



wwPDB X-ray Structure Validation Summary Report

Aug 15, 2022 – 01:17 pm BST

PDB ID : 7PDY
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 wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

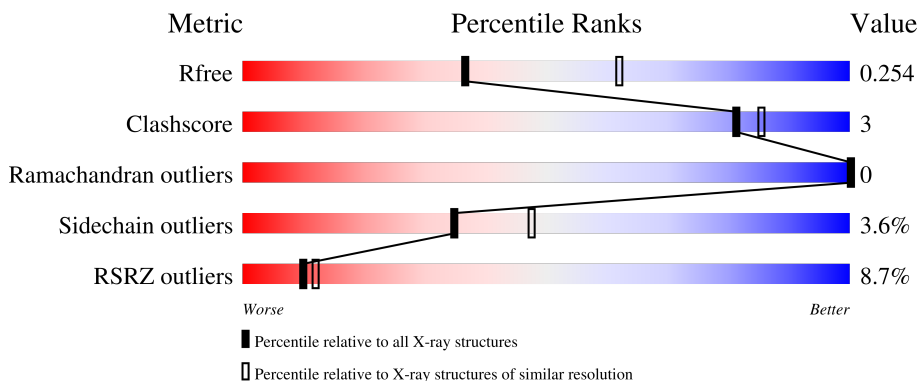
1 Overall quality at a glance

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.



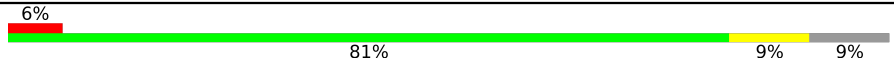
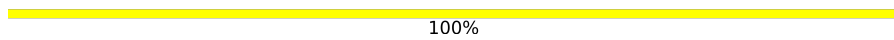
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	 4% 94% ...
1	C	191	 14% 88% 7% ...
1	E	191	 11% 84% 12% .
2	B	225	 5% 80% 10% 9%
2	D	225	 10% 83% 6% . 10%

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Mol	Chain	Length	Quality of chain
2	F	225	 6% 81% 9% 9%
3	G	2	 100%

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	-	-	-
5	GOL	B	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
			Total	C	N	O	S			
1	A	187	1517	978	259	274	6	0	0	0
1	C	184	1452	936	249	261	6	0	0	0
1	E	184	1472	951	249	266	6	0	0	0

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
			Total	C	N	O	S			
2	B	204	1598	1012	274	305	7	0	0	0
2	D	202	1579	1002	267	304	6	0	0	0
2	F	204	1606	1017	277	305	7	0	0	0

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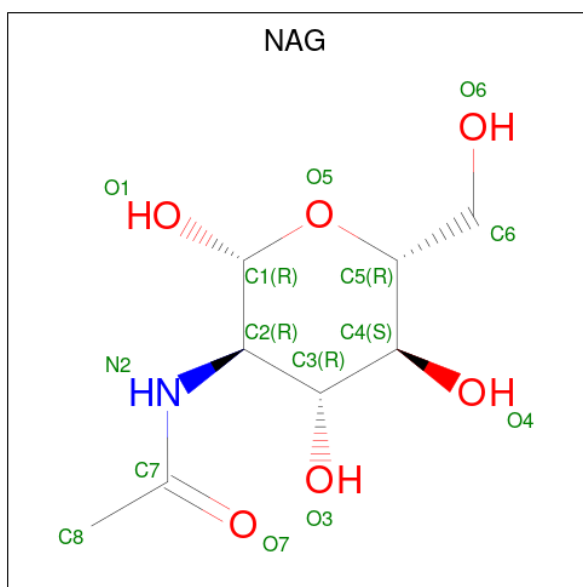
Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	SER	-	linker	UNP P68348
F	-4	GLY	-	linker	UNP P68348
F	-3	GLY	-	linker	UNP P68348
F	-2	GLY	-	linker	UNP P68348
F	-1	GLY	-	linker	UNP P68348
F	0	SER	-	linker	UNP P68348
F	1	GLY	-	linker	UNP P68348
F	2	GLY	-	linker	UNP P68348
F	3	GLY	-	linker	UNP P68348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



