



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 12:32 PM UTC

PDB ID : 8TRL / pdb\_00008trl  
Title : T cell recognition of citrullinated alpha-enolase peptide presented by HLA-DR4  
Authors : Lim, J.J.; Loh, T.J.; Reid, H.H.; Rossjohn, J.  
Deposited on : 2023-08-09  
Resolution : 2.40 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](mailto: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>.

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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

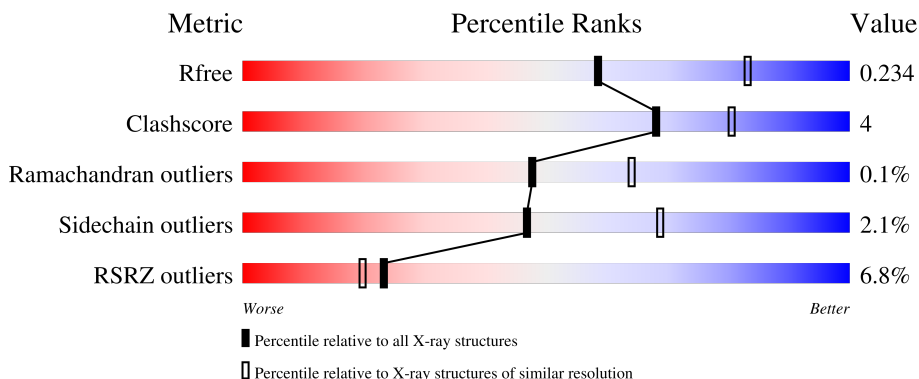
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	181	 90% 9%
1	D	181	 90% 9%
2	B	190	 79% 13% 8%
2	E	190	 83% 12% 6%
3	C	13	 77% 23%

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Mol	Chain	Length	Quality of chain
3	F	13	
4	G	204	
4	I	204	
5	H	245	
5	J	245	
6	K	2	
7	L	6	

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 12917 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
			Total	C	N	O	S			
1	A	179	1441	936	237	263	5	0	0	0
1	D	179	1424	928	234	257	5	0	0	0

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	175	1399	894	243	257	5	0	0	0
2	E	179	1437	914	247	272	4	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	GLU	TRP	variant	UNP P01911
B	11	VAL	PRO	variant	UNP P01911
B	13	HIS	ARG	variant	UNP P01911
B	33	HIS	ASN	variant	UNP P01911
B	37	TYR	SER	variant	UNP P01911
B	47	TYR	PHE	variant	UNP P01911
B	67	LEU	ILE	variant	UNP P01911
B	71	LYS	ALA	variant	UNP P01911
B	86	GLY	VAL	variant	UNP P01911
B	96	TYR	GLN	variant	UNP P01911
B	98	GLU	LYS	variant	UNP P01911
B	104	ALA	SER	variant	UNP P01911
B	120	ASN	SER	variant	UNP P01911
B	133	ARG	LEU	variant	UNP P01911
B	140	THR	ALA	variant	UNP P01911
B	142	VAL	MET	variant	UNP P01911

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	LEU	VAL	variant	UNP P01911
E	9	GLU	TRP	variant	UNP P01911
E	11	VAL	PRO	variant	UNP P01911
E	13	HIS	ARG	variant	UNP P01911
E	33	HIS	ASN	variant	UNP P01911
E	37	TYR	SER	variant	UNP P01911
E	47	TYR	PHE	variant	UNP P01911
E	67	LEU	ILE	variant	UNP P01911
E	71	LYS	ALA	variant	UNP P01911
E	86	GLY	VAL	variant	UNP P01911
E	96	TYR	GLN	variant	UNP P01911
E	98	GLU	LYS	variant	UNP P01911
E	104	ALA	SER	variant	UNP P01911
E	120	ASN	SER	variant	UNP P01911
E	133	ARG	LEU	variant	UNP P01911
E	140	THR	ALA	variant	UNP P01911
E	142	VAL	MET	variant	UNP P01911
E	180	LEU	VAL	variant	UNP P01911

- Molecule 3 is a protein called Alpha-enolase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			99	60	16	23			
3	F	13	Total	C	N	O	0	0	0
			99	60	16	23			

- Molecule 4 is a protein called RA2.7 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	188	Total	C	N	O	S	0	0	0
			1307	816	221	260	10			
4	G	199	Total	C	N	O	S	0	0	0
			1432	903	240	279	10			

- Molecule 5 is a protein called RA2.7 TCR beta chain.

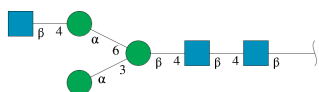
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	240	Total	C	N	O	S	0	0	0
			1857	1189	317	344	7			
5	H	244	Total	C	N	O	S	0	0	0
			1830	1180	305	338	7			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



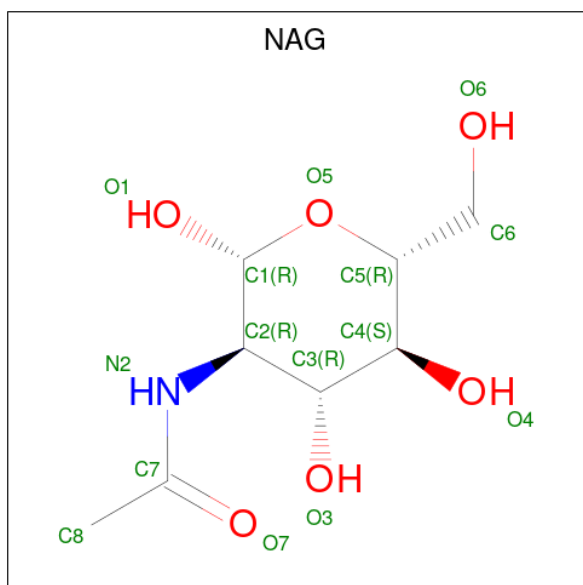
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	K	2	28	16	2	10	0	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



