:ASN:O	2:F:73:GLU:HG2	2.21	0.41
1:A:136:VAL:HA	1:A:154:TYR:O	2.22	0.40
1:E:88:PHE:N	1:E:88:PHE:CD1	2.89	0.40
1:C:107:ASN:HB3	1:C:157:PHE:CE1	2.56	0.40
2:D:108:LEU:HD23	2:D:108:LEU:HA	1.92	0.40
2:F:-14:GLU:HB2	8:F:307:HOH:O	2.20	0.40
2:F:127:GLU:HB3	2:F:175:GLU:HB2	2.04	0.40
2:F:179:LEU:HD13	2:F:183:ILE:HG13	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:203:PEG:C3	7:B:203:PEG:C3[6_554]	1.89	0.31
2:B:54:GLU:OE1	2:B:54:GLU:OE1[6_554]	2.15	0.05
1:A:134:GLU:OE2	1:E:18:GLY:O[3_544]	2.16	0.04

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	185/191 (97%)	179 (97%)	6 (3%)	0	100	100
1	C	180/191 (94%)	179 (99%)	1 (1%)	0	100	100
1	E	180/191 (94%)	176 (98%)	4 (2%)	0	100	100
2	B	200/225 (89%)	196 (98%)	4 (2%)	0	100	100
2	D	198/225 (88%)	191 (96%)	7 (4%)	0	100	100
2	F	200/225 (89%)	194 (97%)	6 (3%)	0	100	100
All	All	1143/1248 (92%)	1115 (98%)	28 (2%)	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	156/162 (96%)	151 (97%)	5 (3%)	34	51
1	C	144/162 (89%)	139 (96%)	5 (4%)	32	48
1	E	149/162 (92%)	140 (94%)	9 (6%)	17	26
2	B	168/188 (89%)	159 (95%)	9 (5%)	20	30
2	D	166/188 (88%)	158 (95%)	8 (5%)	23	35
2	F	169/188 (90%)	161 (95%)	8 (5%)	23	36
All	All	952/1050 (91%)	908 (95%)	44 (5%)	24	36

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	20	ASP
1	A	44	GLN
1	A	123	MET
1	A	179	GLN
2	B	-18	LEU
2	B	-17	MET
2	B	-12	GLN
2	B	84	ILE
2	B	118	VAL
2	B	132	LEU
2	B	137	GLU
2	B	143	SER
2	B	165	ARG
1	C	4	ARG
1	C	109	LEU
1	C	123	MET
1	C	179	GLN
1	C	181	MET
2	D	-18	LEU
2	D	-16	LEU
2	D	65	GLU

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Mol	Chain	Res	Type
2	D	75	ASP
2	D	76	ARG
2	D	90	VAL
2	D	113	ARG
2	D	118	VAL
1	E	4	ARG
1	E	16	SER
1	E	51	GLU
1	E	71	LYS
1	E	82	ASN
1	E	123	MET
1	E	134	GLU
1	E	180	ARG
1	E	185	GLU
2	F	-17	MET
2	F	-14	GLU
2	F	99	ARG
2	F	104	GLN
2	F	118	VAL
2	F	137	GLU
2	F	139	GLU
2	F	153	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	C	61	GLN
1	C	66	ASN
2	D	18	ASN
2	D	34	GLN
2	D	80	HIS
1	E	82	ASN
2	F	-23	HIS
2	F	34	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 ⓘ

2 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	G	1	3	14,14,15	0.44	0	17,19,21	1.15	1 (5%)
3	NAG	G	2	3	14,14,15	0.67	0	17,19,21	2.62	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
3	NAG	G	1	3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	1/1/5/7	3/6/23/26	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(°)
3	G	2	NAG	C1-C2-N2	6.28	120.33	110.43
3	G	2	NAG	C1-O5-C5	-6.04	104.09	112.19
3	G	2	NAG	O5-C1-C2	5.98	120.55	111.29
3	G	1	NAG	O5-C1-C2	-3.43	105.99	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	2	NAG	C1