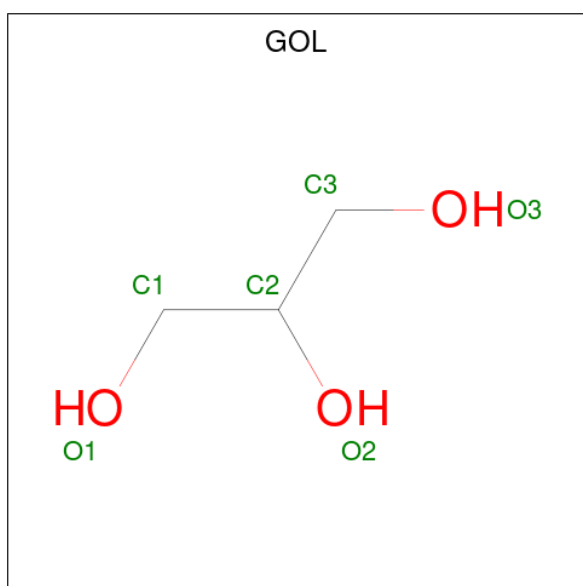
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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 (three-letter code: GOL) (formula: C₃H₈O₃).



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 (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

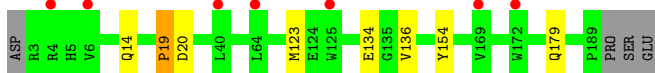
- Molecule 8 is water.

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

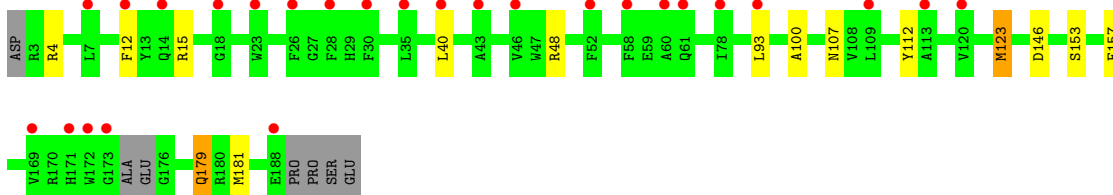
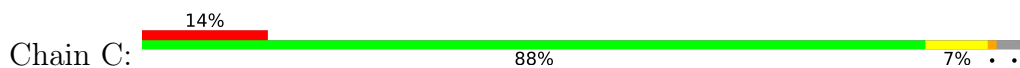
3 Residue-property plots [i](#)

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.

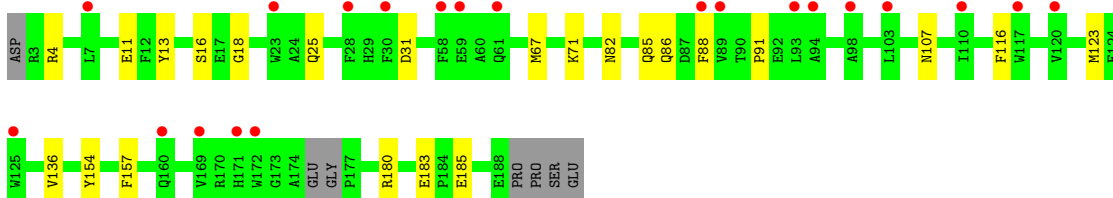
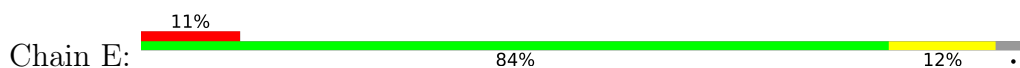
- Molecule 1: MHC class II alpha chain



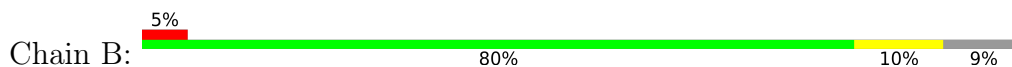
- Molecule 1: MHC class II alpha chain



- Molecule 1: MHC class II alpha chain

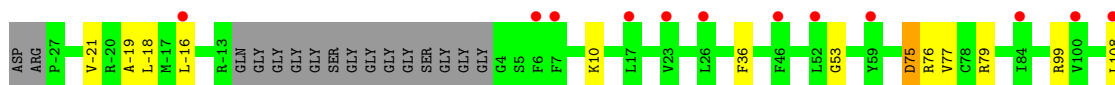
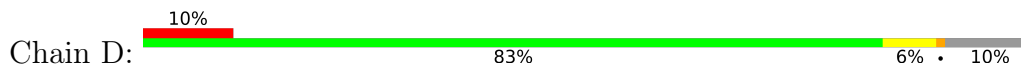