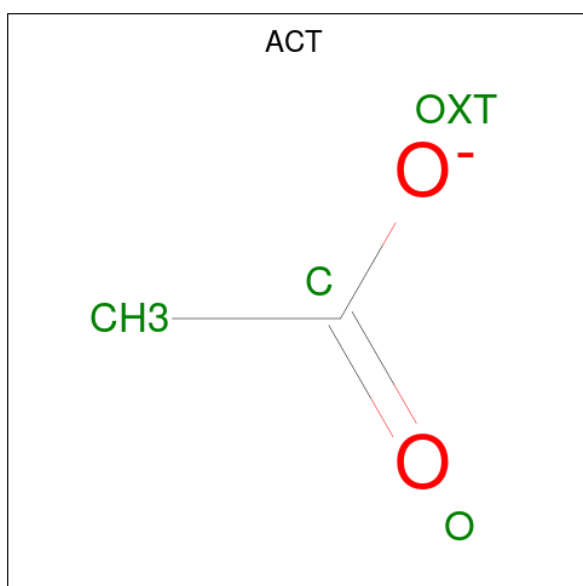
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	L	6	75	42	3	30	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



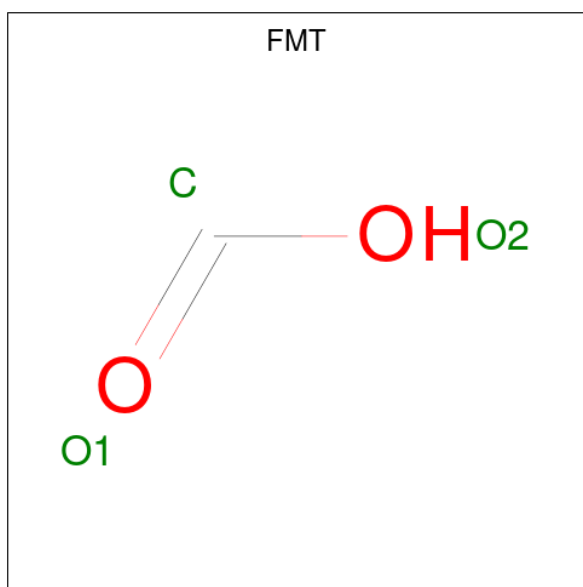
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2^-$ ).



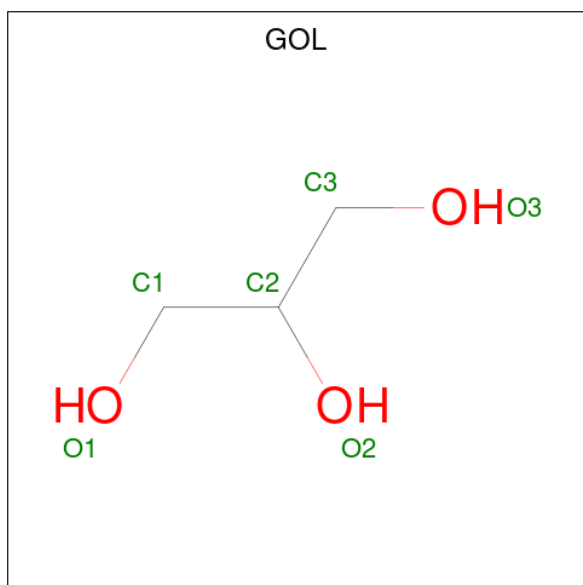
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is FORMIC ACID (CCD ID: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	C O	0	0
			3	1 2		
10	A	1	Total	C O	0	0
			3	1 2		
10	J	1	Total	C O	0	0
			3	1 2		
10	D	1	Total	C O	0	0
			3	1 2		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	60	Total O 60 60	0	0
12	B	65	Total O 65 65	0	0
12	C	8	Total O 8 8	0	0
12	I	20	Total O 20 20	0	0
12	J	30	Total O 30 30	0	0
12	D	54	Total O 54 54	0	0
12	E	50	Total O 50 50	0	0
12	F	7	Total O 7 7	0	0
12	G	22	Total O 22 22	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	H	27	Total	O	0	0
			27	27		

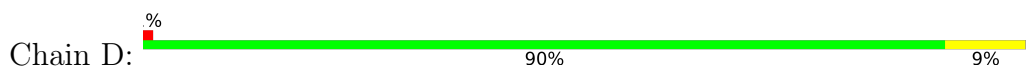
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

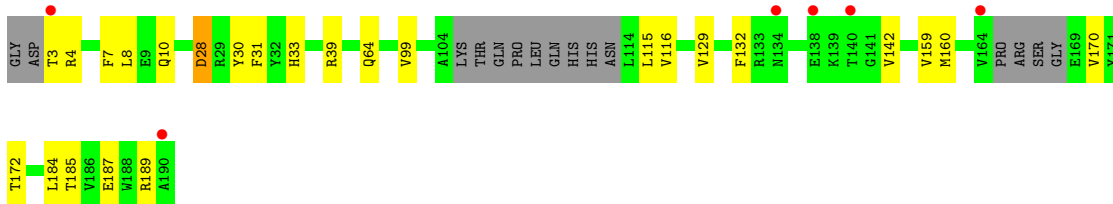
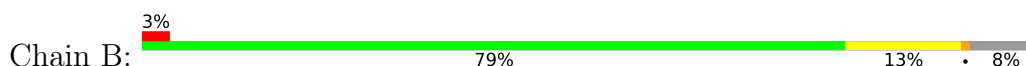
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