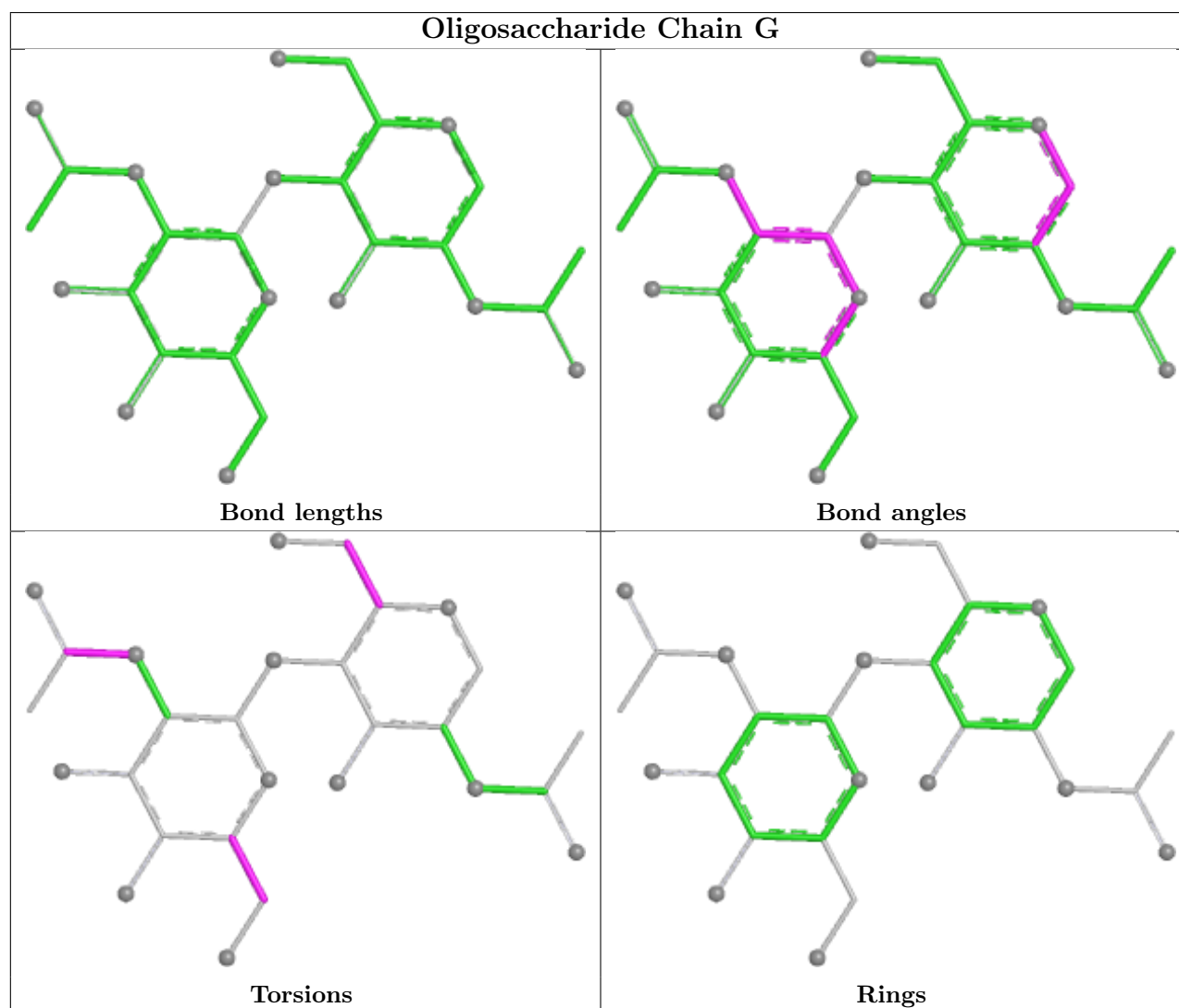
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2