- Molecule 2: 38 kDa phosphoprotein, MHC class II beta chain

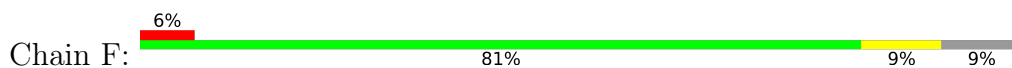




• Molecule 2: 38 kDa phosphoprotein, MHC class II beta chain



• 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 i

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)	Xtrriage
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 (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtrriage
Anisotropy	0.157	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9525	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.64	0/1567	0.87	1/2134 (0.0%)
1	C	0.67	0/1497	0.84	1/2040 (0.0%)
1	E	0.64	0/1518	0.88	1/2066 (0.0%)
2	B	0.70	0/1638	0.80	0/2233
2	D	0.68	0/1619	0.76	0/2210
2	F	0.66	0/1645	0.74	0/2241
All	All	0.67	0/9484	0.81	3/12924 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	LEU	CB-CA-C	-9.39	92.35	110.20
1	A	19	PRO	N-CA-C	-6.36	95.58	112.10
1	E	31	ASP	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1517	0	1423	2	1
1	C	1452	0	1338	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1472	0	1372	11	1
2	B	1598	0	1483	10	1
2	D	1579	0	1457	10	0
2	F	1606	0	1499	14	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	47	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.

The worst 5 of 47 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:MET:HG3	1:C:153:SER:HB2	1.88	0.56
2:D:112:ASP:OD2	1:E:183:GLU:CD	2.45	0.54
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

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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 [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	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 [i](#)

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%)	152 (97%)	4 (3%)	46	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	144/162 (89%)	137 (95%)	7 (5%)	25	34
1	E	149/162 (92%)	142 (95%)	7 (5%)	26	35
2	B	168/188 (89%)	162 (96%)	6 (4%)	35	47
2	D	166/188 (88%)	161 (97%)	5 (3%)	41	55
2	F	169/188 (90%)	164 (97%)	5 (3%)	41	55
All	All	952/1050 (91%)	918 (96%)	34 (4%)	35	47

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	185	GLU
2	F	-14	GLU
2	F	104	GLN
1	C	15	ARG
1	C	12	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	34	GLN
2	F	-23	HIS
2	D	80	HIS
2	D	18	ASN
2	D	91	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.45	0	17,19,21	1.15	1 (5%)
3	NAG	G	2	3	14,14,15	0.69	0	17,19,21	2.52	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-O5-C5	-5.98	104.09	112.19
3	G	2	NAG	O5-C1-C2	5.86	120.55	111.29
3	G	2	NAG	C1-C2-N2	5.76	120.33	110.49
3	G	1	NAG	O5-C1-C2	-3.35	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