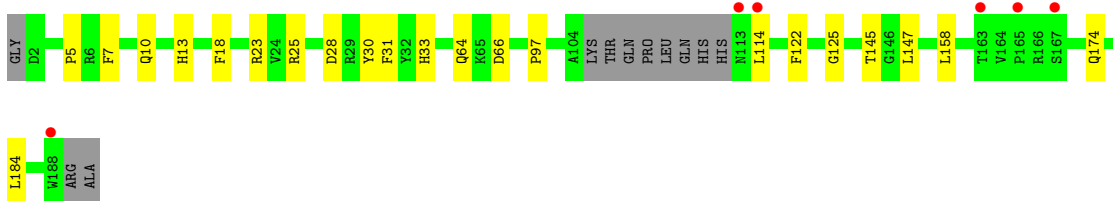
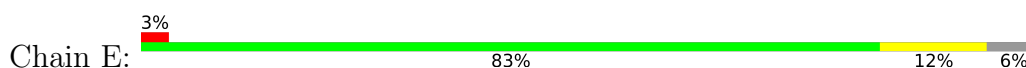
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain




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



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



- Molecule 3: Alpha-enolase

Chain C:  77% 23%




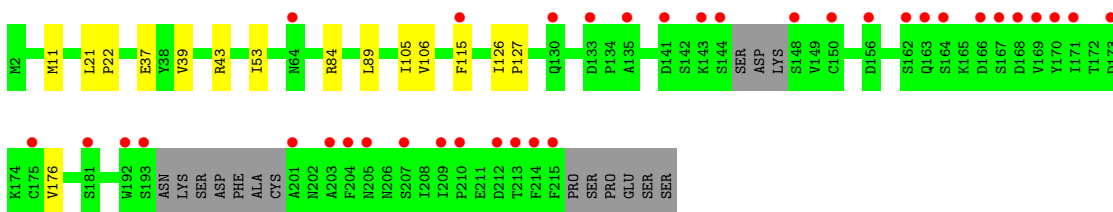
- Molecule 3: Alpha-enolase

Chain F:  69% 31%




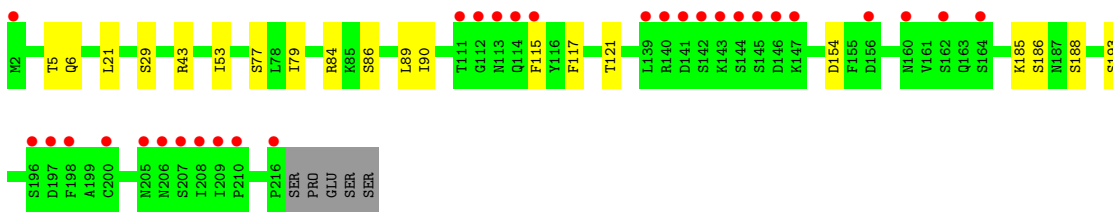
- Molecule 4: RA2.7 TCR alpha chain

Chain I:  18% 85% 7% 8%




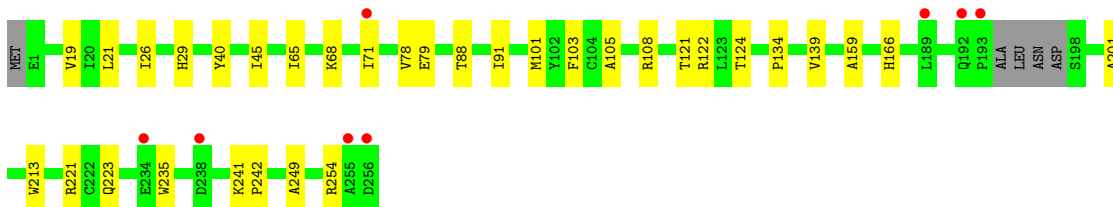
- Molecule 4: RA2.7 TCR alpha chain

Chain G:  15% 88% 10%

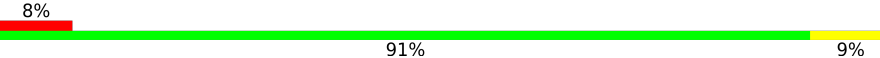


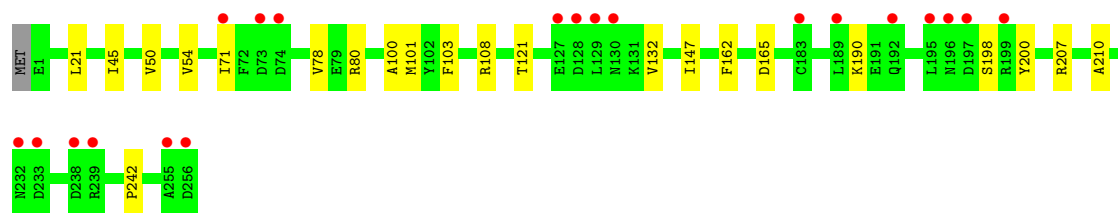
- Molecule 5: RA2.7 TCR beta chain

Chain J:  3% 84% 13%



- Molecule 5: RA2.7 TCR beta chain

Chain H:  8% 91% 9%



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

Chain K: 50% 50%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 33% 17% 50%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.86Å 58.55Å 216.48Å 90.00° 113.60° 90.00°	Depositor
Resolution (Å)	45.87 – 2.40 45.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.87-2.40) 99.9 (45.87-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.210 , 0.234 0.210 , 0.234	Depositor DCC
$R_{free}$ test set	4121 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FMT, BMA, MAN, CIR, NAG, GOL, ACT