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

18 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	D	201	-	14,14,15	0.78	1 (7%)	17,19,21	1.72	1 (5%)
5	GOL	A	202	-	5,5,5	0.21	0	5,5,5	0.27	0
5	GOL	C	204	-	5,5,5	0.20	0	5,5,5	0.41	0
4	NAG	C	201	1	14,14,15	1.15	1 (7%)	17,19,21	1.56	3 (17%)
5	GOL	B	201	-	5,5,5	0.25	0	5,5,5	0.55	0
6	ACT	F	201	-	3,3,3	1.26	0	3,3,3	0.89	0
7	PEG	A	205	-	6,6,6	0.45	0	5,5,5	0.14	0
6	ACT	C	203	-	3,3,3	1.05	0	3,3,3	0.91	0
6	ACT	C	202	-	3,3,3	1.17	0	3,3,3	0.95	0
4	NAG	A	201	1	14,14,15	1.03	1 (7%)	17,19,21	1.36	2 (11%)
4	NAG	F	200	2	14,14,15	0.59	0	17,19,21	1.31	2 (11%)
6	ACT	B	202	-	3,3,3	1.11	0	3,3,3	0.70	0
6	ACT	B	204	-	3,3,3	1.18	0	3,3,3	0.74	0
5	GOL	A	204	-	5,5,5	0.22	0	5,5,5	0.44	0
6	ACT	A	203	-	3,3,3	1.32	0	3,3,3	0.81	0
5	GOL	E	201	-	5,5,5	0.20	0	5,5,5	0.58	0
7	PEG	B	203	-	4,4,6	0.39	0	3,3,5	0.24	0
6	ACT	D	202	-	3,3,3	1.17	0	3,3,3	0.73	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
4	NAG	D	201	-	-	2/6/23/26	0/1/1/1
5	GOL	A	202	-	-	0/4/4/4	-
5	GOL	C	204	-	-	2/4/4/4	-
4	NAG	C	201	1	1/1/5/7	4/6/23/26	0/1/1/1
5	GOL	B	201	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	A	205	-	-	1/4/4/4	-
4	NAG	A	201	1	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	F	200	2	-	4/6/23/26	0/1/1/1
5	GOL	A	204	-	-	2/4/4/4	-
5	GOL	E	201	-	-	2/4/4/4	-
7	PEG	B	203	-	-	1/2/2/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	NAG	O7-C7	2.65	1.29	1.23
4	A	201	NAG	C2-N2	2.23	1.50	1.46
4	D	201	NAG	O7-C7	2.11	1.28	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	NAG	C2-N2-C7	-6.20	114.60	122.90
4	A	201	NAG	O5-C1-C2	3.92	117.36	111.29
4	C	201	NAG	C2-N2-C7	-3.68	117.97	122.90
4	C	201	NAG	O5-C1-C2	3.29	116.38	111.29
4	F	200	NAG	O5-C1-C2	3.08	116.05	111.29
4	C	201	NAG	C1-C2-N2	2.85	114.93	110.43
4	F	200	NAG	C1-C2-N2	2.25	113.97	110.43
4	A	201	NAG	C3-C4-C5	2.25	114.30	110.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	201	NAG	C1
4	C	201	NAG	C1

