W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 25, 2024 – 07:33 PM EST

PDB ID	:	6U3O
Title	:	JR51 DQ2-p.aeru-alpha2a complex
Authors	:	Petersen, J.; Rossjohn, J.
Deposited on	:	2019-08-22
Resolution	:	2.74 Å(reported)

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

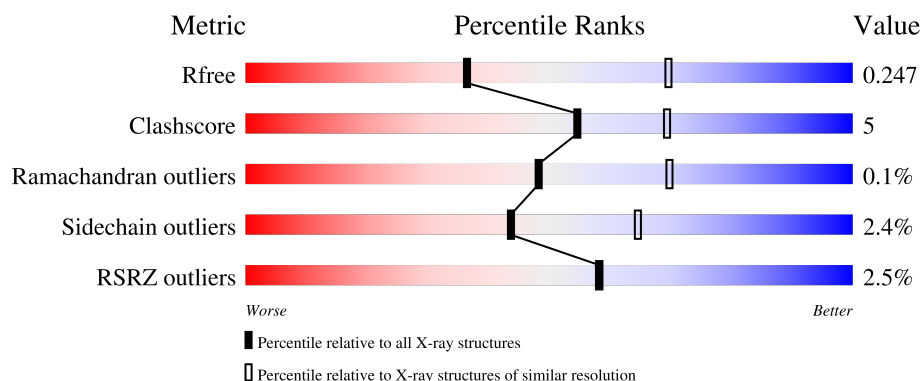|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.74 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		2.4%
RSRZ outliers		2.5%

Worse — *Better*

▮ Percentile relative to all X-ray structures
⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	202	4% · 81% · 14% · ·
1	G	202	5% · 81% · 15% ·
2	B	244	2% · 89% · 10% ··
2	H	244	2% · 90% · 9% ·
3	C	191	2% · 85% · 10% · 5%
3	E	191	% · 82% · 12% · 5%

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Mol	Chain	Length	Quality of chain
4	D	206	2% 73% 14% • 12%
4	F	206	% 69% 18% • 12%
5	I	20	5% 45% 20% 35%
5	J	20	55% 10% 35%
6	K	2	100%
6	L	2	100%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 12888 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 T-CELL RECEPTOR, JR5.1 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	194	Total	C	N	O	S	0	0	0
			1480	924	254	292	10			
1	A	194	Total	C	N	O	S	0	0	0
			1490	931	254	295	10			

- Molecule 2 is a protein called T-CELL RECEPTOR, JR5.1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	242	Total	C	N	O	S	0	0	0
			1877	1182	328	362	5			
2	B	242	Total	C	N	O	S	0	0	0
			1877	1182	328	362	5			

- Molecule 3 is a protein called MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	181	Total	C	N	O	S	0	0	0
			1445	931	236	276	2			
3	E	181	Total	C	N	O	S	0	0	0
			1445	931	236	276	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	44	SER	CYS	conflict	UNP O19705
C	182	THR	-	expression tag	UNP O19705
C	183	SER	-	expression tag	UNP O19705
C	184	GLY	-	expression tag	UNP O19705
C	185	ASP	-	expression tag	UNP O19705
C	186	ASP	-	expression tag	UNP O19705
C	187	ASP	-	expression tag	UNP O19705
C	188	ASP	-	expression tag	UNP O19705

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Chain	Residue	Modelled	Actual	Comment	Reference
C	189	LYS	-	expression tag	UNP O19705
E	44	SER	CYS	conflict	UNP O19705
E	182	THR	-	expression tag	UNP O19705
E	183	SER	-	expression tag	UNP O19705
E	184	GLY	-	expression tag	UNP O19705
E	185	ASP	-	expression tag	UNP O19705
E	186	ASP	-	expression tag	UNP O19705
E	187	ASP	-	expression tag	UNP O19705
E	188	ASP	-	expression tag	UNP O19705
E	189	LYS	-	expression tag	UNP O19705