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	0.14	0/1486	0.35	0/2032
1	D	0.13	0/1469	0.34	0/2011
2	B	0.16	0/1437	0.36	0/1958
2	E	0.14	0/1476	0.33	0/2012
3	C	0.12	0/88	0.24	0/117
3	F	0.12	0/88	0.28	0/117
4	G	0.13	0/1465	0.37	0/2012
4	I	0.15	0/1330	0.38	0/1826
5	H	0.11	0/1887	0.33	0/2591
5	J	0.13	0/1913	0.34	0/2618
All	All	0.14	0/12639	0.35	0/17294

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	F	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	14	SER	Mainchain

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Mol	Chain	Res	Type	Group
3	C	15	CIR	Mainchain
3	F	14	SER	Mainchain
3	F	15	CIR	Mainchain

## 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	1441	0	1359	8	0
1	D	1424	0	1338	8	0
2	B	1399	0	1274	12	0
2	E	1437	0	1302	13	0
3	C	99	0	82	1	0
3	F	99	0	82	1	0
4	G	1432	0	1247	9	1
4	I	1307	0	1120	8	0
5	H	1830	0	1613	12	0
5	J	1857	0	1673	18	0
6	K	28	0	25	0	0
7	L	75	0	64	2	1
8	A	14	0	13	0	0
8	B	14	0	13	0	0
8	D	14	0	13	0	0
8	E	14	0	13	0	0
9	A	8	0	6	0	0
9	H	4	0	3	0	0
10	A	6	0	2	0	0
10	D	3	0	1	0	0
10	J	3	0	1	0	0
11	A	6	0	8	1	0
11	B	6	0	8	0	0
11	D	12	0	16	0	0
11	E	30	0	40	0	0
11	G	12	0	16	0	0
12	A	60	0	0	0	0
12	B	65	0	0	0	0
12	C	8	0	0	0	0
12	D	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	E	50	0	0	0	0
12	F	7	0	0	0	0
12	G	22	0	0	2	0
12	H	27	0	0	0	0
12	I	20	0	0	0	0
12	J	30	0	0	0	0
All	All	12917	0	11332	85	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 85 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)
5:H:45:ILE:HD13	5:H:100:ALA:HB2	1.67	0.77
4:I:43:ARG:HB3	4:I:53:ILE:HD11	1.71	0.73
4:G:43:ARG:HB2	4:G:53:ILE:HD11	1.71	0.72
1:A:141:GLU:HG3	11:A:206:GOL:H32	1.72	0.71
2:B:3:THR:HG22	2:B:4:ARG:H	1.58	0.68

All (1) 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)
4:G:77:SER:OG	7:L:5:NAG:O4[1_545]	2.09	0.11

## 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	177/181 (98%)	175 (99%)	2 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	177/181 (98%)	175 (99%)	2 (1%)	0	100	100
2	B	169/190 (89%)	164 (97%)	5 (3%)	0	100	100
2	E	175/190 (92%)	169 (97%)	6 (3%)	0	100	100
3	C	10/13 (77%)	10 (100%)	0	0	100	100
3	F	10/13 (77%)	10 (100%)	0	0	100	100
4	G	197/204 (97%)	186 (94%)	10 (5%)	1 (0%)	24	37
4	I	182/204 (89%)	167 (92%)	15 (8%)	0	100	100
5	H	242/245 (99%)	234 (97%)	8 (3%)	0	100	100
5	J	236/245 (96%)	230 (98%)	6 (2%)	0	100	100
All	All	1575/1666 (94%)	1520 (96%)	54 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	115	PHE

### 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	156/166 (94%)	153 (98%)	3 (2%)	50	71
1	D	152/166 (92%)	148 (97%)	4 (3%)	40	63
2	B	143/171 (84%)	138 (96%)	5 (4%)	32	53
2	E	149/171 (87%)	147 (99%)	2 (1%)	61	80
3	C	10/10 (100%)	10 (100%)	0	100	100
3	F	10/10 (100%)	9 (90%)	1 (10%)	7	11
4	G	138/184 (75%)	133 (96%)	5 (4%)	31	52
4	I	122/184 (66%)	121 (99%)	1 (1%)	73	86
5	H	178/222 (80%)	176 (99%)	2 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	J	189/222 (85%)	186 (98%)	3 (2%)	55 76
All	All	1247/1506 (83%)	1221 (98%)	26 (2%)	47 69

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	128	VAL
2	E	114	LEU
5	H	80	ARG
2	E	64	GLN
3	F	22	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	206	ASN
5	J	63	ASN
1	D	57	GLN
5	J	237	GLN
4	I	51	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](#)

2 non-standard protein/DNA/RNA residues 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	CIR	F	15	3	9,10,11	0.48	0	6,11,13	0.63	0
3	CIR	C	15	3	9,10,11	0.49	0	6,11,13	0.44	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
3	CIR	F	15	3	-	2/8/9/11	-
3	CIR	C	15	3	-	2/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	15	CIR	O-C-CA-C3
3	F	15	CIR	O-C-CA-C3
3	C	15	CIR	C4-C5-N6-C7
3	F	15	CIR	C4-C5-N6-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