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	NAG	C8-C7-N2-C2
4	A	201	NAG	O7-C7-N2-C2
4	D	201	NAG	C8-C7-N2-C2
4	D	201	NAG	O7-C7-N2-C2
5	A	204	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	201	GOL	C1-C2-C3-O3
5	B	201	GOL	O2-C2-C3-O3
5	C	204	GOL	O1-C1-C2-C3
5	E	201	GOL	C1-C2-C3-O3
4	C	201	NAG	C4-C5-C6-O6
4	F	200	NAG	O5-C5-C6-O6
4	C	201	NAG	O5-C5-C6-O6
4	A	201	NAG	O5-C5-C6-O6
4	C	201	NAG	C8-C7-N2-C2
4	F	200	NAG	C4-C5-C6-O6
4	F	200	NAG	C8-C7-N2-C2
4	F	200	NAG	O7-C7-N2-C2
7	B	203	PEG	O2-C3-C4-O4
4	C	201	NAG	O7-C7-N2-C2
5	B	201	GOL	O1-C1-C2-C3
5	E	201	GOL	O2-C2-C3-O3
7	A	205	PEG	O1-C1-C2-O2
4	A	201	NAG	C4-C5-C6-O6
5	A	204	GOL	O2-C2-C3-O3
5	B	201	GOL	O1-C1-C2-O2
5	C	204	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	204	GOL	1	0
6	C	203	ACT	1	0
7	B	203	PEG	0	1

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	187/191 (97%)	0.21	10 (5%) 32 31	50, 64, 98, 125	0
1	C	184/191 (96%)	0.89	22 (11%) 9 8	56, 78, 122, 159	0
1	E	184/191 (96%)	0.53	17 (9%) 14 14	51, 73, 104, 140	0
2	B	204/225 (90%)	0.72	21 (10%) 12 11	50, 83, 119, 139	0
2	D	202/225 (89%)	1.06	34 (16%) 4 3	59, 94, 127, 158	0
2	F	204/225 (90%)	0.91	28 (13%) 6 5	57, 91, 123, 156	0
All	All	1165/1248 (93%)	0.73	132 (11%) 10 9	50, 81, 121, 159	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	172	TRP	8.2
1	E	174	ALA	8.0
2	D	-13	ARG	6.2
1	E	177	PRO	6.1
1	E	188	GLU	6.1
1	A	189	PRO	5.7
1	A	3	ARG	4.6
1	E	171	HIS	4.6
2	F	-12	GLN	4.6
2	D	117	TYR	4.6
2	D	-27	PRO	4.5
1	C	3	ARG	4.3
1	C	173	GLY	4.3
2	F	189	PRO	4.1
2	D	190	PRO	4.0
1	C	17	GLU	4.0
2	B	-17	MET	3.8
1	E	54	ARG	3.8
2	F	17	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	-18	LEU	3.7
2	D	4	GLY	3.7
2	F	-27	PRO	3.7
2	B	-12	GLN	3.6
2	F	181	GLN	3.6
2	F	-13	ARG	3.6
2	F	45	LYS	3.6
