



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2026 – 10:17 AM EDT

PDB ID : 10TZ / pdb\_000010tz  
Title : Tissue Non-specific Alkaline Phosphatase -S110A bound to ATP  
Authors : Krishnan, S.S.; Carroll, B.L.; Guarne, A.  
Deposited on : 2026-02-09  
Resolution : 2.71 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](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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

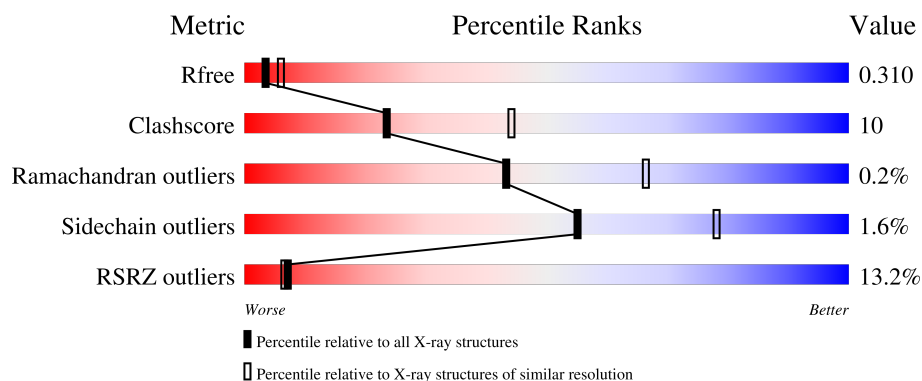
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	493	
1	B	493	
1	C	493	
1	D	493	
2	E	5	

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Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	H	2	 50%50%
3	I	2	 100%
3	J	2	 50%50%
4	G	4	 75%25%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15598 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 Alkaline phosphatase, tissue-nonspecific isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	1	0	0
			3753	2346	670	717	20			
1	B	481	Total	C	N	O	S	1	0	0
			3737	2337	667	713	20			
1	C	482	Total	C	N	O	S	1	0	0
			3743	2340	668	715	20			
1	D	481	Total	C	N	O	S	1	0	0
			3737	2337	667	713	20			

There are 36 discrepancies between the modelled and reference sequences:

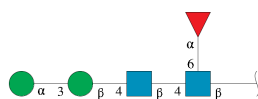
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASP	-	expression tag	UNP P09242
A	16	GLY	-	expression tag	UNP P09242
A	110	ALA	SER	engineered mutation	UNP P09242
A	502	HIS	-	expression tag	UNP P09242
A	503	HIS	-	expression tag	UNP P09242
A	504	HIS	-	expression tag	UNP P09242
A	505	HIS	-	expression tag	UNP P09242
A	506	HIS	-	expression tag	UNP P09242
A	507	HIS	-	expression tag	UNP P09242
B	15	ASP	-	expression tag	UNP P09242
B	16	GLY	-	expression tag	UNP P09242
B	110	ALA	SER	engineered mutation	UNP P09242
B	502	HIS	-	expression tag	UNP P09242
B	503	HIS	-	expression tag	UNP P09242
B	504	HIS	-	expression tag	UNP P09242
B	505	HIS	-	expression tag	UNP P09242
B	506	HIS	-	expression tag	UNP P09242
B	507	HIS	-	expression tag	UNP P09242
C	15	ASP	-	expression tag	UNP P09242
C	16	GLY	-	expression tag	UNP P09242
C	110	ALA	SER	engineered mutation	UNP P09242

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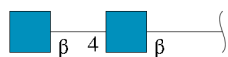
Chain	Residue	Modelled	Actual	Comment	Reference
C	502	HIS	-	expression tag	UNP P09242
C	503	HIS	-	expression tag	UNP P09242
C	504	HIS	-	expression tag	UNP P09242
C	505	HIS	-	expression tag	UNP P09242
C	506	HIS	-	expression tag	UNP P09242
C	507	HIS	-	expression tag	UNP P09242
D	15	ASP	-	expression tag	UNP P09242
D	16	GLY	-	expression tag	UNP P09242
D	110	ALA	SER	engineered mutation	UNP P09242
D	502	HIS	-	expression tag	UNP P09242
D	503	HIS	-	expression tag	UNP P09242
D	504	HIS	-	expression tag	UNP P09242
D	505	HIS	-	expression tag	UNP P09242
D	506	HIS	-	expression tag	UNP P09242
D	507	HIS	-	expression tag	UNP P09242

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



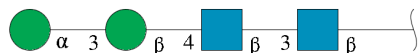
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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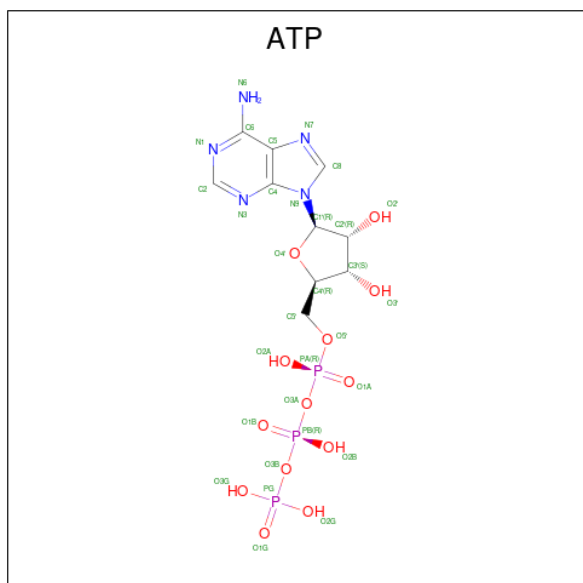
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	18	0
			31	10	5	13	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	B	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

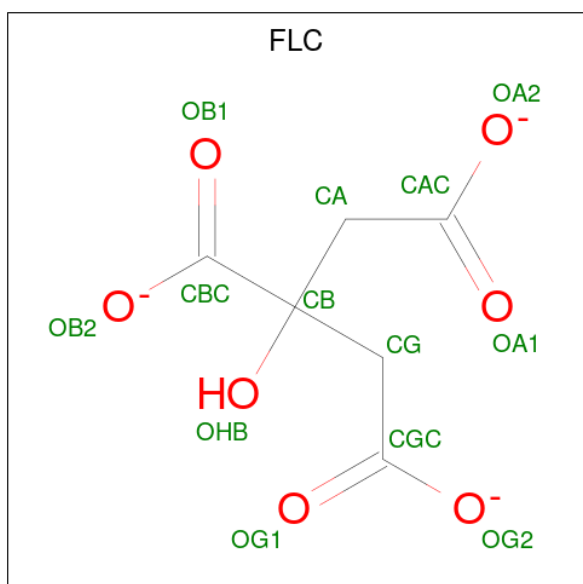
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).





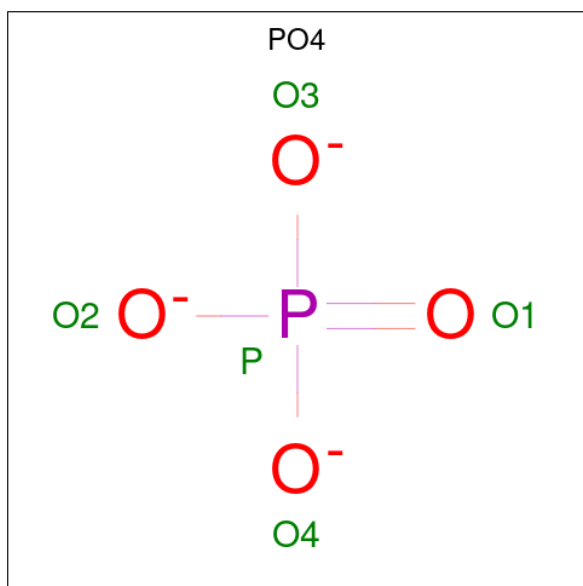
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is CITRATE ANION (CCD ID: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total	O	P	0	0
			5	4	1		