8 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	1,6	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
6	NAG	K	2	6	14,14,15	0.40	0	17,19,21	0.48	0
7	NAG	L	1	1,7	14,14,15	0.23	0	17,19,21	0.70	1 (5%)
7	NAG	L	2	7	14,14,15	0.18	0	17,19,21	0.47	0
7	BMA	L	3	7	11,11,12	1.03	0	15,15,17	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	L	4	7	11,11,12	1.64	3 (27%)	15,15,17	1.43	2 (13%)
7	NAG	L	5	7	14,14,15	0.71	1 (7%)	17,19,21	0.95	1 (5%)
7	MAN	L	6	7	11,11,12	0.71	0	15,15,17	1.21	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
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
7	NAG	L	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	BMA	L	3	7	-	2/2/19/22	0/1/1/1
7	MAN	L	4	7	-	2/2/19/22	0/1/1/1
7	NAG	L	5	7	-	4/6/23/26	0/1/1/1
7	MAN	L	6	7	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	4	MAN	O4-C4	3.48	1.51	1.43
7	L	4	MAN	C4-C5	2.64	1.58	1.53
7	L	4	MAN	O5-C5	2.52	1.48	1.43
7	L	5	NAG	O5-C1	2.15	1.47	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	6	MAN	C1-O5-C5	3.76	117.23	112.19
7	L	4	MAN	C1-O5-C5	3.62	117.04	112.19
7	L	4	MAN	O4-C4-C5	2.65	115.85	109.32
7	L	5	NAG	C1-C2-N2	2.27	114.02	110.43
6	K	1	NAG	C1-O5-C5	2.16	115.08	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

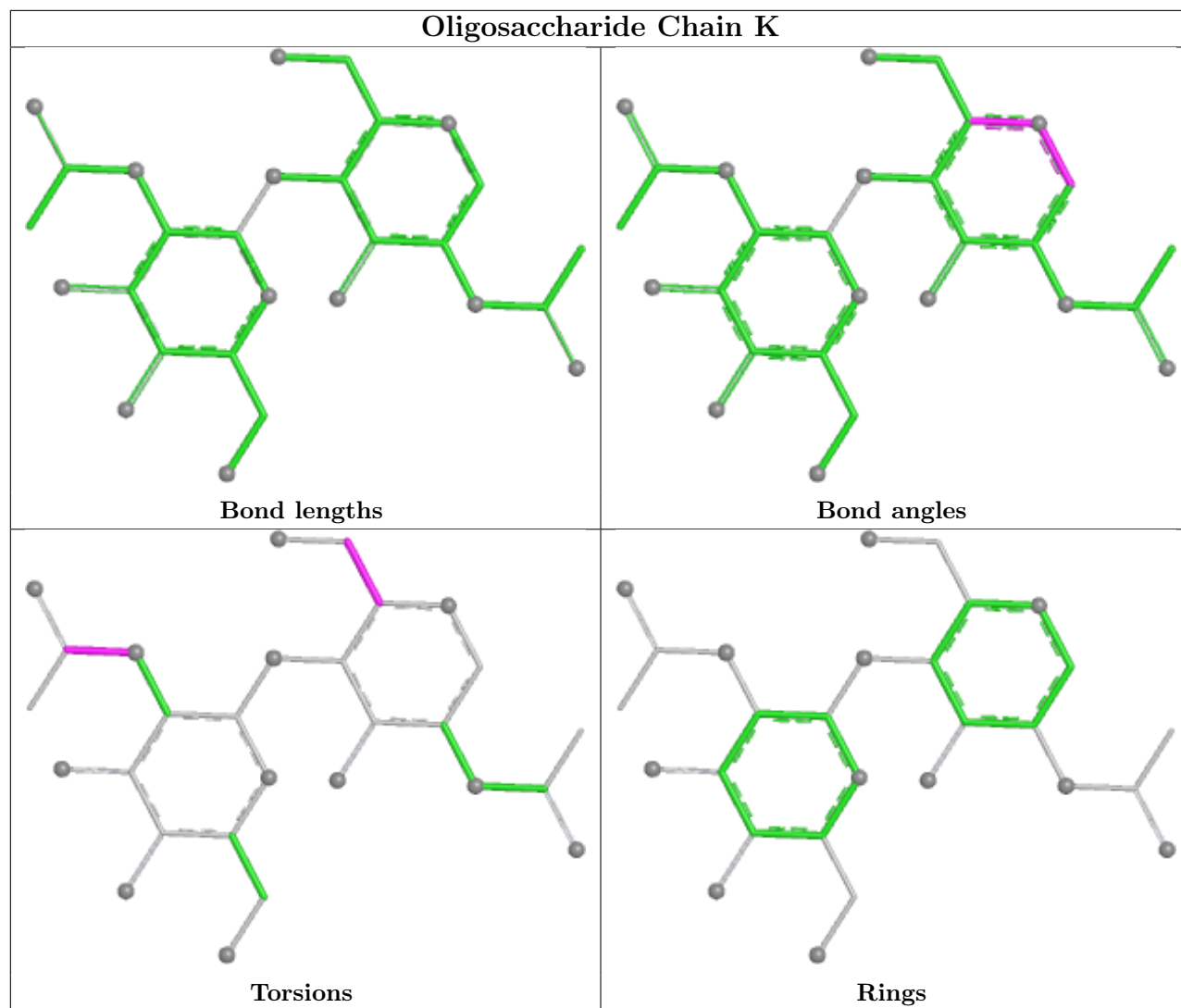
Mol	Chain	Res	Type	Atoms
7	L	4	MAN	C4-C5-C6-O6
7	L	5	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
7	L	4	MAN	O5-C5-C6-O6
7	L	5	NAG	O5-C5-C6-O6

