



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 9BF9 / pdb_00009bf9
Title : Human LAG-3-HLA-DR1 complex
Authors : Petersen, J.; Rossjohn, J.
Deposited on : 2024-04-17
Resolution : 3.40 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

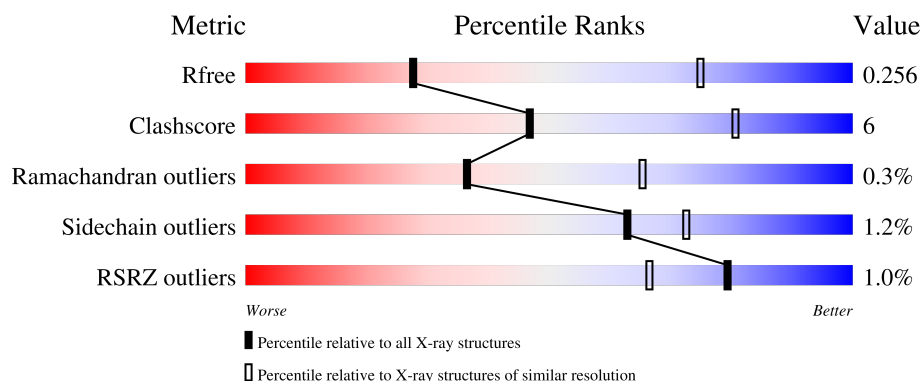
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

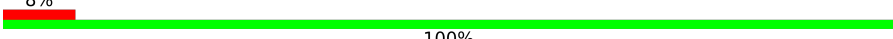
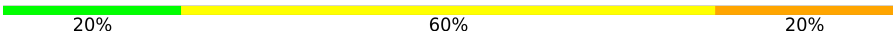
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	189	
2	B	211	
3	G	13	
4	D	418	
5	C	5	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4865 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	182	Total	C	N	O	S	0	0	0
			1480	957	238	280	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ILE	-	expression tag	UNP P01903
A	2	LYS	-	expression tag	UNP P01903
A	3	GLU	-	expression tag	UNP P01903
A	4	GLU	-	expression tag	UNP P01903
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	ASP	-	expression tag	UNP P01903
A	186	ASP	-	expression tag	UNP P01903
A	187	ASP	-	expression tag	UNP P01903
A	188	ASP	-	expression tag	UNP P01903
A	189	LYS	-	expression tag	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	0	0
			1540	968	273	293	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	ASP	-	expression tag	UNP D7RIG0
B	-11	SER	-	expression tag	UNP D7RIG0
B	-10	GLY	-	expression tag	UNP D7RIG0
B	-9	GLY	-	expression tag	UNP D7RIG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP D7RIG0
B	-7	GLY	-	expression tag	UNP D7RIG0
B	-6	SER	-	expression tag	UNP D7RIG0
B	-5	ILE	-	expression tag	UNP D7RIG0
B	-4	GLU	-	expression tag	UNP D7RIG0
B	-3	GLY	-	expression tag	UNP D7RIG0
B	-2	ARG	-	expression tag	UNP D7RIG0
B	-1	GLY	-	expression tag	UNP D7RIG0
B	0	SER	ALA	conflict	UNP D7RIG0
B	191	THR	ARG	conflict	UNP D7RIG0
B	192	GLY	SER	conflict	UNP D7RIG0
B	193	GLY	GLU	conflict	UNP D7RIG0
B	194	ASP	SER	conflict	UNP D7RIG0
B	195	ASP	ALA	conflict	UNP D7RIG0
B	196	ASP	GLN	conflict	UNP D7RIG0
B	197	ASP	SER	conflict	UNP D7RIG0

- Molecule 3 is a protein called Membrane protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	13	Total	C	N	O	0	0	0
			98	62	18	18			

- Molecule 4 is a protein called Lymphocyte activation gene 3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	210	Total	C	N	O	S	0	0	0
			1650	1033	324	286	7			

There are 11 discrepancies between the modelled and reference sequences:

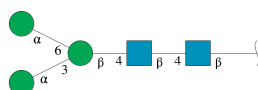
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P18627
D	0	SER	-	expression tag	UNP P18627
D	408	THR	-	expression tag	UNP P18627
D	409	GLY	-	expression tag	UNP P18627
D	410	GLY	-	expression tag	UNP P18627
D	411	LEU	-	expression tag	UNP P18627
D	412	GLU	-	expression tag	UNP P18627
D	413	VAL	-	expression tag	UNP P18627
D	414	LEU	-	expression tag	UNP P18627
D	415	PHE	-	expression tag	UNP P18627

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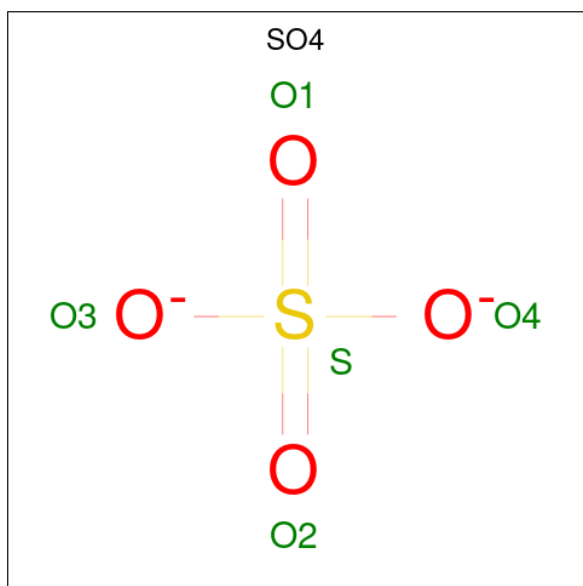
Chain	Residue	Modelled	Actual	Comment	Reference
D	416	GLN	-	expression tag	UNP P18627

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			7	4	3		

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

Chain A: 



- Molecule 2: HLA class II histocompatibility antigen DR beta chain

Chain B: 



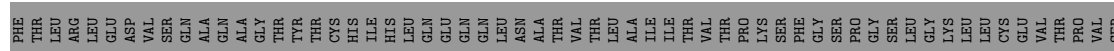
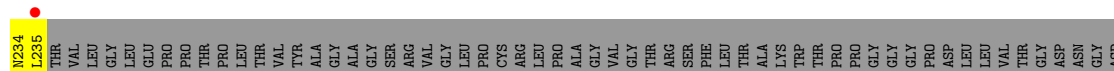
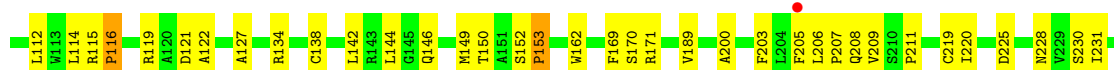
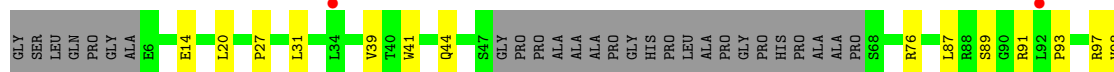
- Molecule 3: Membrane protein

Chain G: 



- Molecule 4: Lymphocyte activation gene 3 protein

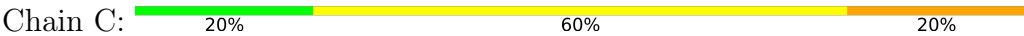
Chain D: 



GLY
GLN
GLU
ARG
PHE
VAL
TRP
SER
SER
LEU
ASP
THR
PRO
SER
GLN
ARG
SER
PHE
SER
SER
GLY
PRO
TRP
LEU
GLU
ALA
GLN
GLU
ALA
GLN
LEU
LEU
SER
GLN
PRO
TRP
GLN
CYS
GLN
LEU
TYR
GLN
GLY
GLU
ARG
LEU
LEU
GLY
ALA
ALA
VAL
TYR
PHE
THR
GLU
THR
THR
GLY
GLY
LEU
GLU
VAL

LEU
PHE
GLN

- Molecule 5: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



MAN1
MAN2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.71Å 148.07Å 85.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.56 – 3.40 81.56 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.56-3.40) 99.6 (81.56-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.253 0.209 , 0.256	Depositor DCC
R_{free} test set	1818 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	134.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 150.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4865	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: SO4, PEG, NAG, MAN, BMA