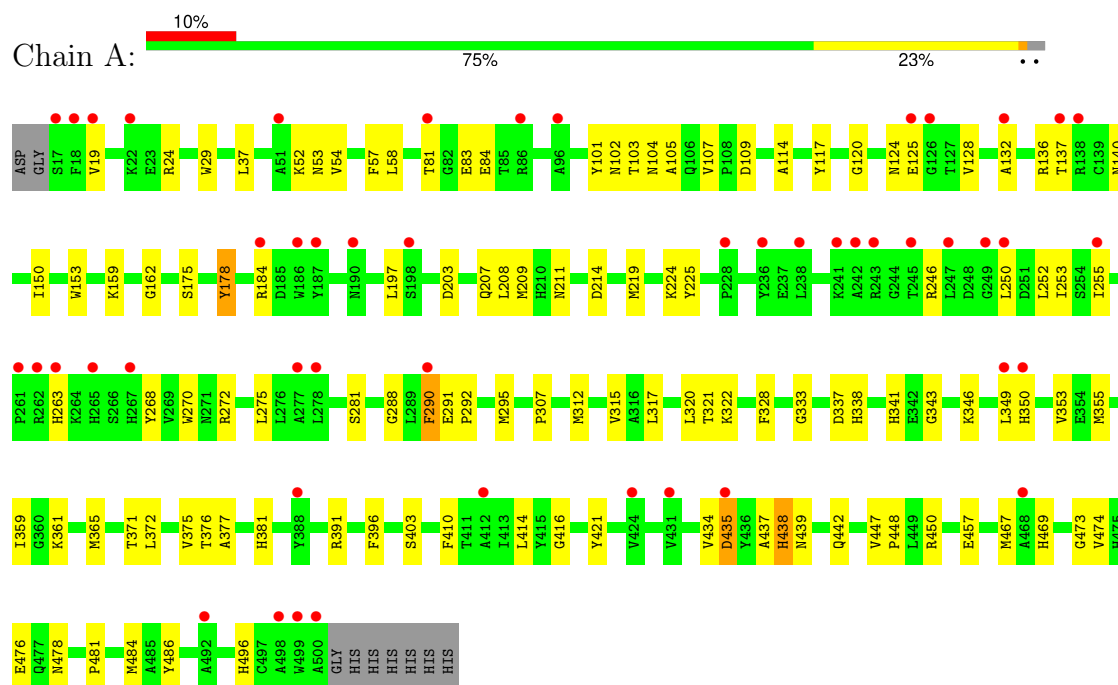
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	26	Total	O	0	0
			26	26		
13	B	20	Total	O	0	0
			20	20		
13	C	35	Total	O	0	0
			35	35		
13	D	42	Total	O	0	0
			42	42		

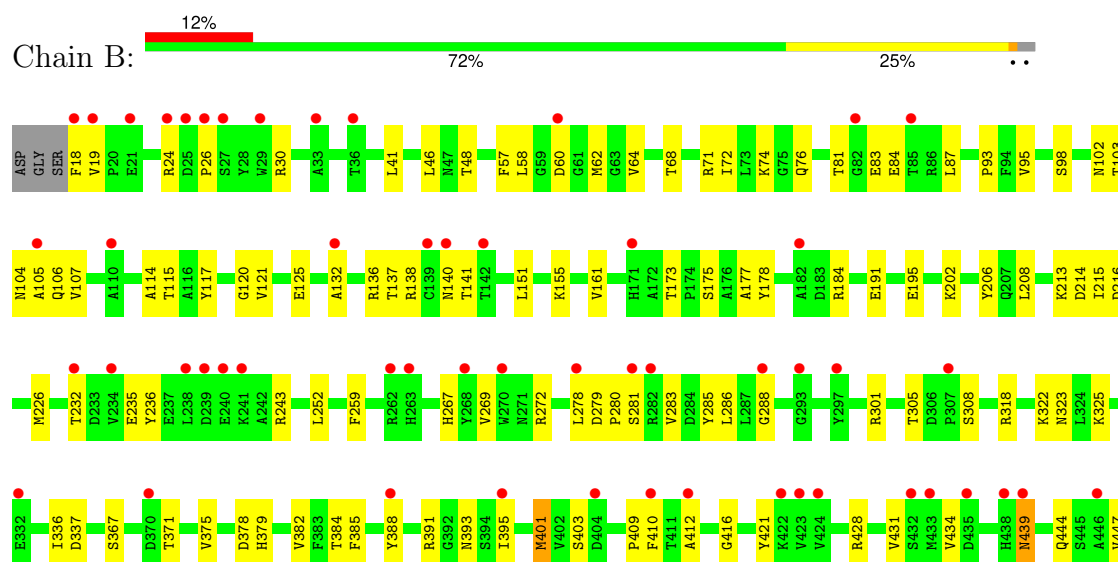
### 3 Residue-property plots

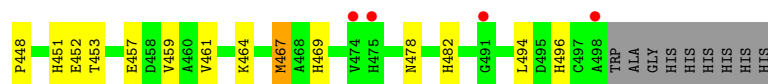
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alkaline phosphatase, tissue-nonspecific isozyme

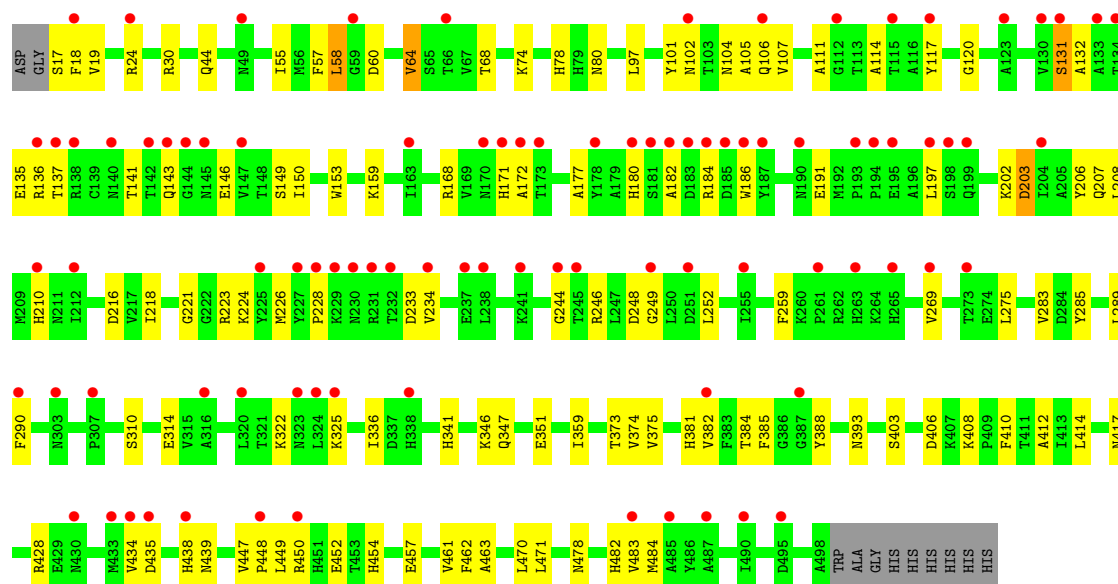
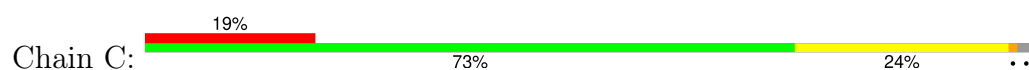


- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

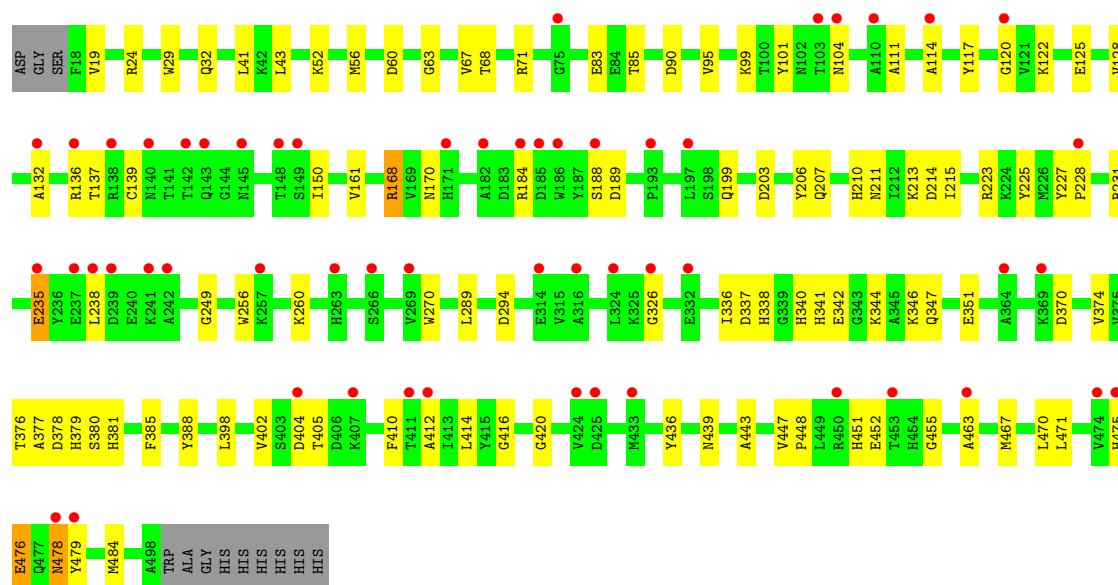
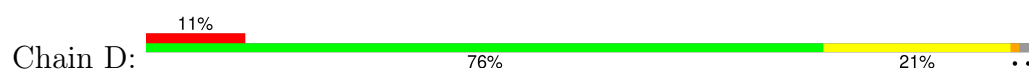





- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



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

Chain E:  80% 20%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



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

Chain G:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.86Å 119.43Å 348.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.71 38.81 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.9 (38.81-2.71) 84.4 (38.81-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.39 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.273 , 0.310 0.273 , 0.310	Depositor DCC
$R_{free}$ test set	3788 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	15598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.32% 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: PO4, FUC, MAN, FLC, GOL, ATP, BMA, ZN, MG, NAG, CA

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	0.15	0/3835	0.39	1/5197 (0.0%)
1	B	0.16	0/3819	0.37	0/5175
1	C	0.17	0/3825	0.36	0/5183
1	D	0.18	0/3819	0.40	2/5175 (0.0%)
All	All	0.17	0/15298	0.38	3/20730 (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	A	290	PHE	CB-CA-C	7.46	121.60	109.07
1	D	235	GLU	CA-C-N	6.41	132.04	123.20
1	D	235	GLU	C-N-CA	6.41	132.04	123.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3753	0	3649	84	0
1	B	3737	0	3637	101	0
1	C	3743	0	3644	89	0
1	D	3737	0	3638	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	60	0	52	0	0
3	F	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
4	G	50	0	43	2	0
5	A	31	0	12	3	0
5	B	31	0	12	1	0
5	C	31	0	12	4	0
5	D	31	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	12	0	16	0	0
9	B	6	0	8	0	0
9	C	24	0	32	3	0
9	D	18	0	24	2	0
10	A	14	0	13	0	0
10	B	14	0	13	0	0
10	C	28	0	26	0	0
10	D	14	0	13	0	0
11	C	13	0	5	2	0
12	D	5	0	0	0	0
13	A	26	0	0	0	0
13	B	20	0	0	1	0
13	C	35	0	0	1	0
13	D	42	0	0	1	0
All	All	15598	0	14961	311	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 10.