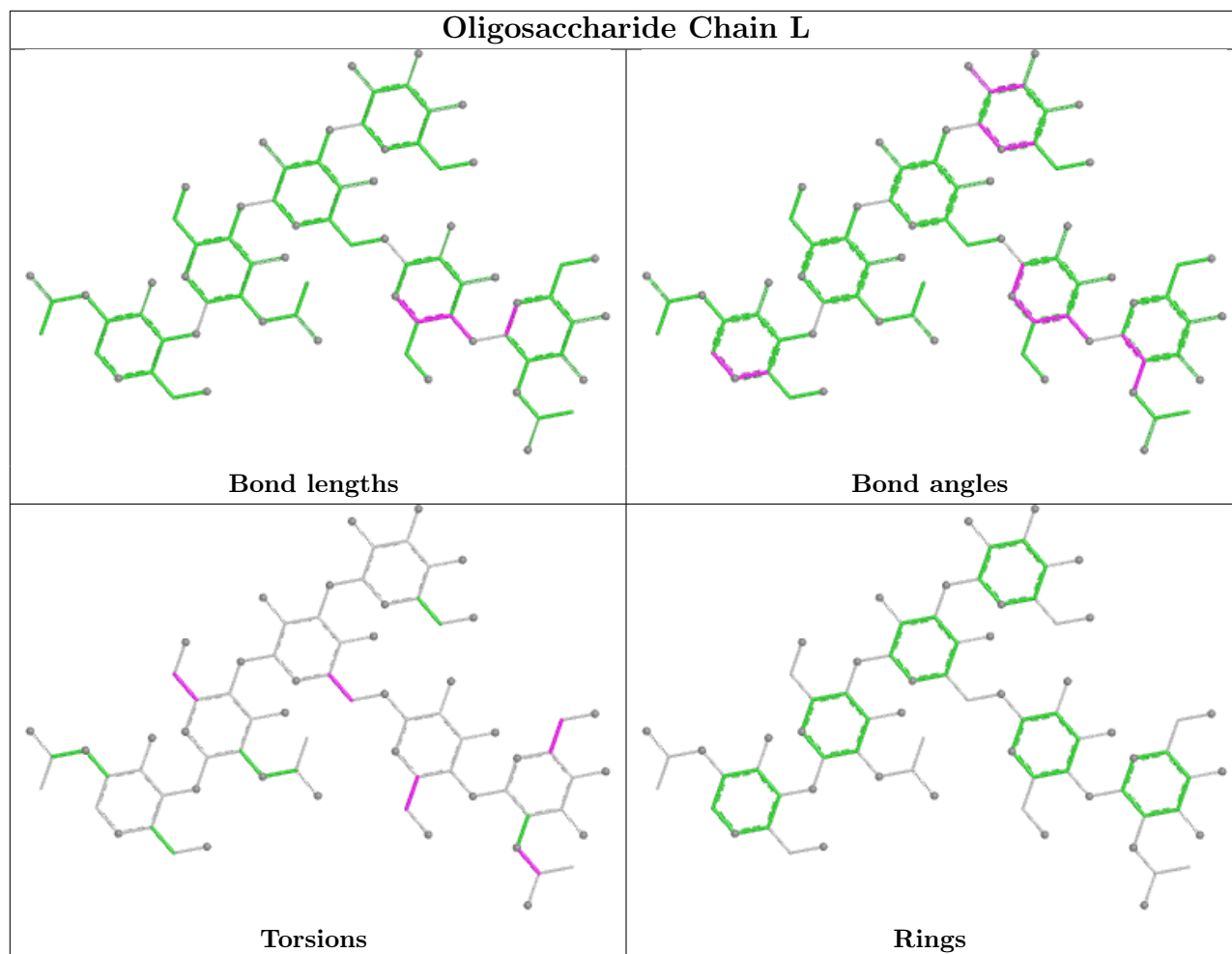
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	4	MAN	1	0
7	L	5	NAG	1	1
7	L	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](#)