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	0.07	0/1525	0.24	0/2082
2	B	0.07	0/1579	0.23	0/2148
3	G	0.04	0/99	0.21	0/131
4	D	0.11	0/1697	0.28	0/2309
All	All	0.08	0/4900	0.25	0/6670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1480	0	1400	14	0
2	B	1540	0	1451	11	0
3	G	98	0	100	0	0
4	D	1650	0	1618	32	0
5	C	61	0	52	1	0
6	A	5	0	0	0	0
6	D	10	0	0	0	0
7	D	14	0	13	1	0
8	D	7	0	10	0	0
All	All	4865	0	4644	54	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 6.

All (54) 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)
4:D:209:VAL:HG13	4:D:211:PRO:HD3	1.61	0.82
1:A:160:VAL:HB	1:A:177:HIS:HE1	1.52	0.73
4:D:97:ARG:NH1	4:D:121:ASP:OD2	2.31	0.63
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.82	0.61
1:A:95:SER:OG	1:A:103:ASN:ND2	2.34	0.59
4:D:122:ALA:HB2	4:D:144:LEU:HD12	1.83	0.59
4:D:127:ALA:HB3	4:D:138:CYS:SG	2.44	0.58
4:D:27:PRO:HG2	4:D:134:ARG:HH21	1.69	0.57
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.87	0.57
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.87	0.56
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.85	0.56
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.88	0.56
1:A:162:ASP:OD1	1:A:177:HIS:ND1	2.40	0.55
1:A:160:VAL:HB	1:A:177:HIS:CE1	2.38	0.55
4:D:162:TRP:HA	4:D:207:PRO:HA	1.89	0.55
4:D:200:ALA:HB3	4:D:203:PHE:HB2	1.90	0.54
4:D:119:ARG:HA	4:D:144:LEU:HD13	1.92	0.52
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.90	0.52
4:D:150:THR:OG1	5:C:1:NAG:O7	2.24	0.52
4:D:208:GLN:HG3	4:D:209:VAL:H	1.74	0.51
1:A:162:ASP:HB3	1:A:175:LEU:HD12	1.93	0.51
4:D:152:SER:OG	4:D:153:PRO:HD3	2.11	0.50
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.47	0.50
2:B:4:ARG:O	2:B:6:ARG:NH1	2.43	0.49
4:D:171:ARG:HH22	4:D:225:ASP:CG	2.20	0.48
4:D:169:PHE:HD2	4:D:171:ARG:HB2	1.78	0.48
4:D:41:TRP:CD2	4:D:127:ALA:HB2	2.49	0.48
4:D:91:ARG:HG3	4:D:93:PRO:HD2	1.96	0.47
4:D:228:ASN:OD1	7:D:501:NAG:N2	2.46	0.47
4:D:44:GLN:HB2	4:D:76:ARG:HG2	1.96	0.47
4:D:98:VAL:HG12	4:D:114:LEU:HD22	1.96	0.47
4:D:115:ARG:HB3	4:D:116:PRO:HD2	1.98	0.46
1:A:8:ILE:HB	1:A:25:ASP:HB3	1.99	0.45
4:D:20:LEU:HD21	4:D:142:LEU:HD12	1.99	0.44
1:A:70:LEU:HD13	2:B:9:TRP:HB2	1.99	0.44
1:A:76:ARG:HH12	2:B:57:ASP:CG	2.25	0.44
4:D:20:LEU:HD12	4:D:112:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:ALA:HB2	4:D:205:PHE:HE2	1.83	0.43
4:D:149:MET:HE3	4:D:231:ILE:HG23	2.01	0.43
4:D:14:GLU:OE2	4:D:119:ARG:HB2	2.19	0.43
4:D:146:GLN:H	4:D:170:SER:HB3	1.84	0.43
2:B:145:THR:HG22	4:D:89:SER:HB3	2.01	0.42
4:D:97:ARG:HB2	4:D:115:ARG:O	2.18	0.42
4:D:220:ILE:HG12	4:D:230:SER:HB3	2.01	0.42
1:A:132:VAL:HG12	1:A:151:LEU:HD13	2.01	0.42
1:A:164:ARG:NH1	1:A:166:GLU:OE2	2.52	0.42
4:D:41:TRP:CE2	4:D:112:LEU:HB2	2.54	0.42
2:B:106:THR:HG21	2:B:114:LEU:HD21	2.02	0.42
2:B:105:LYS:C	2:B:107:GLN:H	2.28	0.42
4:D:87:LEU:HD23	4:D:87:LEU:HA	1.90	0.41
4:D:31:LEU:HD12	4:D:31:LEU:HA	1.93	0.41
1:A:94:ASN:HB3	1:A:106:ILE:HD11	2.04	0.40
2:B:8:LEU:HB3	2:B:33:ASN:HA	2.03	0.40
4:D:234:ASN:HB3	4:D:235:LEU:H	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/189 (95%)	175 (97%)	5 (3%)	0	100	100
2	B	189/211 (90%)	183 (97%)	6 (3%)	0	100	100
3	G	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
4	D	206/418 (49%)	189 (92%)	15 (7%)	2 (1%)	12	40
All	All	586/831 (70%)	556 (95%)	28 (5%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	116	PRO
4	D	153	PRO