2	B	59	TYR	3.5
1	C	23	TRP	3.5
1	E	88	PHE	3.5
2	B	18	ASN	3.5
1	E	3	ARG	3.3
2	F	22	ARG	3.3
2	D	-17	MET	3.3
1	C	42	ALA	3.3
2	D	62	SER	3.2
1	E	187	PRO	3.2
2	D	10	LYS	3.2
2	F	187	TRP	3.2
1	E	172	TRP	3.1
1	A	175	GLU	3.1
2	D	161	GLU	3.1
2	F	-17	MET	3.1
1	A	18	GLY	3.1
1	C	88	PHE	3.1
2	B	187	TRP	3.1
2	D	17	LEU	3.1
2	B	-27	PRO	3.1
2	D	5	SER	3.1
1	E	170	ARG	3.1
2	F	43	VAL	3.1
2	D	22	ARG	3.0
2	B	-26	ALA	3.0
1	C	176	GLY	3.0
1	C	51	GLU	2.9
2	B	43	VAL	2.9
1	C	171	HIS	2.9
1	A	4	ARG	2.9
2	F	33	ARG	2.9
2	F	168	ASP	2.8
2	D	180	ARG	2.8
1	C	43	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	190	PRO	2.7
1	C	170	ARG	2.7
1	E	104	GLU	2.7
1	C	71	LYS	2.7
2	D	-16	LEU	2.7
2	F	10	LYS	2.6
1	C	19	PRO	2.6
2	D	189	PRO	2.6
2	D	-15	ALA	2.6
1	C	187	PRO	2.5
1	A	174	ALA	2.5
2	B	177	ALA	2.5
2	F	-20	ARG	2.5
2	F	60	TRP	2.5
2	D	23	VAL	2.5
2	D	-26	ALA	2.5
2	B	3	GLY	2.5
2	F	36	PHE	2.4
1	C	50	PRO	2.4
1	E	19	PRO	2.4
2	B	189	PRO	2.4
2	F	-18	LEU	2.4
1	A	8	LEU	2.4
2	B	166	ARG	2.4
2	F	59	TYR	2.4
2	D	-25	VAL	2.4
2	F	20	THR	2.3
2	F	62	SER	2.3
2	F	-26	ALA	2.3
1	E	18	GLY	2.3
2	D	167	GLY	2.3
2	D	108	LEU	2.3
2	D	166	ARG	2.3
2	D	111	THR	2.3
2	F	188	GLU	2.3
2	B	180	ARG	2.3
1	C	44	GLN	2.2
2	D	93	SER	2.2
2	D	21	GLU	2.2
1	A	19	PRO	2.2
1	C	14	GLN	2.2
2	D	112	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	59	GLU	2.2
1	C	188	GLU	2.2
1	C	122	THR	2.2
2	B	46	PHE	2.2
2	F	16	TYR	2.2
2	B	-13	ARG	2.2
1	A	14	GLN	2.1
2	B	-16	LEU	2.1
1	A	61	GLN	2.1
1	C	90	THR	2.1
2	B	86	GLU	2.1
2	F	180	ARG	2.1
1	E	55	PHE	2.1
2	D	100	VAL	2.1
2	F	-19	ALA	2.1
2	D	129	LYS	2.1
1	E	4	ARG	2.1
2	D	52	LEU	2.1
2	F	-28	ARG	2.1
2	B	188	GLU	2.1
2	F	137	GLU	2.1
2	D	-19	ALA	2.0
1	E	23	TRP	2.0
2	D	138	THR	2.0
1	E	181	MET	2.0
2	D	140	ARG	2.0
2	D	165	ARG	2.0
2	B	-19	ALA	2.0
2	B	17	LEU	2.0