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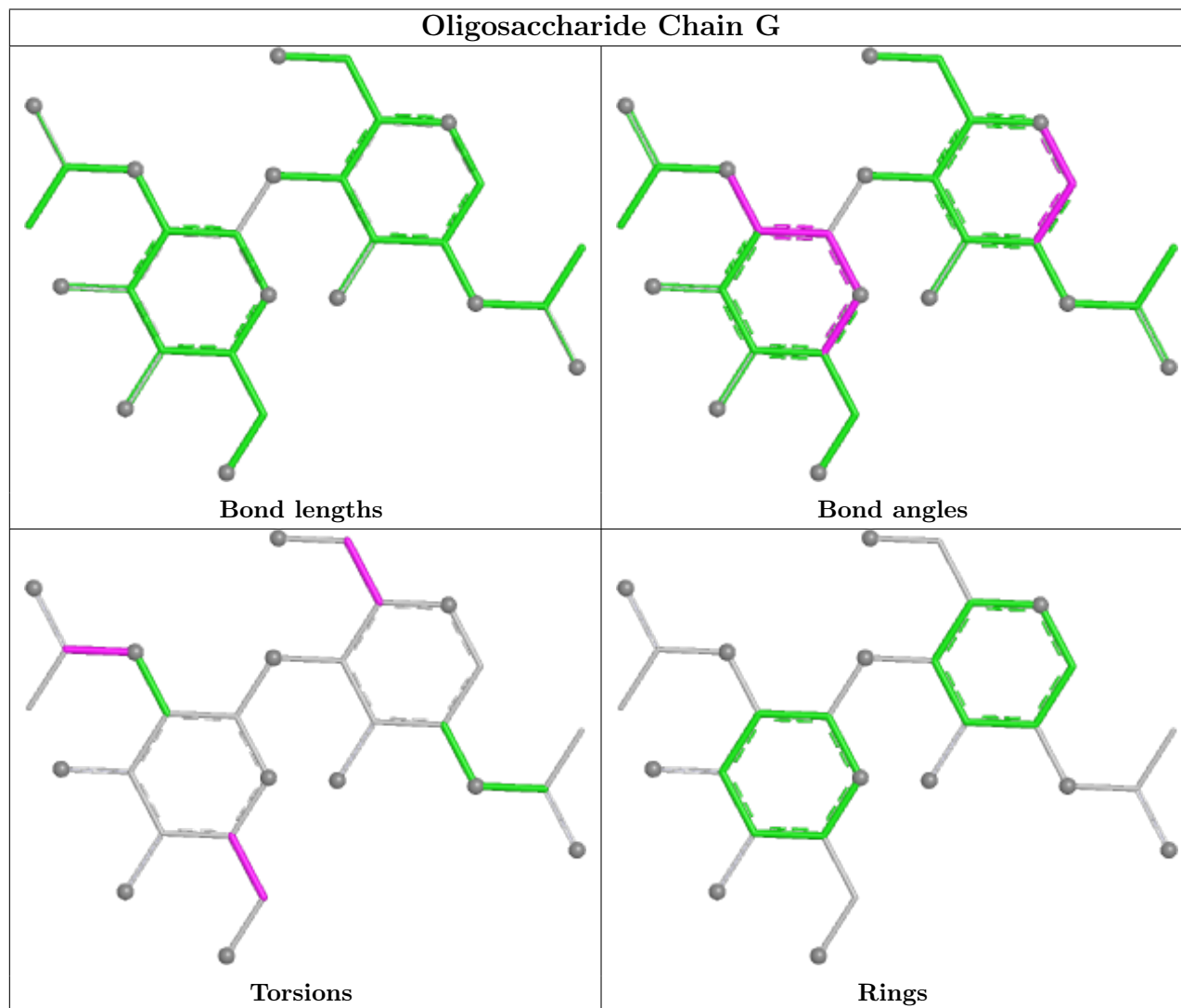
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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C8-C7-N2-C2

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 [i](#)