- Molecule 4 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	181	Total 1480	C 935	N 264	O 274	S 7	0	0	0
4	F	181	Total 1480	C 935	N 264	O 274	S 7	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP O19712
D	-4	GLY	-	expression tag	UNP O19712
D	-3	SER	-	expression tag	UNP O19712
D	-2	GLY	-	expression tag	UNP O19712
D	-1	ALA	-	expression tag	UNP O19712
D	0	SER	-	expression tag	UNP O19712
D	193	THR	-	expression tag	UNP O19712
D	194	GLY	-	expression tag	UNP O19712
D	195	GLY	-	expression tag	UNP O19712
D	196	ASP	-	expression tag	UNP O19712
D	197	ASP	-	expression tag	UNP O19712
D	198	ASP	-	expression tag	UNP O19712
D	199	ASP	-	expression tag	UNP O19712
D	200	LYS	-	expression tag	UNP O19712
F	-5	GLY	-	expression tag	UNP O19712
F	-4	GLY	-	expression tag	UNP O19712
F	-3	SER	-	expression tag	UNP O19712
F	-2	GLY	-	expression tag	UNP O19712
F	-1	ALA	-	expression tag	UNP O19712
F	0	SER	-	expression tag	UNP O19712

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Chain	Residue	Modelled	Actual	Comment	Reference
F	193	THR	-	expression tag	UNP O19712
F	194	GLY	-	expression tag	UNP O19712
F	195	GLY	-	expression tag	UNP O19712
F	196	ASP	-	expression tag	UNP O19712
F	197	ASP	-	expression tag	UNP O19712
F	198	ASP	-	expression tag	UNP O19712
F	199	ASP	-	expression tag	UNP O19712
F	200	LYS	-	expression tag	UNP O19712

- Molecule 5 is a protein called Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	13	Total	C	N	O	0	0	0
			96	61	14	21			
5	J	13	Total	C	N	O	0	0	0
			96	61	14	21			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
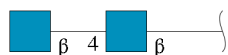
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	9	Total	O	0	0
			9	9		
7	H	6	Total	O	0	0
			6	6		
7	A	12	Total	O	0	0
			12	12		
7	B	2	Total	O	0	0
			2	2		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	10	Total 10	O 10	0	0
7	D	9	Total 9	O 9	0	0
7	E	11	Total 11	O 11	0	0
7	F	6	Total 6	O 6	0	0
7	I	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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. 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. 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.
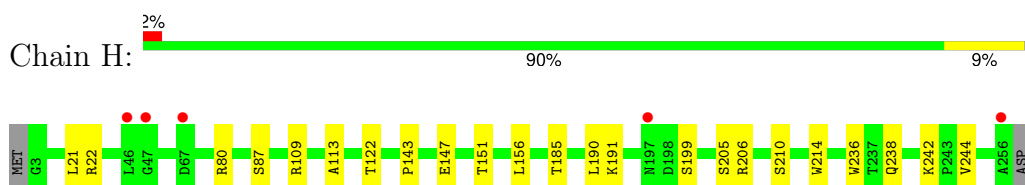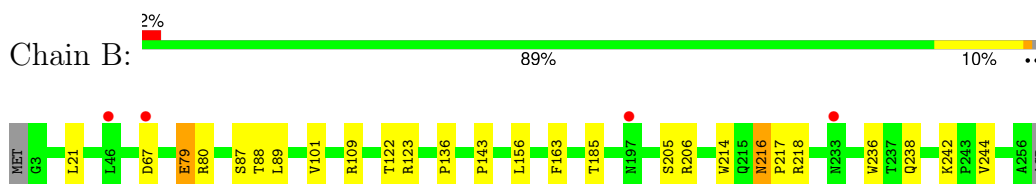
• Molecule 1: T-CELL RECEPTOR, JR5.1 alpha
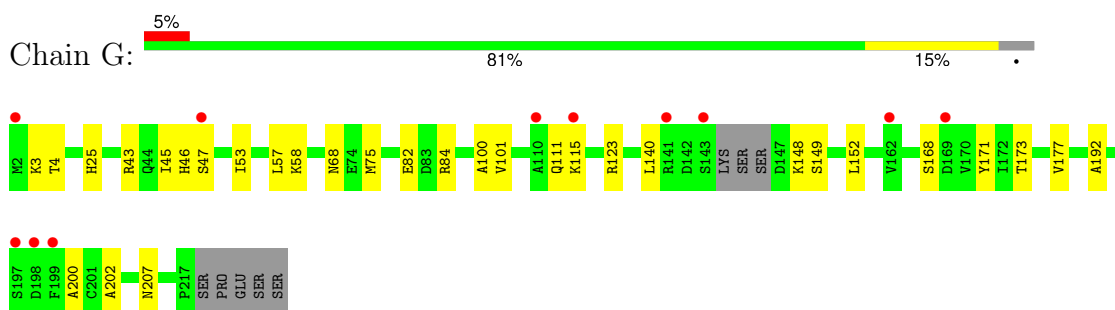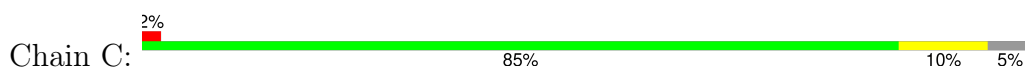