All (311) 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:A:184:ARG:NH2	5:A:601:ATP:O3G	2.05	0.88
1:D:228:PRO:HB3	1:D:249:GLY:HA2	1.62	0.82
1:B:24:ARG:HA	1:C:132:ALA:HB3	1.62	0.81
1:A:132:ALA:HB3	1:D:24:ARG:HA	1.64	0.80
1:D:56:MET:HB2	1:D:484:MET:HE1	1.68	0.75
1:B:235:GLU:HG2	1:B:236:TYR:CE1	2.21	0.74
1:B:457:GLU:HA	1:C:68:THR:HG21	1.68	0.74
1:C:135:GLU:HG3	1:C:141:THR:HG21	1.70	0.74
1:A:57:PHE:HB2	1:A:375:VAL:HG22	1.71	0.73
1:A:24:ARG:HA	1:D:132:ALA:HB3	1.70	0.72
1:C:203:ASP:OD1	1:C:203:ASP:N	2.24	0.70
1:B:76:GLN:NE2	1:B:393:ASN:O	2.24	0.70
1:B:19:VAL:HG22	1:C:104:ASN:HB3	1.73	0.69
1:D:117:TYR:HE2	1:D:378:ASP:HB3	1.58	0.68
1:C:463:ALA:HB2	1:C:471:LEU:HD12	1.77	0.66
1:B:132:ALA:HB3	1:C:24:ARG:HA	1.78	0.66
1:B:62:MET:O	13:B:701:HOH:O	2.13	0.66
1:A:104:ASN:HB3	1:D:19:VAL:HG22	1.78	0.65
1:B:482:HIS:HE1	1:C:30:ARG:HA	1.62	0.65
1:D:374:VAL:HB	1:D:484:MET:HE3	1.78	0.65
1:D:337:ASP:OD1	1:D:341:HIS:CD2	2.50	0.64
1:B:226:MET:HA	1:B:252:LEU:HD12	1.79	0.63
1:C:57:PHE:HB2	1:C:375:VAL:HG22	1.81	0.63
1:D:463:ALA:HB2	1:D:471:LEU:HD12	1.80	0.62
1:D:223:ARG:HH11	1:D:270:TRP:HB2	1.65	0.62
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.35	0.61
1:D:467:MET:HE3	1:D:470:LEU:HD11	1.82	0.61
1:C:228:PRO:HB3	1:C:249:GLY:HA2	1.83	0.61
1:A:457:GLU:HA	1:D:68:THR:HG21	1.83	0.61
1:B:388:TYR:CD2	5:C:602:ATP:H1'	2.36	0.61
1:A:54:VAL:HG22	1:A:372:LEU:HB3	1.83	0.60
1:A:346:LYS:HD3	1:A:439:ASN:HA	1.83	0.60
1:B:283:VAL:O	1:B:322:LYS:NZ	2.29	0.60
1:D:478:ASN:HD22	1:D:479:TYR:N	2.00	0.60
1:D:478:ASN:HD22	1:D:479:TYR:H	1.50	0.60
1:B:447:VAL:HG21	1:C:410:PHE:HB2	1.83	0.60
1:A:102:ASN:HB2	1:A:105:ALA:HB3	1.84	0.60
1:C:208:LEU:HD11	1:C:218:ILE:HD13	1.84	0.60
1:B:64:VAL:HG11	1:C:64:VAL:HG21	1.83	0.59
1:D:370:ASP:OD2	9:D:606:GOL:O2	2.16	0.59
1:A:19:VAL:HG22	1:D:104:ASN:HB3	1.83	0.59
1:A:346:LYS:NZ	1:A:437:ALA:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ARG:HB2	1:D:404:ASP:OD2	2.02	0.59
1:B:226:MET:HB3	1:B:252:LEU:HB2	1.85	0.59
1:B:107:VAL:HB	1:C:388:TYR:HA	1.85	0.58
1:B:136:ARG:HG2	1:B:137:THR:HG23	1.86	0.58
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.39	0.58
1:A:478:ASN:ND2	1:D:29:TRP:HB3	2.18	0.58
1:B:448:PRO:O	1:C:403:SER:OG	2.20	0.58
1:D:223:ARG:NH1	1:D:270:TRP:HB2	2.19	0.58
1:A:53:ASN:HB2	1:A:371:THR:HG23	1.84	0.57
1:A:410:PHE:HB2	1:D:447:VAL:HG21	1.85	0.57
1:C:347:GLN:O	1:C:351:GLU:HG2	2.04	0.57
1:C:191:GLU:N	1:C:191:GLU:OE1	2.37	0.57
1:B:216:ASP:HA	1:B:285:TYR:HD1	1.69	0.57
1:A:473:GLY:HA2	1:D:95:VAL:HG23	1.86	0.57
1:B:191:GLU:OE1	1:B:191:GLU:N	2.38	0.56
1:C:102:ASN:HB2	1:C:105:ALA:HB3	1.86	0.56
1:A:281:SER:HA	1:A:322:LYS:HD3	1.88	0.56
1:A:403:SER:OG	1:D:448:PRO:O	2.16	0.56
1:C:136:ARG:HG2	1:C:137:THR:HG23	1.87	0.56
1:C:223:ARG:NE	1:C:233:ASP:OD2	2.25	0.56
1:D:117:TYR:CE2	1:D:378:ASP:HB3	2.40	0.56
1:B:114:ALA:HA	1:B:117:TYR:CE1	2.40	0.56
1:B:104:ASN:HB3	1:C:19:VAL:HG22	1.88	0.56
1:B:184:ARG:NH1	5:B:601:ATP:O3G	2.39	0.56
1:B:384:THR:HB	1:C:382:VAL:HG12	1.87	0.56
1:D:214:ASP:OD1	1:D:214:ASP:N	2.38	0.56
1:B:403:SER:OG	1:C:448:PRO:O	2.16	0.55
1:B:57:PHE:HB2	1:B:375:VAL:HG22	1.89	0.55
1:B:279:ASP:OD2	1:B:281:SER:OG	2.25	0.55
1:D:347:GLN:O	1:D:351:GLU:HG2	2.07	0.55
1:D:125:GLU:OE1	1:D:136:ARG:NH1	2.40	0.55
1:D:136:ARG:HG2	1:D:137:THR:HG23	1.88	0.55
1:A:337:ASP:OD1	1:A:381:HIS:NE2	2.39	0.55
1:B:267:HIS:ND1	1:B:278:LEU:HD22	2.22	0.55
1:B:388:TYR:CE2	5:C:602:ATP:H1'	2.41	0.55
1:B:46:LEU:HD13	1:B:469:HIS:CD2	2.42	0.55
1:A:467:MET:HA	1:A:469:HIS:CE1	2.42	0.54
1:B:388:TYR:HB3	5:C:602:ATP:C5	2.43	0.54
1:B:388:TYR:HB3	5:C:602:ATP:C4	2.44	0.53
1:A:361:LYS:O	1:A:365:MET:HG3	2.08	0.53
1:A:184:ARG:NH2	5:A:601:ATP:O1B	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE2	1:A:359:ILE:HD11	1.90	0.53
1:D:83:GLU:OE1	1:D:83:GLU:N	2.42	0.53
1:C:60:ASP:O	1:C:336:ILE:HB	2.09	0.52
1:B:74:LYS:HD3	1:B:87:LEU:HD23	1.91	0.52
1:D:19:VAL:HB	1:D:24:ARG:NH1	2.24	0.52
1:C:19:VAL:HB	1:C:24:ARG:NH1	2.25	0.52
1:B:388:TYR:OH	1:C:341:HIS:HE1	1.93	0.52
1:B:68:THR:O	1:B:72:ILE:HG13	2.10	0.52
1:D:188:SER:HB3	1:D:225:TYR:HD1	1.74	0.52
1:B:138:ARG:O	1:B:141:THR:OG1	2.28	0.52
1:C:283:VAL:O	1:C:322:LYS:NZ	2.28	0.52
1:C:159:LYS:NZ	1:C:325:LYS:O	2.33	0.51
1:B:421:TYR:HB3	1:B:448:PRO:HB3	1.92	0.51
1:D:225:TYR:OH	13:D:701:HOH:O	2.15	0.51
1:C:80:ASN:ND2	13:C:702:HOH:O	2.33	0.51
1:A:58:LEU:O	1:A:333:GLY:N	2.40	0.51
1:D:168:ARG:HB2	1:D:170:ASN:OD1	2.10	0.51
1:A:117:TYR:HA	1:A:481:PRO:HD3	1.92	0.51
1:A:338:HIS:HA	1:A:341:HIS:HB2	1.93	0.51
1:A:447:VAL:HG21	1:D:410:PHE:HB2	1.92	0.51
1:C:248:ASP:OD2	9:C:608:GOL:O3	2.29	0.51
1:B:301:ARG:CZ	1:B:308:SER:HB3	2.41	0.51
1:D:168:ARG:NH1	1:D:294:ASP:OD2	2.44	0.51
1:A:275:LEU:HD11	1:A:315:VAL:HG11	1.93	0.50
1:D:235:GLU:HG3	1:D:270:TRP:HZ3	1.76	0.50
1:B:202:LYS:HD3	1:B:206:TYR:CE1	2.46	0.50
1:C:146:GLU:HB3	1:C:180:HIS:ND1	2.26	0.50
1:D:71:ARG:HD3	1:D:85:THR:O	2.11	0.50
1:A:214:ASP:OD1	1:A:214:ASP:N	2.44	0.50
1:A:24:ARG:NH1	1:D:132:ALA:O	2.45	0.50
1:D:184:ARG:NH2	5:D:603:ATP:O1G	2.45	0.50
1:A:250:LEU:HD22	1:A:255:ILE:HD11	1.94	0.50
4:G:2:NAG:O7	4:G:2:NAG:O3	2.22	0.50
1:C:346:LYS:HD3	1:C:439:ASN:HA	1.93	0.49
1:B:410:PHE:HB2	1:C:447:VAL:HG21	1.93	0.49
1:B:428:ARG:NH1	1:B:444:GLN:OE1	2.46	0.49
1:C:210:HIS:ND1	11:C:609:FLC:OA2	2.45	0.49
1:D:378:ASP:OD1	1:D:378:ASP:N	2.37	0.49
1:C:417:ASN:HB2	1:C:449:LEU:HD12	1.95	0.49
1:D:376:THR:OG1	1:D:377:ALA:N	2.42	0.49
1:C:111:ALA:HB2	1:C:184:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLU:HG2	1:B:236:TYR:CD1	2.47	0.48
1:C:223:ARG:NH1	1:C:289:LEU:O	2.41	0.48
1:D:101:TYR:OH	1:D:476:GLU:OE2	2.29	0.48
1:A:349:LEU:O	1:A:353:VAL:HG23	2.13	0.48
1:B:382:VAL:HG12	1:C:384:THR:HB	1.95	0.48
1:D:342:GLU:HB3	1:D:344:LYS:HE3	1.95	0.48
1:B:60:ASP:HB2	1:B:337:ASP:HB2	1.95	0.48
1:D:256:TRP:O	1:D:260:LYS:HD3	2.14	0.48
1:D:451:HIS:N	9:D:601:GOL:O3	2.45	0.48
1:A:81:THR:HG22	1:A:83:GLU:OE1	2.13	0.48
1:A:29:TRP:CE2	1:D:122:LYS:HB2	2.49	0.48
1:D:398:LEU:HG	1:D:436:TYR:CZ	2.49	0.48
1:A:101:TYR:CG	1:D:83:GLU:HB3	2.49	0.48
1:A:447:VAL:HG11	1:D:410:PHE:HB3	1.96	0.48
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.48	0.48
1:C:149:SER:OG	1:C:177:ALA:O	2.19	0.48
1:A:162:GLY:HA3	1:A:320:LEU:HD11	1.95	0.48
1:A:84:GLU:O	1:D:99:LYS:NZ	2.47	0.47
1:A:376:THR:OG1	1:A:377:ALA:N	2.46	0.47
1:B:272:ARG:N	1:B:305:THR:O	2.39	0.47
1:B:103:THR:HB	1:C:19:VAL:HG13	1.95	0.47
1:B:195:GLU:H	1:B:195:GLU:CD	2.21	0.47
1:B:26:PRO:HB2	1:B:30:ARG:NH1	2.29	0.47
1:B:401:MET:SD	1:B:401:MET:N	2.87	0.47
1:B:26:PRO:HD3	1:C:131:SER:HB3	1.96	0.47
1:B:280:PRO:HG2	1:B:318:ARG:HD3	1.96	0.47
1:B:72:ILE:HG21	1:C:106:GLN:OE1	2.15	0.47
1:B:452:GLU:HG2	1:B:453:THR:N	2.30	0.47
1:C:381:HIS:HB3	1:C:452:GLU:OE2	2.13	0.47
1:D:203:ASP:OD1	1:D:206:TYR:N	2.40	0.47
1:C:146:GLU:HB3	1:C:180:HIS:HD1	1.79	0.47