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
5	GOL	A	202	-	5,5,5	0.21	0	5,5,5	0.28	0
7	PEG	B	203	-	4,4,6	0.38	0	3,3,5	0.23	0
6	ACT	B	204	-	3,3,3	1.11	0	3,3,3	0.73	0
5	GOL	E	201	-	5,5,5	0.20	0	5,5,5	0.57	0
6	ACT	A	203	-	3,3,3	1.24	0	3,3,3	0.80	0
6	ACT	F	201	-	3,3,3	1.18	0	3,3,3	0.89	0
5	GOL	C	204	-	5,5,5	0.20	0	5,5,5	0.41	0
6	ACT	B	202	-	3,3,3	1.05	0	3,3,3	0.70	0
7	PEG	A	205	-	6,6,6	0.45	0	5,5,5	0.15	0
6	ACT	D	202	-	3,3,3	1.10	0	3,3,3	0.72	0
4	NAG	F	200	2	14,14,15	0.57	0	17,19,21	1.28	2 (11%)
4	NAG	A	201	1	14,14,15	1.00	1 (7%)	17,19,21	1.35	2 (11%)
5	GOL	A	204	-	5,5,5	0.22	0	5,5,5	0.44	0
5	GOL	B	201	-	5,5,5	0.24	0	5,5,5	0.54	0
4	NAG	C	201	1	14,14,15	1.13	1 (7%)	17,19,21	1.49	3 (17%)
6	ACT	C	203	-	3,3,3	0.99	0	3,3,3	0.92	0
4	NAG	D	201	-	14,14,15	0.76	1 (7%)	17,19,21	1.69	2 (11%)
6	ACT	C	202	-	3,3,3	1.10	0	3,3,3	0.95	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	GOL	A	202	-	-	0/4/4/4	-
7	PEG	B	203	-	-	1/2/2/4	-
5	GOL	E	201	-	-	2/4/4/4	-
5	GOL	C	204	-	-	3/4/4/4	-
7	PEG	A	205	-	-	1/4/4/4	-
4	NAG	F	200	2	-	4/6/23/26	0/1/1/1
4	NAG	A	201	1	1/1/5/7	4/6/23/26	0/1/1/1
5	GOL	A	204	-	-	2/4/4/4	-
5	GOL	B	201	-	-	4/4/4/4	-
4	NAG	C	201	1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	201	-	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	NAG	O7-C7	2.63	1.29	1.23
4	A	201	NAG	C2-N2	2.14	1.50	1.46
4	D	201	NAG	O7-C7	2.09	1.28	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	NAG	C2-N2-C7	-5.83	114.60	122.90
4	A	201	NAG	O5-C1-C2	3.84	117.36	111.29
4	C	201	NAG	C2-N2-C7	-3.47	117.97	122.90
4	C	201	NAG	O5-C1-C2	3.22	116.38	111.29
4	F	200	NAG	O5-C1-C2	3.02	116.05	111.29

All (2) chirality outliers are listed below:

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

5 of 27 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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	203	PEG	0	1
5	C	204	GOL	1	0
6	C	203	ACT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.80	7 (3%) 41 48	50, 64, 98, 125	0
1	C	184/191 (96%)	1.06	26 (14%) 2 3	56, 78, 122, 159	0
1	E	184/191 (96%)	0.96	21 (11%) 5 6	51, 73, 104, 140	0
2	B	204/225 (90%)	0.77	11 (5%) 25 30	50, 83, 119, 139	0
2	D	202/225 (89%)	0.92	22 (10%) 5 7	59, 94, 127, 158	0
2	F	204/225 (90%)	0.84	14 (6%) 16 20	57, 91, 123, 156	0
All	All	1165/1248 (93%)	0.89	101 (8%) 10 12	50, 81, 121, 159	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	117	TYR	5.5
2	D	-16	LEU	5.4
1	C	40	LEU	4.3
2	F	36	PHE	4.0
1	E	172	TRP	3.8