• Molecule 1: T-CELL RECEPTOR, JR5.1 alpha
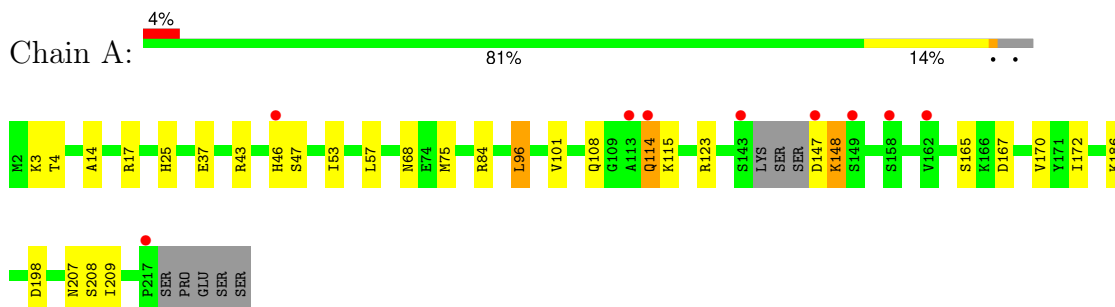
• Molecule 2: T-CELL RECEPTOR, JR5.1 beta
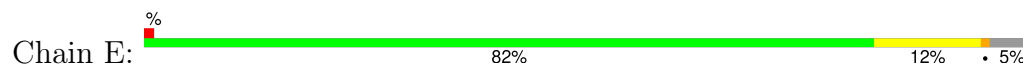

• Molecule 2: T-CELL RECEPTOR, JR5.1 beta

• Molecule 3: MHC class II HLA-DQ-alpha chain

• Molecule 3: MHC class II HLA-DQ-alpha chain

Chain E:

• Molecule 4: MHC class II HLA-DQ-beta-1

Chain D:

• Molecule 4: MHC class II HLA-DQ-beta-1

Chain F:

• Molecule 5: Peptide
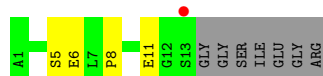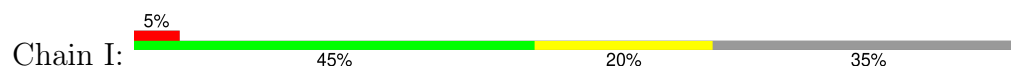
Chain I:

• Molecule 5: Peptide
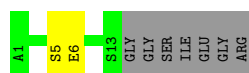
Chain J:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain K:

100%

NAG1
NAG2

● Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain L:

100%

NAG1
NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.06Å 157.65Å 106.10Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	47.03 – 2.74 47.03 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.03-2.74) 99.3 (47.03-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.73Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.214 , 0.247	Depositor DCC
R_{free} test set	56987 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12888	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.25	0/1523	0.47	0/2074
1	G	0.25	0/1512	0.49	0/2060
2	B	0.25	0/1926	0.46	0/2624
2	H	0.25	0/1926	0.45	0/2624
3	C	0.25	0/1487	0.44	0/2031
3	E	0.25	0/1487	0.44	0/2031
4	D	0.23	0/1513	0.43	0/2056
4	F	0.24	0/1513	0.43	0/2056
5	I	0.22	0/98	0.37	0/134
5	J	0.24	0/98	0.39	0/134
All	All	0.25	0/13083	0.45	0/17824