1:A:224:LYS:HE3	1:A:225:TYR:CZ	2.50	0.47
1:B:83:GLU:HB3	1:C:101:TYR:CD2	2.50	0.47
1:A:58:LEU:HD21	1:A:117:TYR:OH	2.15	0.47
1:B:46:LEU:HB3	1:B:469:HIS:CE1	2.49	0.47
1:C:226:MET:SD	1:C:252:LEU:HD12	2.55	0.47
1:B:467:MET:HE2	1:B:496:HIS:CE1	2.50	0.46
1:B:68:THR:HG21	1:C:457:GLU:HA	1.97	0.46
1:D:227:TYR:HB3	1:D:231:ARG:HD3	1.97	0.46
1:A:203:ASP:OD2	1:A:246:ARG:NH1	2.35	0.46
1:B:469:HIS:NE2	1:C:44:GLN:OE1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:VAL:HA	1:C:462:PHE:O	2.16	0.46
1:D:381:HIS:HB3	1:D:452:GLU:OE2	2.15	0.46
1:A:272:ARG:HG3	1:A:307:PRO:HB3	1.97	0.46
1:B:178:TYR:CE2	1:B:208:LEU:HD13	2.50	0.46
1:B:385:PHE:HA	1:B:412:ALA:O	2.16	0.46
1:A:54:VAL:HG12	1:A:328:PHE:HD1	1.80	0.46
1:B:367:SER:O	1:B:371:THR:HB	2.16	0.46
1:B:439:ASN:N	1:B:439:ASN:OD1	2.48	0.46
1:A:291:GLU:HG3	1:A:295:MET:HA	1.96	0.46
1:B:388:TYR:HA	1:C:107:VAL:HB	1.98	0.46
1:C:114:ALA:HA	1:C:117:TYR:CE2	2.51	0.46
1:C:223:ARG:HH12	1:C:290:PHE:C	2.24	0.46
1:C:470:LEU:HD12	1:C:483:VAL:HG13	1.98	0.46
1:D:60:ASP:O	1:D:336:ILE:HB	2.16	0.46
1:A:120:GLY:C	1:A:478:ASN:HB2	2.40	0.46
1:B:175:SER:HA	1:B:178:TYR:CZ	2.50	0.46
1:A:474:VAL:HG21	1:D:90:ASP:HA	1.97	0.45
1:C:182:ALA:HB3	1:C:186:TRP:CH2	2.51	0.45
1:A:37:LEU:HD11	1:D:470:LEU:HD13	1.98	0.45
1:C:58:LEU:HD13	1:C:117:TYR:CZ	2.51	0.45
1:B:102:ASN:HB2	1:B:105:ALA:HB3	1.98	0.45
1:D:63:GLY:O	1:D:67:VAL:HG23	2.16	0.45
1:A:224:LYS:HG2	1:A:292:PRO:O	2.16	0.45
1:C:203:ASP:OD2	1:C:246:ARG:NH2	2.41	0.45
1:D:256:TRP:CD1	1:D:260:LYS:HZ3	2.35	0.45
1:D:337:ASP:OD2	1:D:379:HIS:CE1	2.70	0.45
1:B:120:GLY:C	1:B:478:ASN:HB2	2.42	0.45
1:C:120:GLY:HA3	1:C:482:HIS:NE2	2.30	0.45
1:C:150:ILE:HA	1:C:153:TRP:CD2	2.51	0.45
1:D:346:LYS:HD3	1:D:439:ASN:HA	1.99	0.45
1:A:84:GLU:H	1:A:84:GLU:CD	2.24	0.45
1:C:374:VAL:HB	1:C:484:MET:HE2	1.99	0.45
1:A:178:TYR:CE2	1:A:208:LEU:HD13	2.52	0.45
1:A:219:MET:HE1	1:A:312:MET:O	2.16	0.44
1:A:317:LEU:O	1:A:321:THR:HG23	2.17	0.44
1:B:447:VAL:HG13	1:C:428:ARG:CZ	2.47	0.44
1:B:451:HIS:HB2	9:C:607:GOL:H12	2.00	0.44
1:D:238:LEU:HD23	1:D:238:LEU:HA	1.84	0.44
1:D:380:SER:O	1:D:455:GLY:N	2.46	0.44
1:A:107:VAL:HB	1:D:388:TYR:HA	1.99	0.44
1:A:207:GLN:HB3	1:A:211:ASN:ND2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:SER:OG	1:C:18:PHE:N	2.50	0.44
1:C:168:ARG:HA	1:C:221:GLY:C	2.43	0.44
1:C:210:HIS:ND1	11:C:609:FLC:OB1	2.51	0.44
1:A:29:TRP:HB3	1:D:478:ASN:OD1	2.18	0.44
1:B:388:TYR:HE1	1:C:454:HIS:CG	2.36	0.44
1:A:81:THR:HG21	1:A:391:ARG:HG3	2.00	0.44
1:A:476:GLU:HG3	1:D:32:GLN:OE1	2.18	0.44
1:C:385:PHE:HA	1:C:412:ALA:O	2.17	0.44
1:B:151:LEU:HD13	1:B:177:ALA:HB1	1.98	0.44
1:A:288:GLY:HA3	1:A:290:PHE:CZ	2.53	0.44
1:B:58:LEU:HD21	1:B:117:TYR:OH	2.17	0.44
1:C:171:HIS:CG	1:C:172:ALA:N	2.86	0.44
1:C:216:ASP:HA	1:C:285:TYR:CD1	2.53	0.44
1:D:270:TRP:HE1	3:J:1:NAG:H62	1.83	0.44
1:B:84:GLU:CD	1:B:84:GLU:H	2.25	0.44
1:B:95:VAL:HA	1:B:461:VAL:O	2.17	0.44
1:D:207:GLN:HB3	1:D:211:ASN:ND2	2.33	0.44
1:A:184:ARG:NH2	5:A:601:ATP:PG	2.90	0.43
1:D:385:PHE:HA	1:D:412:ALA:O	2.18	0.43
1:A:270:TRP:CZ2	3:F:1:NAG:H2	2.53	0.43
1:B:93:PRO:HD2	1:B:464:LYS:HB3	1.99	0.43
1:C:310:SER:O	1:C:314:GLU:HG3	2.18	0.43
1:D:111:ALA:HB1	1:D:128:VAL:HG13	2.00	0.43
1:D:114:ALA:HA	1:D:117:TYR:CZ	2.53	0.43
1:B:155:LYS:HE2	1:B:161:VAL:HG22	1.99	0.43
1:C:384:THR:OG1	1:C:414:LEU:O	2.27	0.43
1:D:189:ASP:OD1	1:D:189:ASP:N	2.52	0.43
1:B:269:VAL:HG22	1:B:286:LEU:HD11	2.00	0.43
1:C:55:ILE:HB	1:C:373:THR:HG23	2.01	0.43
1:D:338:HIS:HA	1:D:341:HIS:HB2	2.01	0.43
1:A:203:ASP:O	1:A:207:GLN:HG3	2.19	0.43
1:C:120:GLY:C	1:C:478:ASN:HB2	2.44	0.43
1:C:224:LYS:HB2	1:C:244:GLY:HA2	1.99	0.43
1:D:139:CYS:HB3	1:D:199:GLN:OE1	2.19	0.43
1:A:253:ILE:HG21	1:A:268:TYR:CD2	2.54	0.42
1:B:98:SER:HB3	1:B:459:VAL:HG23	2.01	0.42
1:B:409:PRO:HG2	1:B:431:VAL:HG22	2.00	0.42
1:C:450:ARG:N	9:C:601:GOL:O3	2.52	0.42
1:A:421:TYR:HB3	1:A:448:PRO:HB3	2.01	0.42
1:D:184:ARG:HH12	5:D:603:ATP:PG	2.42	0.42
1:D:210:HIS:O	1:D:213:LYS:NZ	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:NE2	1:C:393:ASN:O	2.50	0.42
1:D:43:LEU:HD23	1:D:43:LEU:HA	1.87	0.42
1:B:18:PHE:HE2	1:B:81:THR:HG21	1.85	0.42
1:B:269:VAL:O	1:B:288:GLY:HA2	2.20	0.42
1:C:461:VAL:HG11	1:C:471:LEU:HD13	2.01	0.42
1:A:178:TYR:CE1	1:A:208:LEU:HB2	2.53	0.42
1:B:125:GLU:H	1:B:125:GLU:HG3	1.71	0.42
1:A:101:TYR:CD1	1:D:83:GLU:HB3	2.54	0.42
1:A:128:VAL:HG11	1:A:175:SER:OG	2.20	0.42
1:C:74:LYS:O	1:C:78:HIS:ND1	2.47	0.42
1:C:150:ILE:HA	1:C:153:TRP:CE3	2.55	0.42
1:B:391:ARG:HB2	1:C:104:ASN:HA	2.01	0.42
1:C:434:VAL:HG12	1:C:435:ASP:N	2.35	0.42
1:B:115:THR:HG22	1:B:121:VAL:O	2.20	0.42
1:A:136:ARG:HG2	1:A:137:THR:HG23	2.01	0.41
1:D:104:ASN:HD21	1:D:125:GLU:H	1.67	0.41
1:A:54:VAL:HG13	1:A:484:MET:HE2	2.02	0.41
1:A:140:ASN:OD1	1:A:140:ASN:N	2.53	0.41
1:A:448:PRO:HB2	1:D:405:THR:HG21	2.02	0.41
1:A:346:LYS:HG3	1:A:396:PHE:CZ	2.55	0.41
1:B:416:GLY:O	1:C:414:LEU:HD13	2.20	0.41
1:C:97:LEU:HD23	1:C:97:LEU:HA	1.88	0.41
1:A:343:GLY:O	1:A:442:GLN:HA	2.21	0.41
1:B:232:THR:HG22	1:B:243:ARG:NH1	2.35	0.41
1:B:232:THR:HG22	1:B:243:ARG:HH12	1.85	0.41
1:C:202:LYS:HE2	1:C:206:TYR:CE2	2.55	0.41
1:C:202:LYS:HB2	1:C:207:GLN:HE21	1.86	0.41
1:D:136:ARG:O	1:D:137:THR:OG1	2.34	0.41
1:D:340:HIS:O	1:D:452:GLU:HB3	2.21	0.41
1:B:60:ASP:O	1:B:336:ILE:HB	2.21	0.41
1:B:323:ASN:OD1	1:B:325:LYS:HE3	2.21	0.41
1:B:175:SER:HA	1:B:178:TYR:CE2	2.56	0.41
1:B:213:LYS:HB3	1:B:259:PHE:HB3	2.03	0.41
1:B:235:GLU:CG	1:B:236:TYR:CE1	2.98	0.41
1:C:228:PRO:HA	1:C:246:ARG:HB2	2.03	0.41
1:D:161:VAL:HG23	1:D:215:ILE:HA	2.03	0.41
4:G:2:NAG:HO3	4:G:2:NAG:C7	2.27	0.41
1:A:52:LYS:O	1:A:159:LYS:NZ	2.53	0.41
1:A:150:ILE:HA	1:A:153:TRP:CD2	2.56	0.41
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.94	0.41
1:A:486:TYR:CZ	1:A:496:HIS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASP:OD1	1:B:214:ASP:N	2.51	0.41
1:B:216:ASP:HA	1:B:285:TYR:CD1	2.54	0.41
1:B:395:ILE:HD13	1:B:395:ILE:HA	1.79	0.41
1:C:269:VAL:HG21	1:C:275:LEU:HB2	2.02	0.41
1:C:406:ASP:O	1:C:408:LYS:HE3	2.20	0.41
1:D:120:GLY:O	1:D:478:ASN:HB2	2.20	0.41
1:B:41:LEU:HD23	1:C:470:LEU:HD21	2.01	0.41
1:B:60:ASP:OD1	1:B:60:ASP:N	2.54	0.41
1:C:359:ILE:HD13	1:C:375:VAL:HG21	2.02	0.41
1:D:223:ARG:HD3	1:D:289:LEU:O	2.20	0.41
1:A:416:GLY:O	1:D:414:LEU:HD13	2.21	0.40
1:A:435:ASP:O	1:A:438:HIS:HB2	2.21	0.40
1:B:68:THR:HG23	1:B:71:ARG:NH1	2.36	0.40
1:B:279:ASP:O	1:B:283:VAL:HG23	2.21	0.40
1:D:41:LEU:HD23	1:D:41:LEU:HA	1.90	0.40
1:D:420:GLY:HA3	1:D:443:ALA:O	2.21	0.40
1:A:209:MET:HG3	1:A:252:LEU:HB3	2.03	0.40
1:B:378:ASP:OD1	1:B:379:HIS:N	2.54	0.40
1:A:103:THR:OG1	1:A:124:ASN:OD1	2.39	0.40
1:D:52:LYS:O	1:D:326:GLY:HA3	2.22	0.40
1:A:109:ASP:HB3	1:A:125:GLU:OE2	2.22	0.40
1:A:414:LEU:HD13	1:D:416:GLY:O	2.20	0.40
1:B:161:VAL:HG23	1:B:215:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