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	164/173 (95%)	163 (99%)	1 (1%)	78	80
2	B	167/185 (90%)	166 (99%)	1 (1%)	78	80
3	G	9/9 (100%)	9 (100%)	0	100	100
4	D	175/341 (51%)	171 (98%)	4 (2%)	44	63
All	All	515/708 (73%)	509 (99%)	6 (1%)	63	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
2	B	98	LYS
4	D	39	VAL
4	D	189	VAL
4	D	206	LEU
4	D	219	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	29	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 ⓘ

5 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$
5	NAG	C	1	5,4	14,14,15	0.66	1 (7%)	17,19,21	0.76	0
5	NAG	C	2	5	14,14,15	0.53	0	17,19,21	0.52	0
5	BMA	C	3	5	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
5	MAN	C	4	5	11,11,12	0.73	0	15,15,17	1.27	2 (13%)
5	MAN	C	5	5	11,11,12	0.77	0	15,15,17	1.15	2 (13%)

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	NAG	C	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1
5	MAN	C	5	5	-	0/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	NAG	C1-C2	2.01	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4	MAN	C1-O5-C5	3.93	117.46	112.19
5	C	3	BMA	C1-O5-C5	3.65	117.08	112.19
5	C	5	MAN	C1-O5-C5	3.47	116.83	112.19
5	C	4	MAN	O2-C2-C3	-2.16	105.68	110.15
5	C	5	MAN	O2-C2-C3	-2.12	105.77	110.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6