22 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	$\# Z  > 2$
11	GOL	E	205	-	5,5,5	0.94	0	5,5,5	1.04	0
8	NAG	D	201	1	14,14,15	0.52	0	17,19,21	0.46	0
11	GOL	E	202	-	5,5,5	1.00	0	5,5,5	1.00	0
11	GOL	B	202	-	5,5,5	0.84	0	5,5,5	1.10	0
11	GOL	G	302	-	5,5,5	0.98	0	5,5,5	1.00	0
11	GOL	A	206	-	5,5,5	0.97	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	GOL	E	206	-	5,5,5	1.02	0	5,5,5	0.94	0
8	NAG	B	201	2	14,14,15	0.35	0	17,19,21	0.44	0
8	NAG	A	201	1	14,14,15	0.25	0	17,19,21	0.64	1 (5%)
8	NAG	E	201	2	14,14,15	0.47	0	17,19,21	0.47	0
11	GOL	D	203	-	5,5,5	0.95	0	5,5,5	1.06	0
11	GOL	E	203	-	5,5,5	0.92	0	5,5,5	1.08	0
10	FMT	A	204	-	2,2,2	0.70	0	1,1,1	0.20	0
10	FMT	D	202	-	2,2,2	0.69	0	1,1,1	0.13	0
9	ACT	A	205	-	3,3,3	1.42	1 (33%)	3,3,3	1.35	0
10	FMT	J	301	-	2,2,2	0.75	0	1,1,1	0.28	0
11	GOL	D	204	-	5,5,5	0.99	0	5,5,5	1.00	0
9	ACT	A	202	-	3,3,3	1.41	1 (33%)	3,3,3	1.40	0
10	FMT	A	203	-	2,2,2	0.71	0	1,1,1	0.13	0
11	GOL	G	301	-	5,5,5	0.92	0	5,5,5	1.12	0
11	GOL	E	204	-	5,5,5	1.02	0	5,5,5	1.04	0
9	ACT	H	301	-	3,3,3	1.60	1 (33%)	3,3,3	1.36	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	NAG	A	201	1	-	0/6/23/26	0/1/1/1
8	NAG	E	201	2	-	2/6/23/26	0/1/1/1
11	GOL	D	204	-	-	4/4/4/4	-
11	GOL	D	203	-	-	0/4/4/4	-
11	GOL	E	205	-	-	1/4/4/4	-
11	GOL	E	203	-	-	2/4/4/4	-
8	NAG	D	201	1	-	1/6/23/26	0/1/1/1
11	GOL	G	301	-	-	4/4/4/4	-
11	GOL	E	202	-	-	0/4/4/4	-
11	GOL	G	302	-	-	2/4/4/4	-
11	GOL	A	206	-	-	1/4/4/4	-
11	GOL	E	204	-	-	2/4/4/4	-
11	GOL	E	206	-	-	2/4/4/4	-
8	NAG	B	201	2	-	2/6/23/26	0/1/1/1
11	GOL	B	202	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	301	ACT	CH3-C	2.40	1.58	1.49
9	A	205	ACT	CH3-C	2.08	1.57	1.49
9	A	202	ACT	CH3-C	2.07	1.57	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	201	NAG	C1-O5-C5	2.17	115.09	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	202	GOL	C1-C2-C3-O3
11	E	203	GOL	C1-C2-C3-O3
11	G	302	GOL	C1-C2-C3-O3
8	B	201	NAG	O5-C5-C6-O6
8	E	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	206	GOL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	179/181 (98%)	-0.05	2 (1%) 78 74	35, 49, 70, 81	0
1	D	179/181 (98%)	-0.09	1 (0%) 85 83	35, 50, 68, 84	0
2	B	175/190 (92%)	0.11	6 (3%) 48 44	35, 47, 81, 93	0
2	E	179/190 (94%)	0.19	6 (3%) 48 44	36, 50, 91, 102	0
3	C	12/13 (92%)	0.04	0 100 100	37, 40, 58, 61	0
3	F	12/13 (92%)	0.14	0 100 100	37, 42, 58, 59	0
4	G	199/204 (97%)	0.83	30 (15%) 5 4	42, 64, 111, 129	0
4	I	188/204 (92%)	1.05	36 (19%) 3 2	40, 69, 119, 139	0
5	H	244/245 (99%)	0.69	20 (8%) 17 14	40, 76, 102, 117	0
5	J	240/245 (97%)	0.57	8 (3%) 49 45	39, 77, 110, 132	0
All	All	1607/1666 (96%)	0.43	109 (6%) 23 20	35, 58, 108, 139	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	144	SER	6.6
4	I	168	ASP	5.0
4	G	147	LYS	4.8
4	I	193	SER	4.7
4	G	144	SER	4.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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	CIR	F	15	11/12	0.93	0.12	34,37,45,47	0
3	CIR	C	15	11/12	0.95	0.08	34,39,41,43	0

### 6.3 Carbohydrates [i](#)

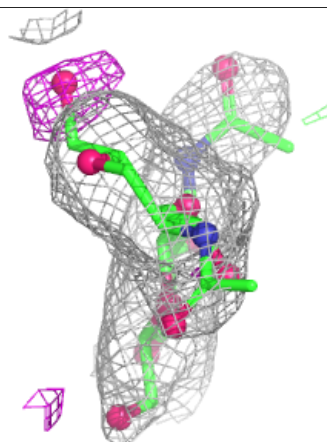
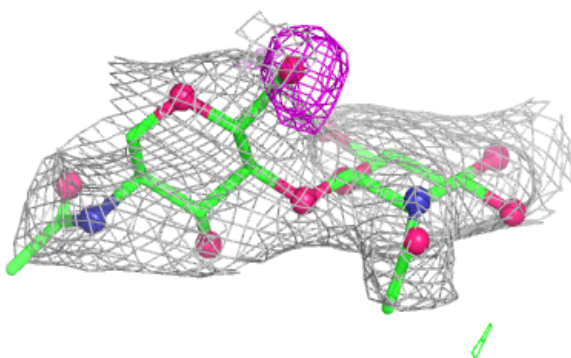
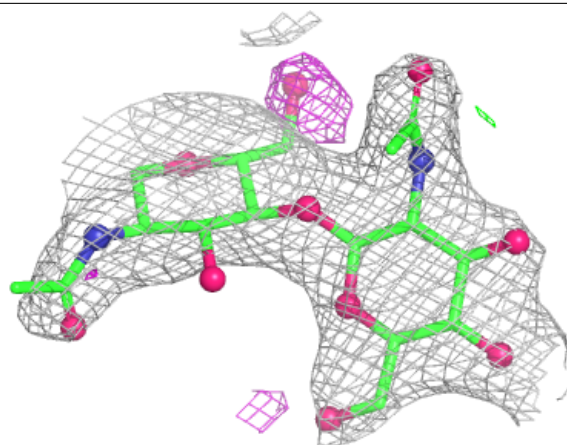
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