## 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	482/493 (98%)	451 (94%)	30 (6%)	1 (0%)	43 66
1	B	479/493 (97%)	448 (94%)	30 (6%)	1 (0%)	43 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	480/493 (97%)	461 (96%)	19 (4%)	0	100	100
1	D	479/493 (97%)	455 (95%)	23 (5%)	1 (0%)	43	66
All	All	1920/1972 (97%)	1815 (94%)	102 (5%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	476	GLU
1	B	140	ASN
1	A	178	TYR

### 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	397/405 (98%)	392 (99%)	5 (1%)	61	81
1	B	396/405 (98%)	389 (98%)	7 (2%)	51	76
1	C	397/405 (98%)	388 (98%)	9 (2%)	44	71
1	D	396/405 (98%)	391 (99%)	5 (1%)	61	81
All	All	1586/1620 (98%)	1560 (98%)	26 (2%)	55	78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	350	HIS
1	A	434	VAL
1	A	435	ASP
1	A	438	HIS
1	B	48	THR
1	B	173	THR
1	B	401	MET
1	B	434	VAL

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Mol	Chain	Res	Type
1	B	439	ASN
1	B	467	MET
1	B	494	LEU
1	C	58	LEU
1	C	64	VAL
1	C	131	SER
1	C	143	GLN
1	C	197	LEU
1	C	203	ASP
1	C	234	VAL
1	C	259	PHE
1	C	438	HIS
1	D	150	ILE
1	D	168	ARG
1	D	402	VAL
1	D	475	HIS
1	D	478	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	171	HIS
1	A	350	HIS
1	B	44	GLN
1	B	47	ASN
1	B	190	ASN
1	B	475	HIS
1	B	477	GLN
1	B	478	ASN
1	B	482	HIS
1	C	180	HIS
1	C	300	ASN
1	C	393	ASN
1	C	440	ASN
1	D	49	ASN
1	D	171	HIS
1	D	211	ASN
1	D	393	ASN
1	D	493	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 ⓘ

17 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
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.32	0	17,19,21	0.50	0
2	BMA	E	3	2	11,11,12	0.68	0	15,15,17	0.75	0
2	MAN	E	4	2	11,11,12	0.74	0	15,15,17	1.29	2 (13%)
2	FUC	E	5	2	10,10,11	0.78	0	14,14,16	0.93	0
3	NAG	F	1	1,3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.64	1 (7%)	17,19,21	0.45	0
4	NAG	G	1	4,1	14,14,15	0.32	0	17,19,21	0.80	1 (5%)
4	NAG	G	2	4	14,14,15	0.49	0	17,19,21	0.74	1 (5%)
4	BMA	G	3	4	11,11,12	0.98	1 (9%)	15,15,17	1.29	2 (13%)
4	MAN	G	4	4	11,11,12	0.60	0	15,15,17	1.27	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.37	0	17,19,21	0.46	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.48	0	17,19,21	0.57	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	J	1	1,3	14,14,15	0.60	1 (7%)	17,19,21	0.74	0
3	NAG	J	2	3	14,14,15	0.19	0	17,19,21	0.50	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	FUC	E	5	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	O5-C1	-2.10	1.40	1.43
3	F	2	NAG	C1-C2	2.09	1.55	1.52
4	G	3	BMA	O5-C1	-2.07	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	4.16	117.77	112.19
4	G	4	MAN	C1-O5-C5	3.90	117.41	112.19
4	G	3	BMA	C3-C4-C5	2.97	115.62	110.23
4	G	1	NAG	C1-O5-C5	2.63	115.71	112.19
3	H	2	NAG	C1-O5-C5	2.23	115.17	112.19
4	G	2	NAG	C2-N2-C7	2.20	125.85	122.90
4	G	3	BMA	C2-C3-C4	2.20	114.73	110.86
2	E	4	MAN	O2-C2-C3	-2.15	105.70	110.15
4	G	4	MAN	O2-C2-C3	-2.08	105.84	110.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