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	1490	0	1381	18	0
1	G	1480	0	1369	14	0
2	B	1877	0	1776	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1877	0	1776	12	2
3	C	1445	0	1397	13	0
3	E	1445	0	1397	12	1
4	D	1480	0	1443	18	0
4	F	1480	0	1443	24	0
5	I	96	0	92	3	0
5	J	96	0	92	1	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
7	A	12	0	0	0	0
7	B	2	0	0	0	0
7	C	10	0	0	0	0
7	D	9	0	0	0	0
7	E	11	0	0	0	0
7	F	6	0	0	0	0
7	G	9	0	0	0	0
7	H	6	0	0	0	0
7	I	1	0	0	0	0
All	All	12888	0	12216	117	2

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 5.

The worst 5 of 117 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:109:ARG:NH2	3:C:62:ASN:OD1	2.18	0.76
2:H:109:ARG:NH2	3:E:62:ASN:OD1	2.22	0.73
3:E:96:PRO:HD3	4:F:120:THR:HG21	1.74	0.70
4:D:10:GLN:HB2	4:D:31:ILE:HB	1.73	0.69
3:C:96:PRO:HD3	4:D:120:THR:HG21	1.74	0.69

All (2) 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)
2:H:210:SER:OG	3:E:159:GLU:OE1[1_556]	2.10	0.10
2:H:22:ARG:NH2	2:B:79:GLU:OE2[2_458]	2.19	0.01

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	190/202 (94%)	177 (93%)	12 (6%)	1 (0%)	25	41
1	G	190/202 (94%)	175 (92%)	15 (8%)	0	100	100
2	B	240/244 (98%)	232 (97%)	8 (3%)	0	100	100
2	H	240/244 (98%)	232 (97%)	8 (3%)	0	100	100
3	C	179/191 (94%)	177 (99%)	2 (1%)	0	100	100
3	E	179/191 (94%)	177 (99%)	2 (1%)	0	100	100
4	D	177/206 (86%)	171 (97%)	6 (3%)	0	100	100
4	F	177/206 (86%)	171 (97%)	6 (3%)	0	100	100
5	I	11/20 (55%)	11 (100%)	0	0	100	100
5	J	11/20 (55%)	11 (100%)	0	0	100	100
All	All	1594/1726 (92%)	1534 (96%)	59 (4%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASN

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	162/181 (90%)	157 (97%)	5 (3%)	35	56
1	G	159/181 (88%)	151 (95%)	8 (5%)	20	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	200/209 (96%)	195 (98%)	5 (2%)	42	63
2	H	200/209 (96%)	198 (99%)	2 (1%)	73	84
3	C	165/174 (95%)	164 (99%)	1 (1%)	84	90
3	E	165/174 (95%)	161 (98%)	4 (2%)	44	64
4	D	164/184 (89%)	161 (98%)	3 (2%)	54	72
4	F	164/184 (89%)	160 (98%)	4 (2%)	44	64
5	I	11/15 (73%)	10 (91%)	1 (9%)	7	14
5	J	11/15 (73%)	10 (91%)	1 (9%)	7	14
All	All	1401/1526 (92%)	1367 (98%)	34 (2%)	44	64

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

Mol	Chain	Res	Type
4	F	19	ASN
4	F	21	THR
5	I	6	GLU
1	A	115	LYS
1	A	114	GLN

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

Mol	Chain	Res	Type
2	B	216	ASN

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 ⓘ

4 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	$\#|Z| > 2$
6	NAG	K	1	6,3	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	K	2	6	14,14,15	0.45	0	17,19,21	0.43	0
6	NAG	L	1	6,3	14,14,15	0.33	0	17,19,21	0.41	0
6	NAG	L	2	6	14,14,15	0.42	0	17,19,21	0.45	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
6	NAG	K	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	NAG	L	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
6	L	2	NAG	O5-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.