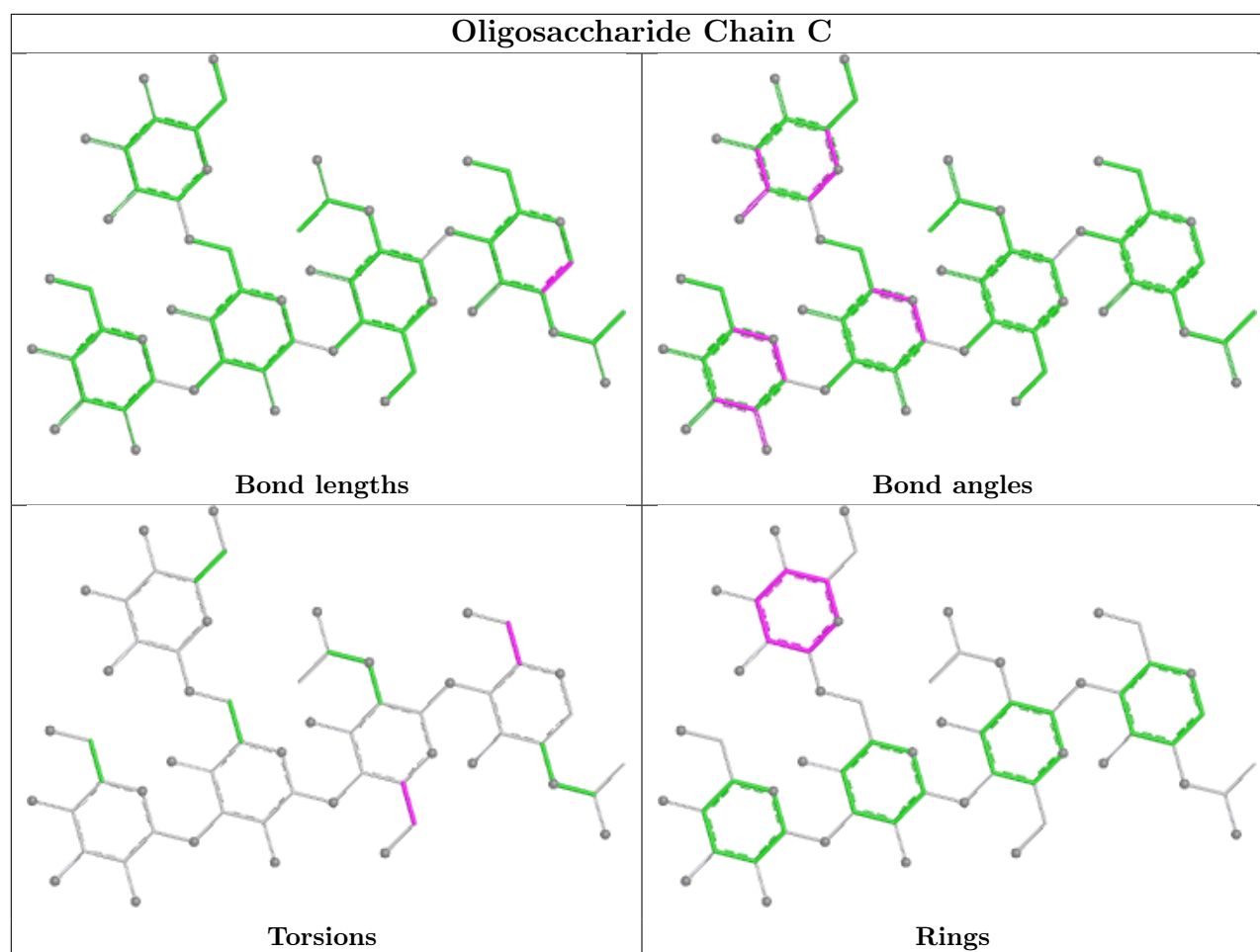
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	5	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	1	0

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](#)

5 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	$\# Z > 2$
6	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.08	0
7	NAG	D	501	4	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
8	PEG	D	502	-	6,6,6	0.11	0	5,5,5	0.10	0
6	SO4	A	201	-	4,4,4	0.23	0	6,6,6	0.07	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
8	PEG	D	502	-	-	1/4/4/4	-
7	NAG	D	501	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	502	PEG	O1-C1-C2-O2
7	D	501	NAG	C3-C2-N2-C7
7	D	501	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	501	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 [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	182/189 (96%)	-0.18	0 100 100	108, 151, 200, 250	0
2	B	191/211 (90%)	-0.21	1 (0%) 87 78	88, 138, 202, 232	0
3	G	13/13 (100%)	-0.03	1 (7%) 19 16	125, 156, 181, 184	0
4	D	210/418 (50%)	-0.02	4 (1%) 66 51	82, 132, 225, 272	0
All	All	596/831 (71%)	-0.13	6 (1%) 79 66	82, 141, 207, 272	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	152	ASP	5.5
4	D	34	LEU	3.4
4	D	92	LEU	3.0
4	D	205	PHE	3.0
3	G	13	GLY	2.5
4	D	235	LEU	2.3