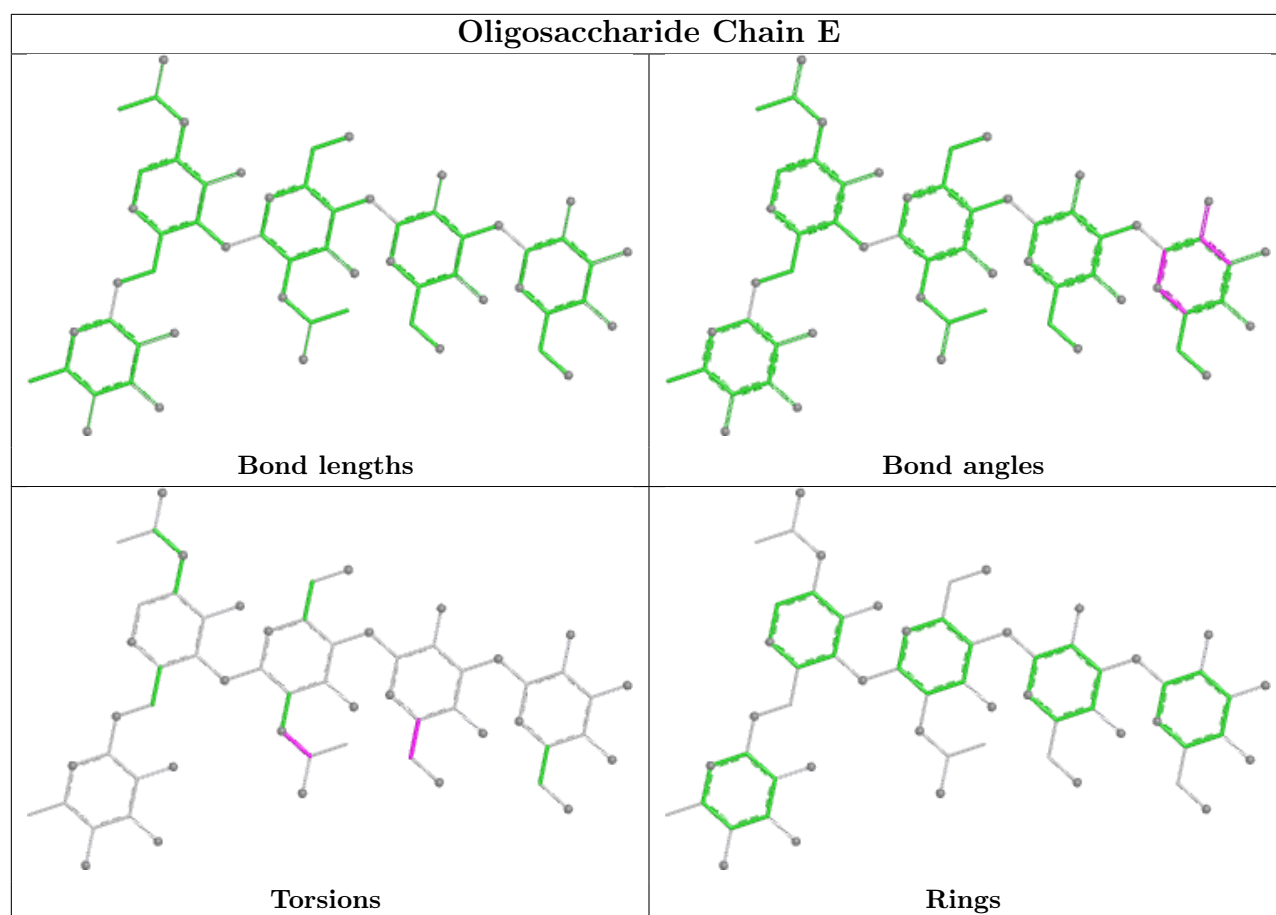
Mol	Chain	Res	Type	Atoms
3	J	1	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7

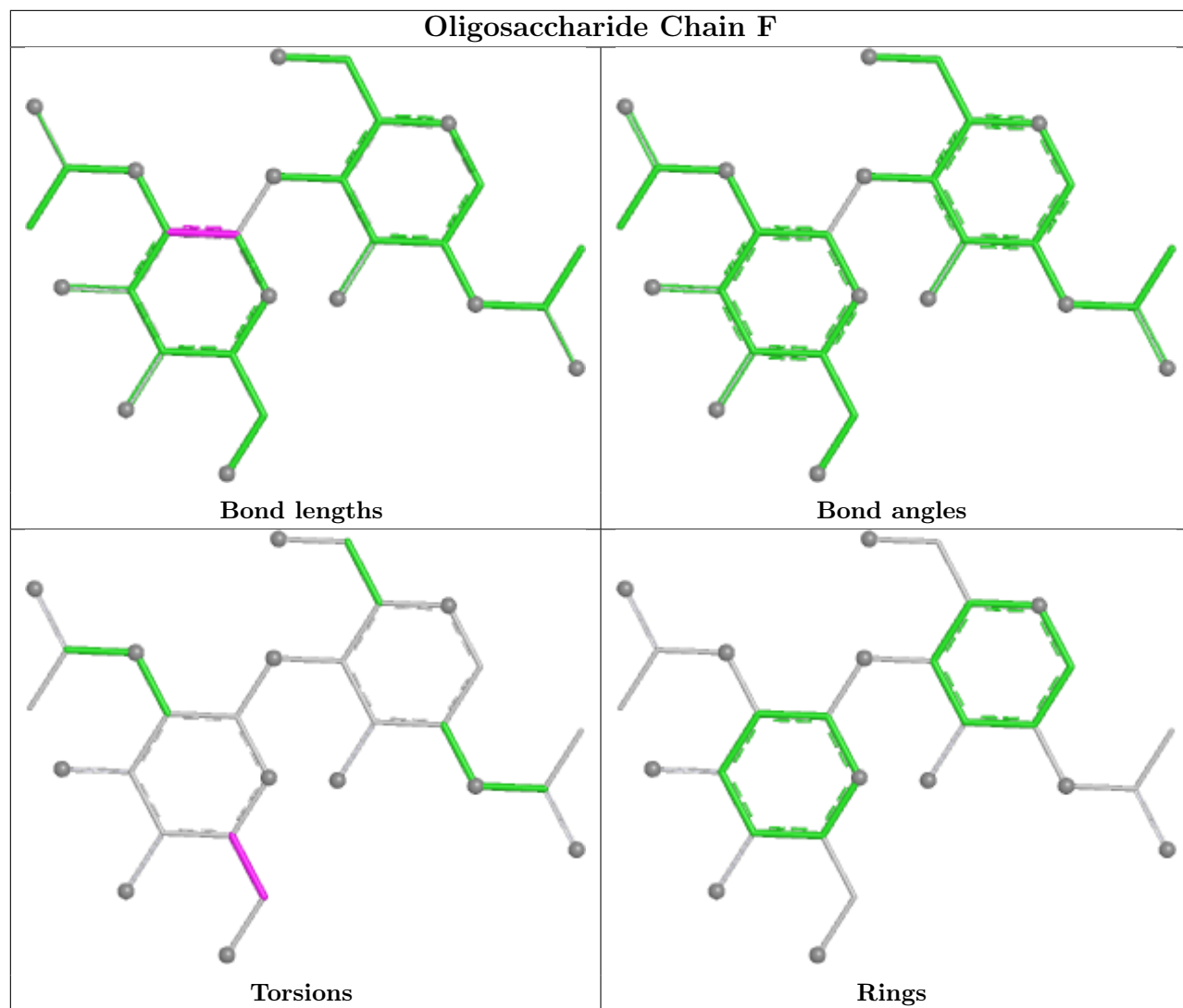
There are no ring outliers.