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L
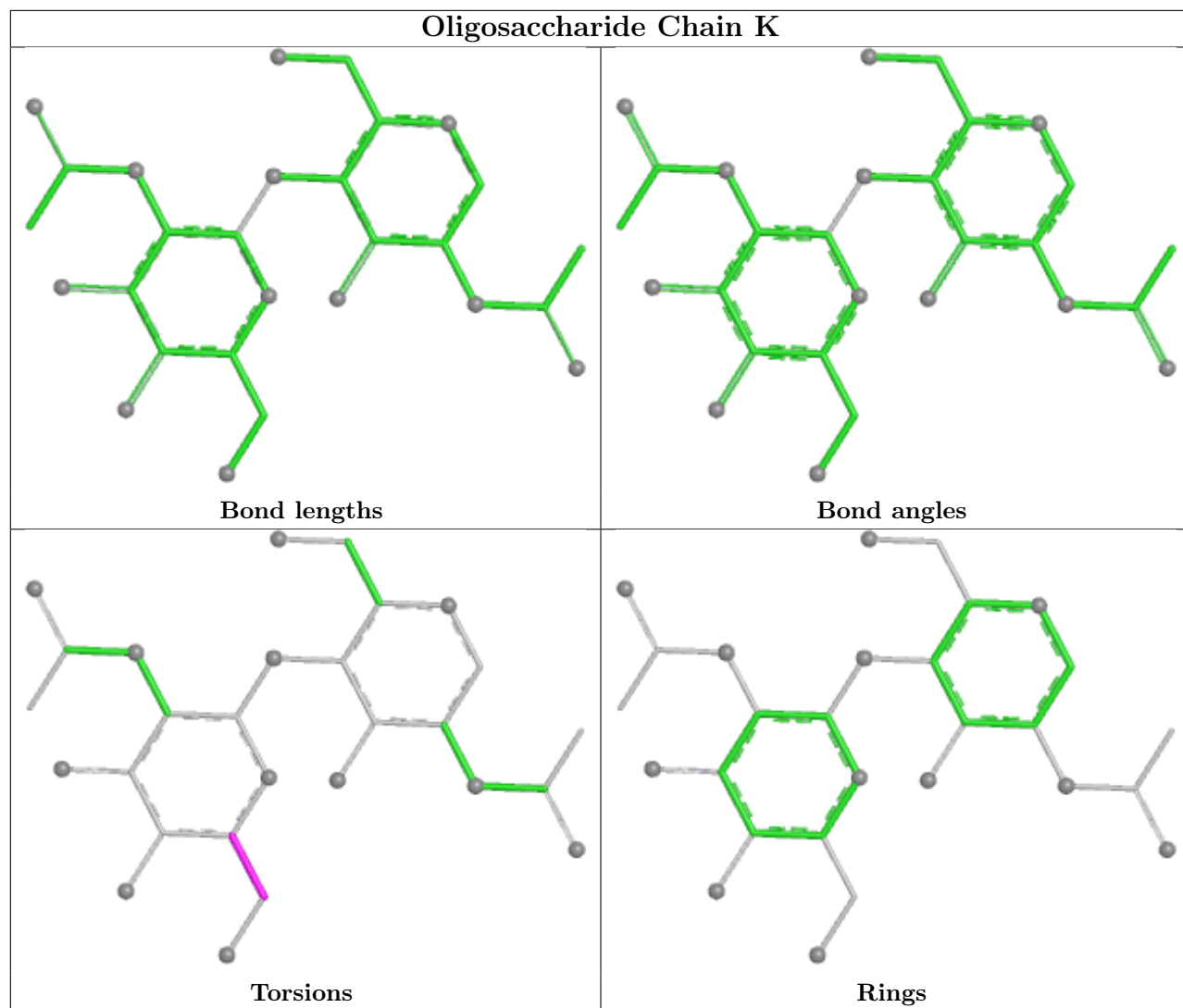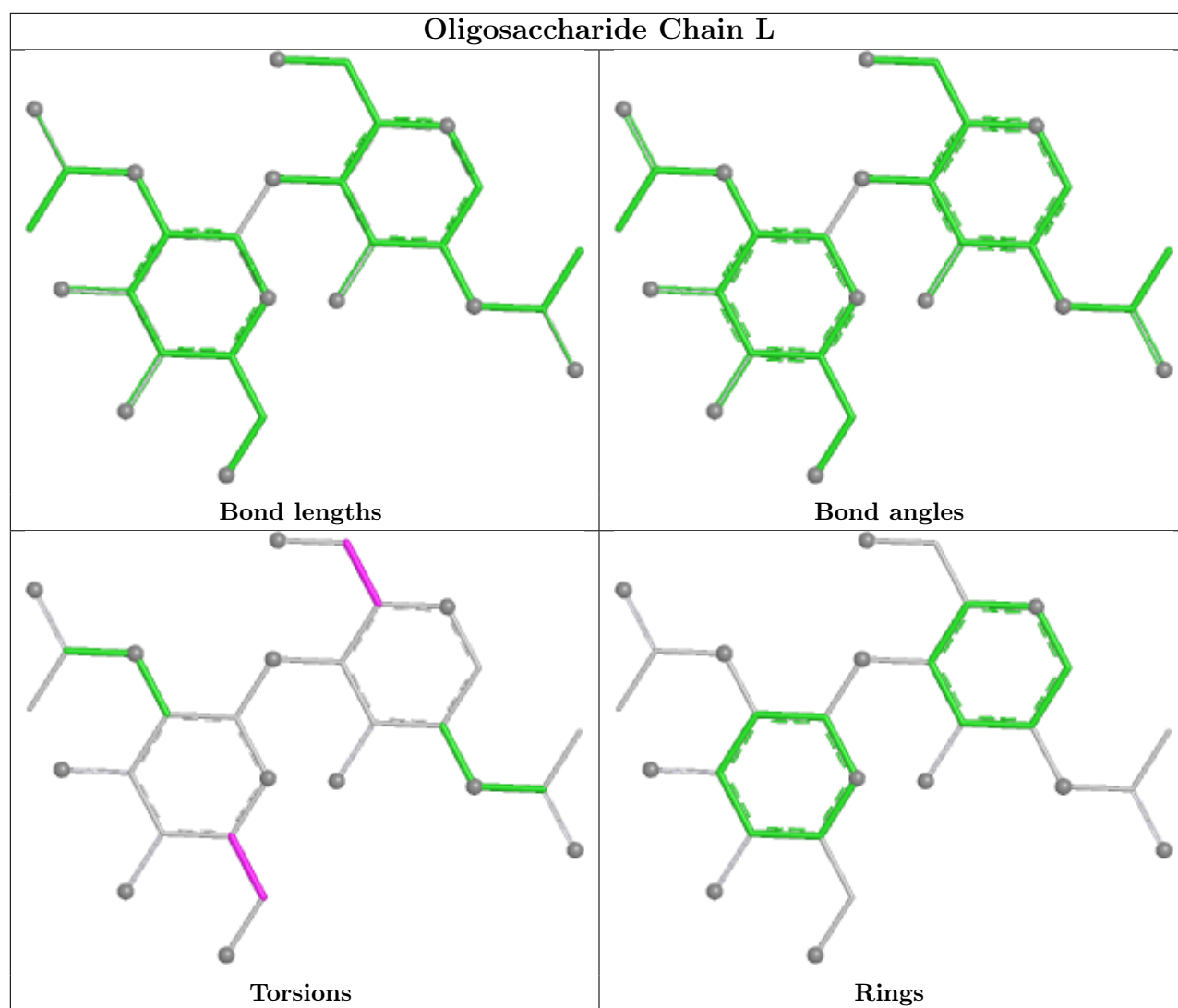
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