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

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

6.3 Carbohydrates [i](#)

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

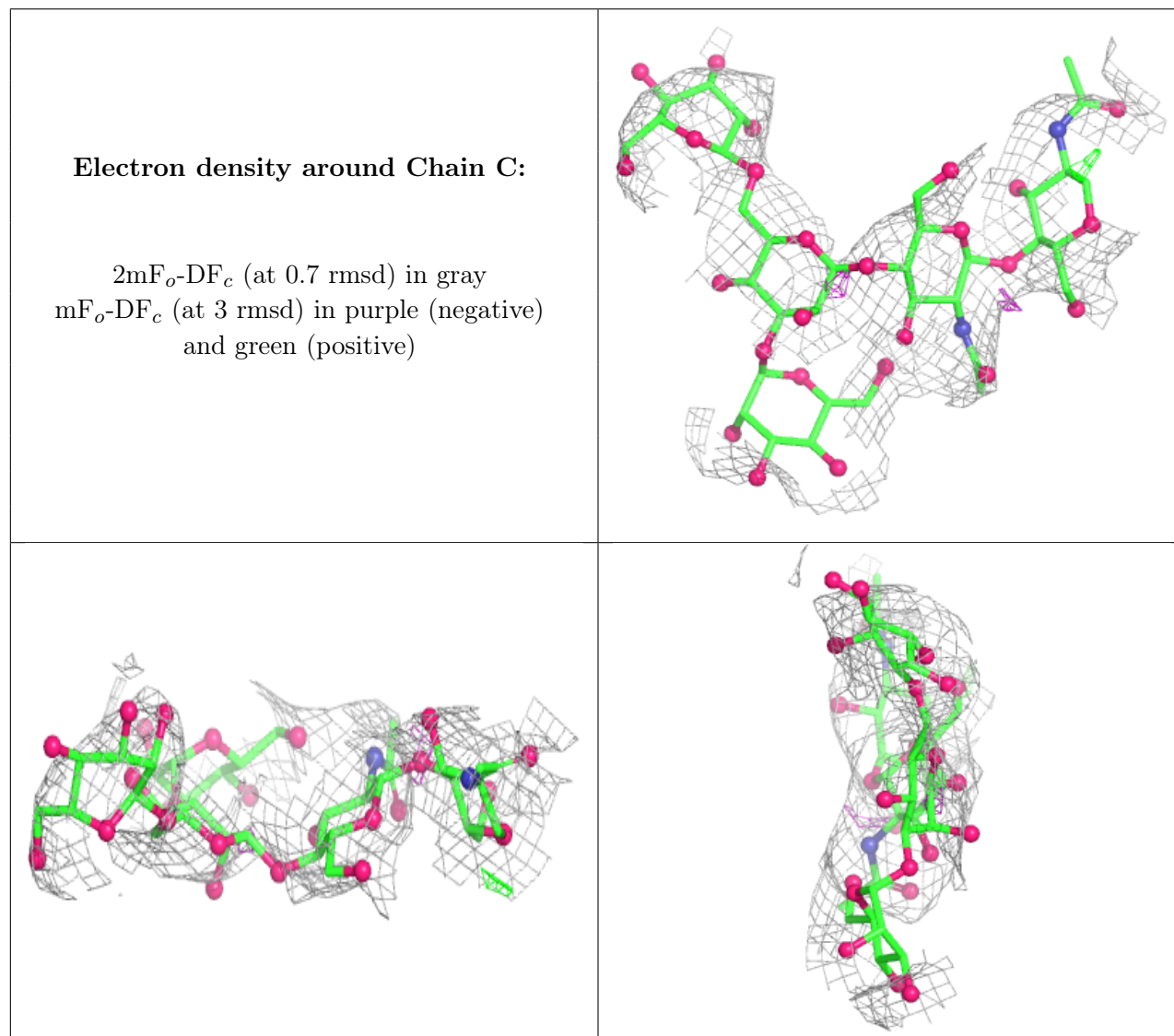
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	135,178,195,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	2	14/15	-	-	167,193,216,239	0
5	BMA	C	3	11/12	-	-	216,238,248,250	0
5	MAN	C	4	11/12	-	-	200,229,234,236	0
5	MAN	C	5	11/12	-	-	204,234,238,243	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	SO4	D	503	5/5	0.59	0.11	146,172,197,205	0
6	SO4	A	201	5/5	0.62	0.07	182,194,218,243	0
6	SO4	D	504	5/5	0.63	0.08	155,170,218,232	0
7	NAG	D	501	14/15	0.74	0.07	137,190,208,214	0
8	PEG	D	502	7/7	0.86	0.15	114,139,163,173	0

6.5 Other polymers [i](#)

There are no such residues in this entry.