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

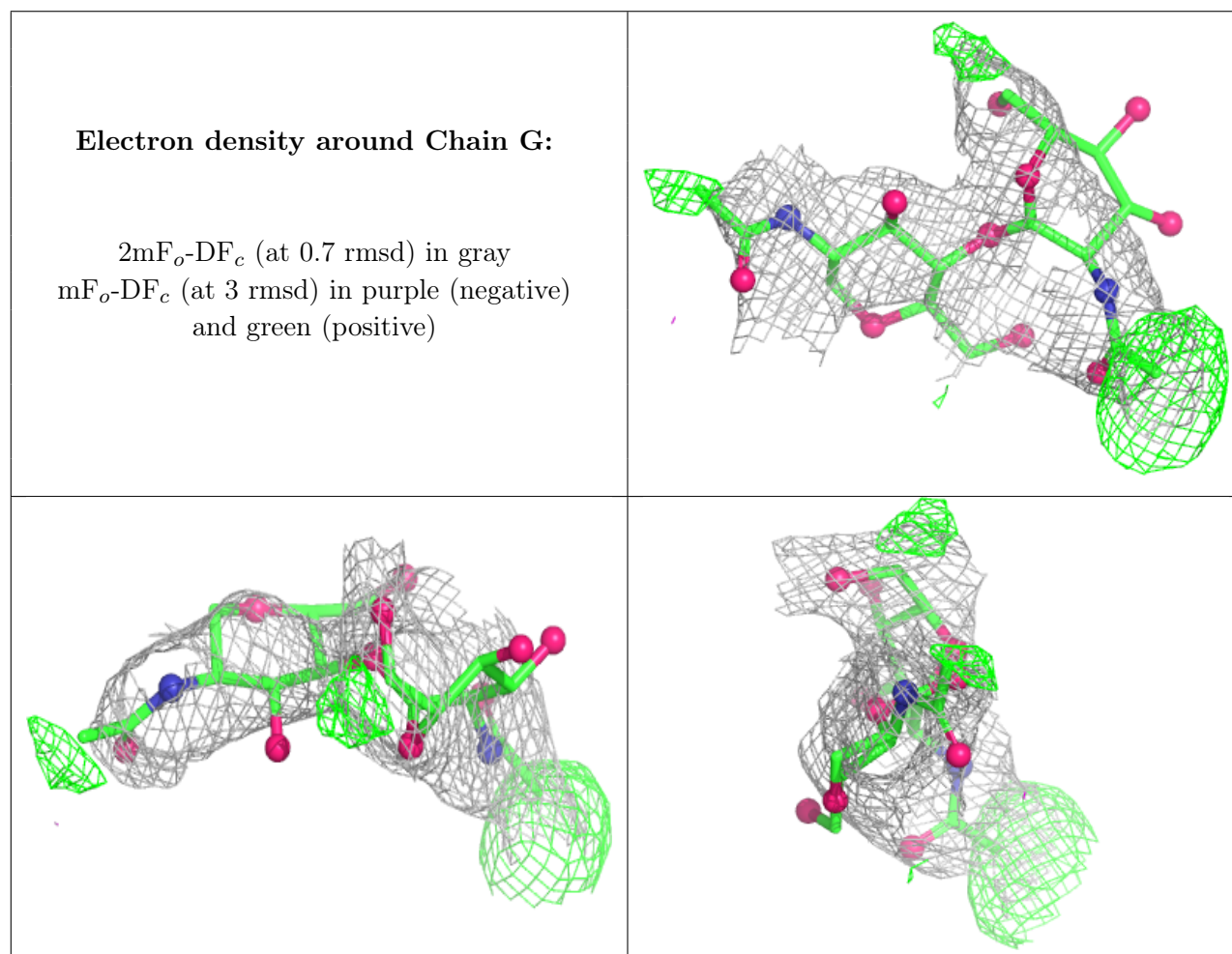
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
3	NAG	G	2	14/15	-0.17	0.18	164,194,201,202	0
3	NAG	G	1	14/15	0.69	0.18	156,189,202,204	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
4	NAG	F	200	14/15	0.17	0.20	161,176,182,183	0
4	NAG	A	201	14/15	0.35	0.21	124,149,157,163	0
4	NAG	D	201	14/15	0.47	0.18	170,178,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	201	14/15	0.60	0.19	138,144,149,150	0
5	GOL	A	204	6/6	0.79	0.19	96,99,100,106	0
5	GOL	C	204	6/6	0.81	0.19	89,94,100,100	0
7	PEG	A	205	7/7	0.81	0.23	76,96,100,102	0
6	ACT	B	204	4/4	0.83	0.22	84,85,89,94	0
7	PEG	B	203	5/7	0.83	0.20	95,97,108,120	0
6	ACT	B	202	4/4	0.84	0.24	110,110,110,112	0
5	GOL	A	202	6/6	0.84	0.15	70,80,86,90	0
6	ACT	F	201	4/4	0.85	0.20	80,85,91,92	0
6	ACT	A	203	4/4	0.88	0.20	76,83,85,89	0
6	ACT	D	202	4/4	0.89	0.19	86,96,99,99	0
5	GOL	B	201	6/6	0.89	0.23	94,103,106,106	0
6	ACT	C	202	4/4	0.90	0.23	95,101,104,104	0
6	ACT	C	203	4/4	0.91	0.13	87,90,91,93	0
5	GOL	E	201	6/6	0.92	0.12	77,81,87,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.