<mark>Warning: The R factor obtained from EDS is 0.2144, which does not match the depositor's R factor of 0.0. Please interpret the results in this section carefully.</mark>

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	194/202 (96%)	0.17	9 (4%)	38	39	45, 78, 158, 191	0
1	G	194/202 (96%)	0.27	11 (5%)	30	32	42, 78, 172, 218	0
2	B	242/244 (99%)	0.02	4 (1%)	69	69	42, 83, 146, 178	0
2	H	242/244 (99%)	-0.02	5 (2%)	63	63	44, 84, 141, 197	0
3	C	181/191 (94%)	-0.22	3 (1%)	69	69	42, 68, 117, 205	0
3	E	181/191 (94%)	-0.32	2 (1%)	77	79	38, 62, 104, 144	0
4	D	181/206 (87%)	0.08	4 (2%)	62	61	48, 81, 160, 199	0
4	F	181/206 (87%)	-0.08	2 (1%)	77	79	41, 73, 179, 225	0
5	I	13/20 (65%)	-0.02	1 (7%)	21	23	46, 50, 71, 74	0
5	J	13/20 (65%)	0.03	0	100	100	58, 66, 92, 93	0
All	All	1622/1726 (93%)	-0.01	41 (2%)	58	58	38, 77, 156, 225	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	ILE	5.6
3	E	1	ILE	5.1
1	G	2	MET	4.1
2	H	256	ALA	3.7
1	G	110	ALA	3.5