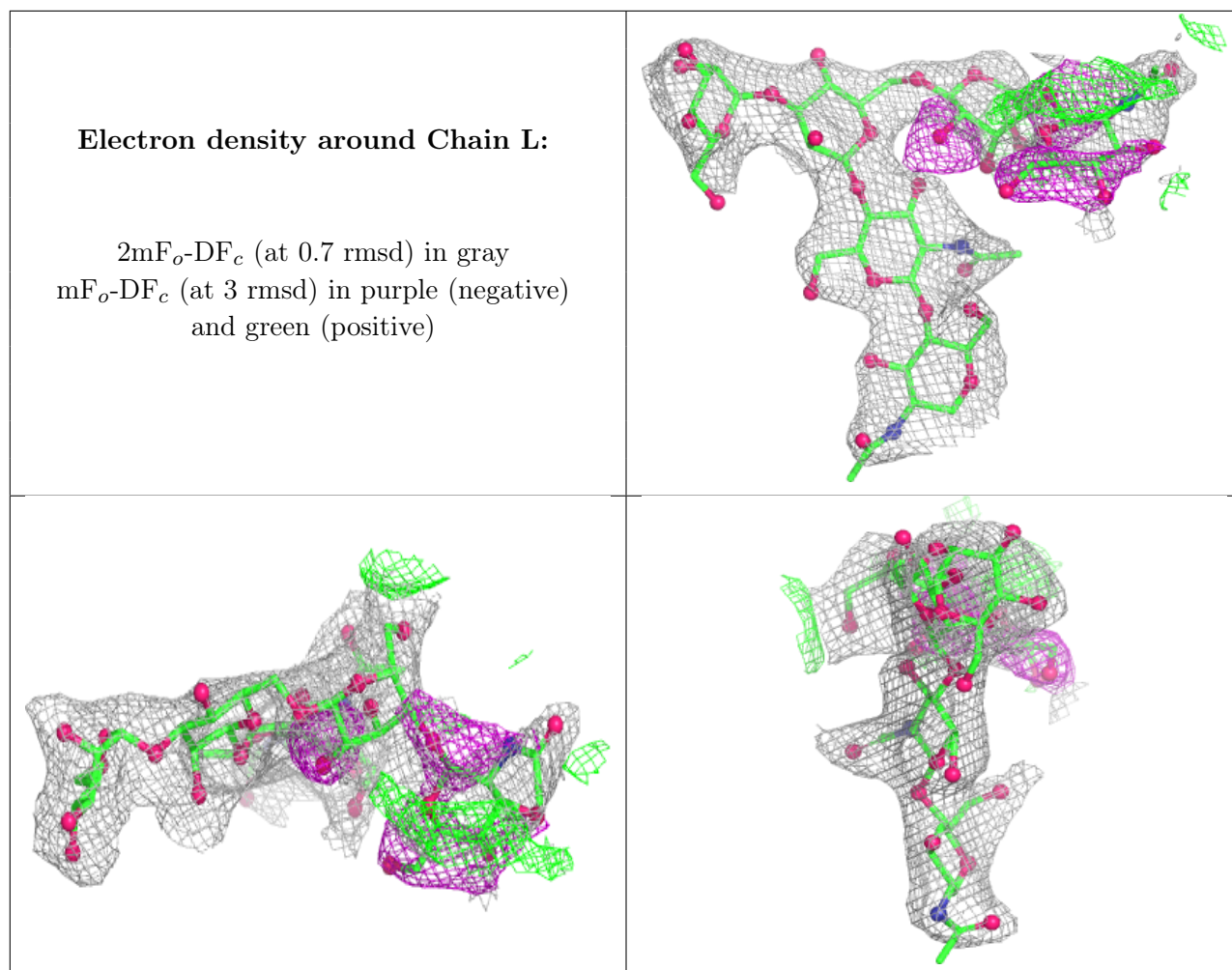
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	L	5	14/15	0.46	0.23	64,71,75,76	0
7	MAN	L	6	11/12	0.58	0.13	80,87,90,92	0
7	MAN	L	4	11/12	0.59	0.18	58,69,79,86	0
6	NAG	K	2	14/15	0.62	0.14	76,81,85,87	0
6	NAG	K	1	14/15	0.75	0.15	67,78,83,92	0
7	NAG	L	2	14/15	0.78	0.11	70,76,79,81	0
7	BMA	L	3	11/12	0.84	0.09	75,80,81,85	0
7	NAG	L	1	14/15	0.85	0.11	67,72,77,77	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)





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	NAG	E	201	14/15	0.54	0.15	78,83,87,98	0
9	ACT	H	301	4/4	0.60	0.23	49,54,54,62	0
11	GOL	G	302	6/6	0.61	0.23	58,58,58,58	0
10	FMT	J	301	3/3	0.65	0.20	66,66,73,79	0
9	ACT	A	205	4/4	0.69	0.20	66,71,72,72	0
11	GOL	D	203	6/6	0.70	0.13	70,74,77,77	0
11	GOL	G	301	6/6	0.74	0.14	70,74,79,82	0
8	NAG	A	201	14/15	0.77	0.12	61,67,72,76	0
11	GOL	E	205	6/6	0.77	0.19	55,59,62,64	0
11	GOL	E	203	6/6	0.79	0.11	78,83,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NAG	D	201	14/15	0.79	0.13	52,74,86,86	0
8	NAG	B	201	14/15	0.81	0.11	62,68,74,76	0
9	ACT	A	202	4/4	0.82	0.20	58,59,60,61	0
10	FMT	A	204	3/3	0.82	0.16	52,52,53,53	0
10	FMT	D	202	3/3	0.83	0.21	36,36,53,53	0
11	GOL	E	204	6/6	0.84	0.16	54,57,58,58	0
10	FMT	A	203	3/3	0.86	0.21	44,44,44,46	0
11	GOL	E	202	6/6	0.87	0.14	51,56,56,58	0
11	GOL	B	202	6/6	0.88	0.15	58,60,61,61	0
11	GOL	A	206	6/6	0.89	0.18	46,49,51,51	0
11	GOL	E	206	6/6	0.90	0.12	45,46,47,51	0
11	GOL	D	204	6/6	0.91	0.15	44,49,49,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.