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

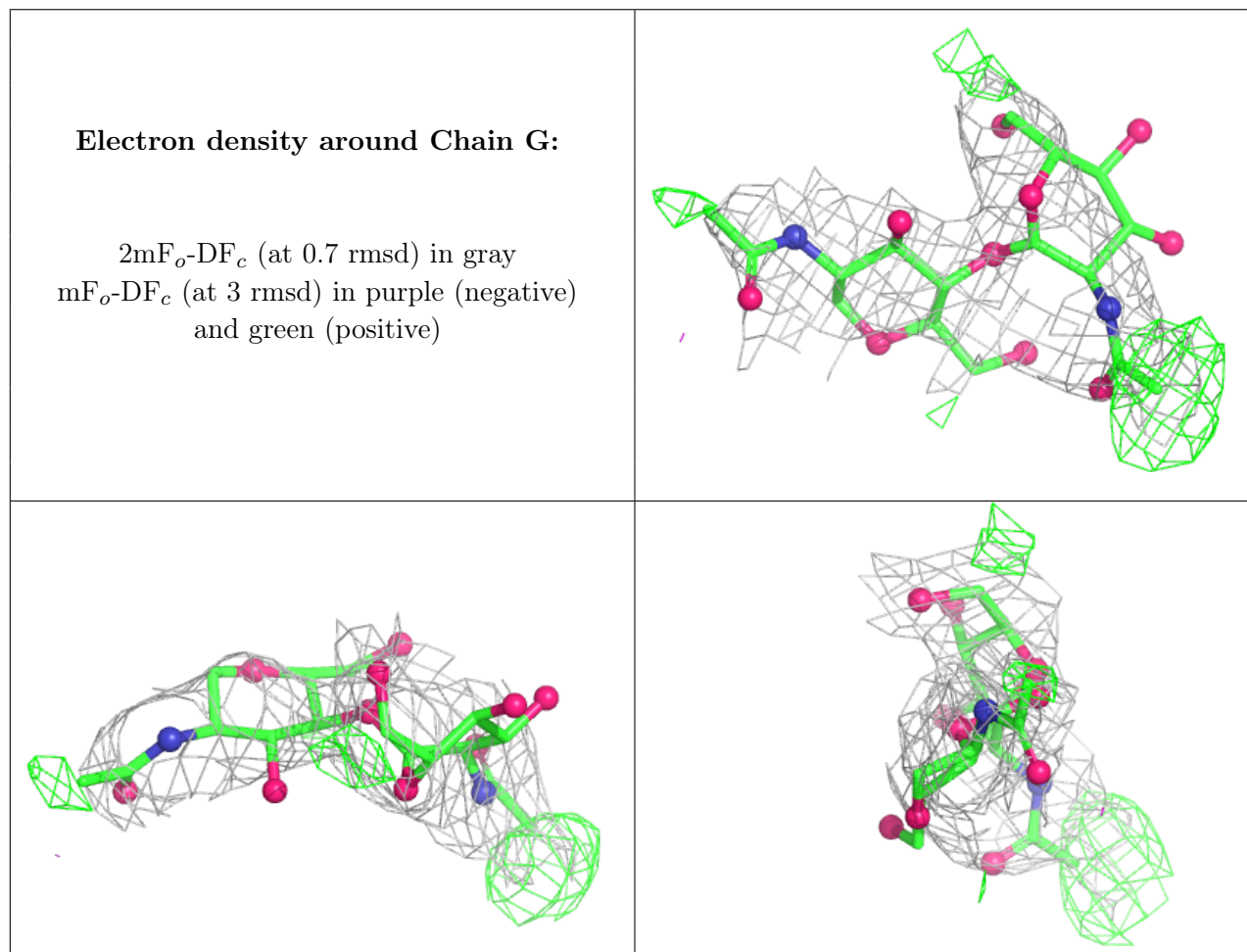
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	G	2	14/15	0.63	0.21	164,194,201,202	0
3	NAG	G	1	14/15	0.74	0.26	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(\AA^2)	Q<0.9
4	NAG	F	200	14/15	0.27	0.28	161,176,182,183	0
4	NAG	A	201	14/15	0.47	0.21	124,149,157,163	0
4	NAG	D	201	14/15	0.52	0.23	170,178,180,180	0
4	NAG	C	201	14/15	0.61	0.21	138,144,149,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	204	6/6	0.64	0.30	96,99,100,106	0
5	GOL	C	204	6/6	0.73	0.27	89,94,100,100	0
7	PEG	A	205	7/7	0.73	0.24	76,96,100,102	0
5	GOL	B	201	6/6	0.75	0.47	94,103,106,106	0
6	ACT	C	203	4/4	0.76	0.20	87,90,91,93	0
6	ACT	B	202	4/4	0.81	0.26	110,110,110,112	0
6	ACT	D	202	4/4	0.84	0.26	86,96,99,99	0
6	ACT	C	202	4/4	0.84	0.42	95,101,104,104	0
6	ACT	A	203	4/4	0.86	0.22	76,83,85,89	0
5	GOL	E	201	6/6	0.86	0.23	77,81,87,91	0
7	PEG	B	203	5/7	0.86	0.13	95,97,108,120	0
6	ACT	F	201	4/4	0.88	0.15	80,85,91,92	0
6	ACT	B	204	4/4	0.89	0.20	84,85,89,94	0
5	GOL	A	202	6/6	0.93	0.18	70,80,86,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.