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

There are no non-standard protein/DNA/RNA residues in this entry.
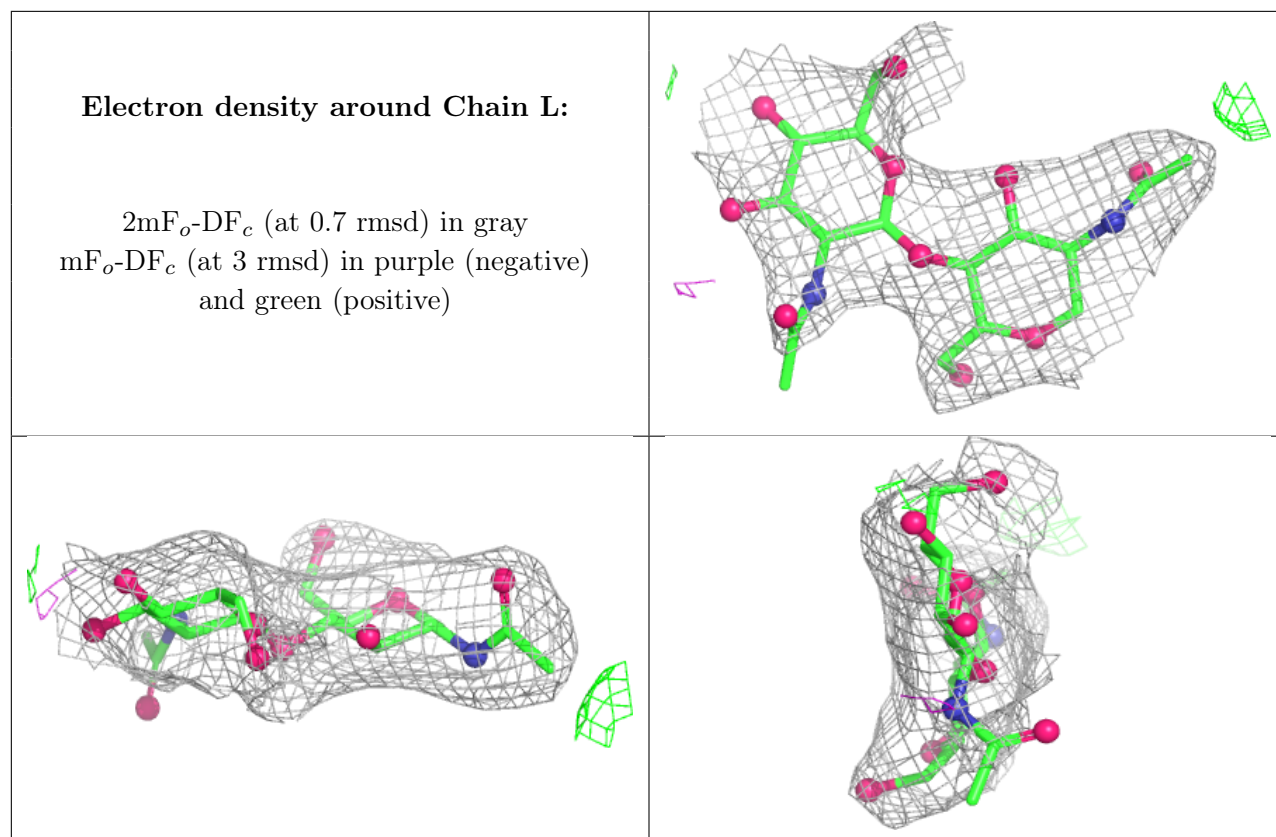
WORLDWIDE
wwPDB
PROTEIN DATA BANK

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($Å^2$)	Q<0.9
6	NAG	L	2	14/15	0.57	0.15	117,124,126,126	0
6	NAG	K	1	14/15	0.70	0.13	65,76,85,91	0
6	NAG	K	2	14/15	0.73	0.13	86,92,98,100	0
6	NAG	L	1	14/15	0.89	0.08	59,82,99,107	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.

Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
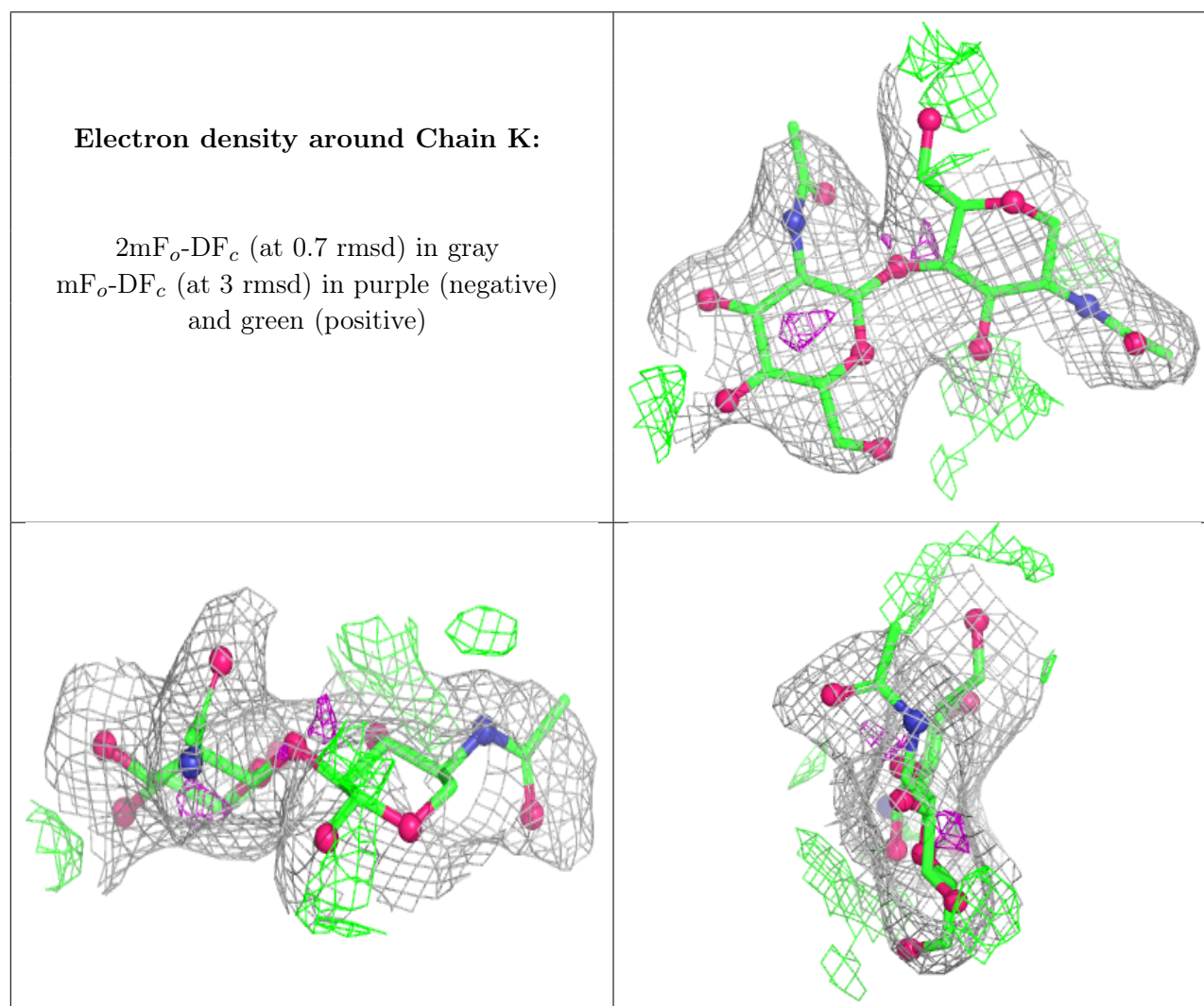
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.