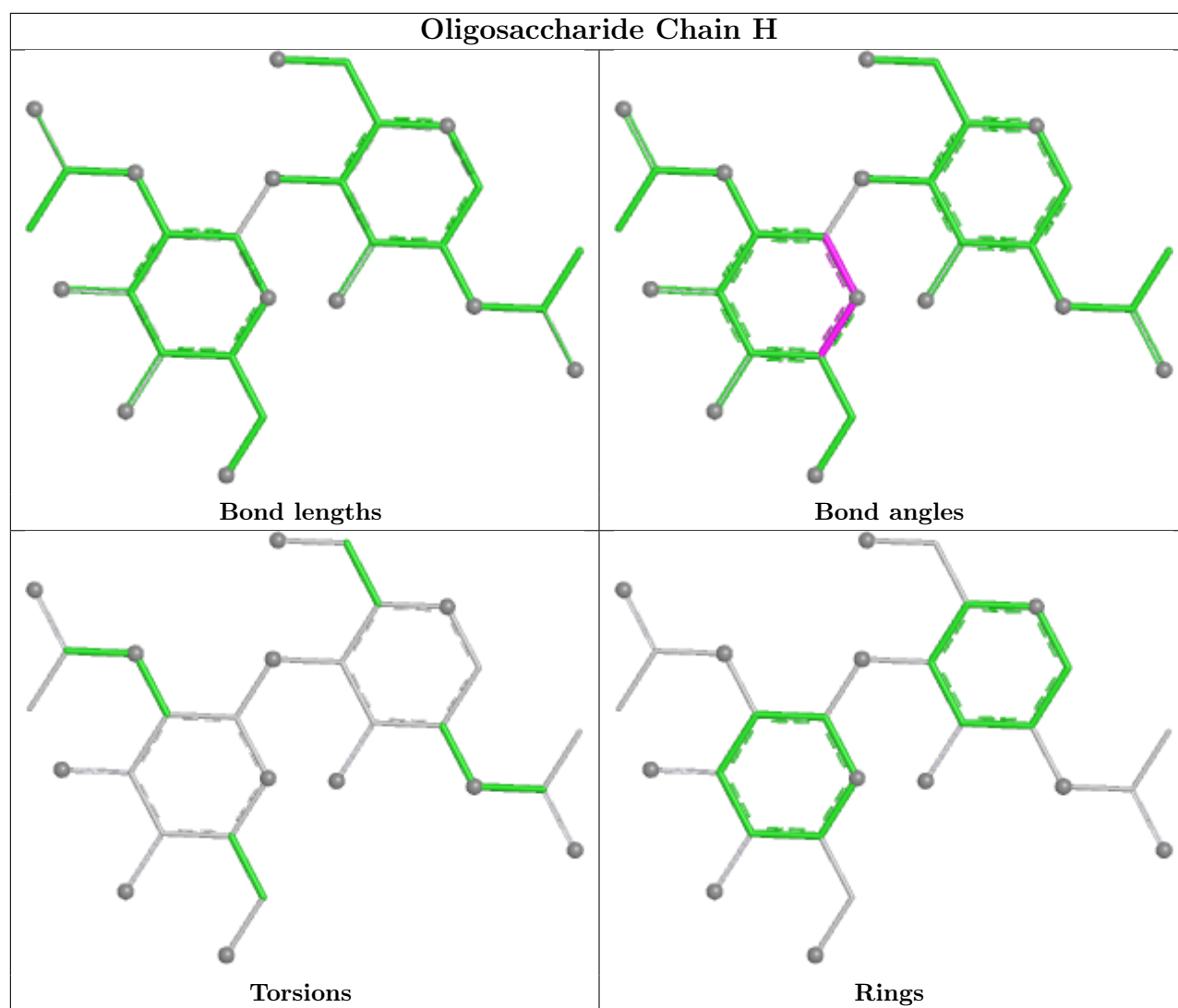
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	2	0
3	J	1	NAG	1	0
3	F	1	NAG	1	0

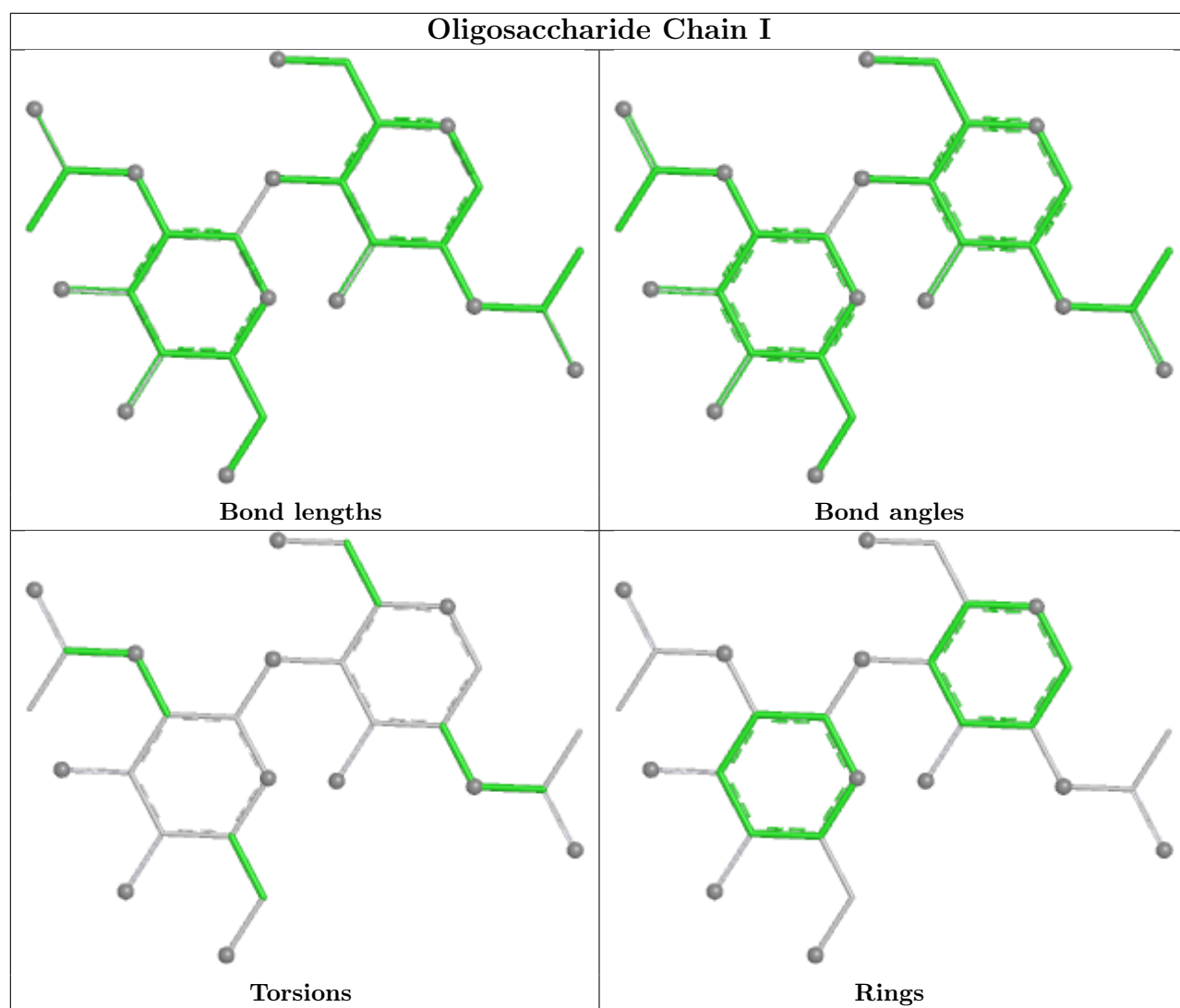
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

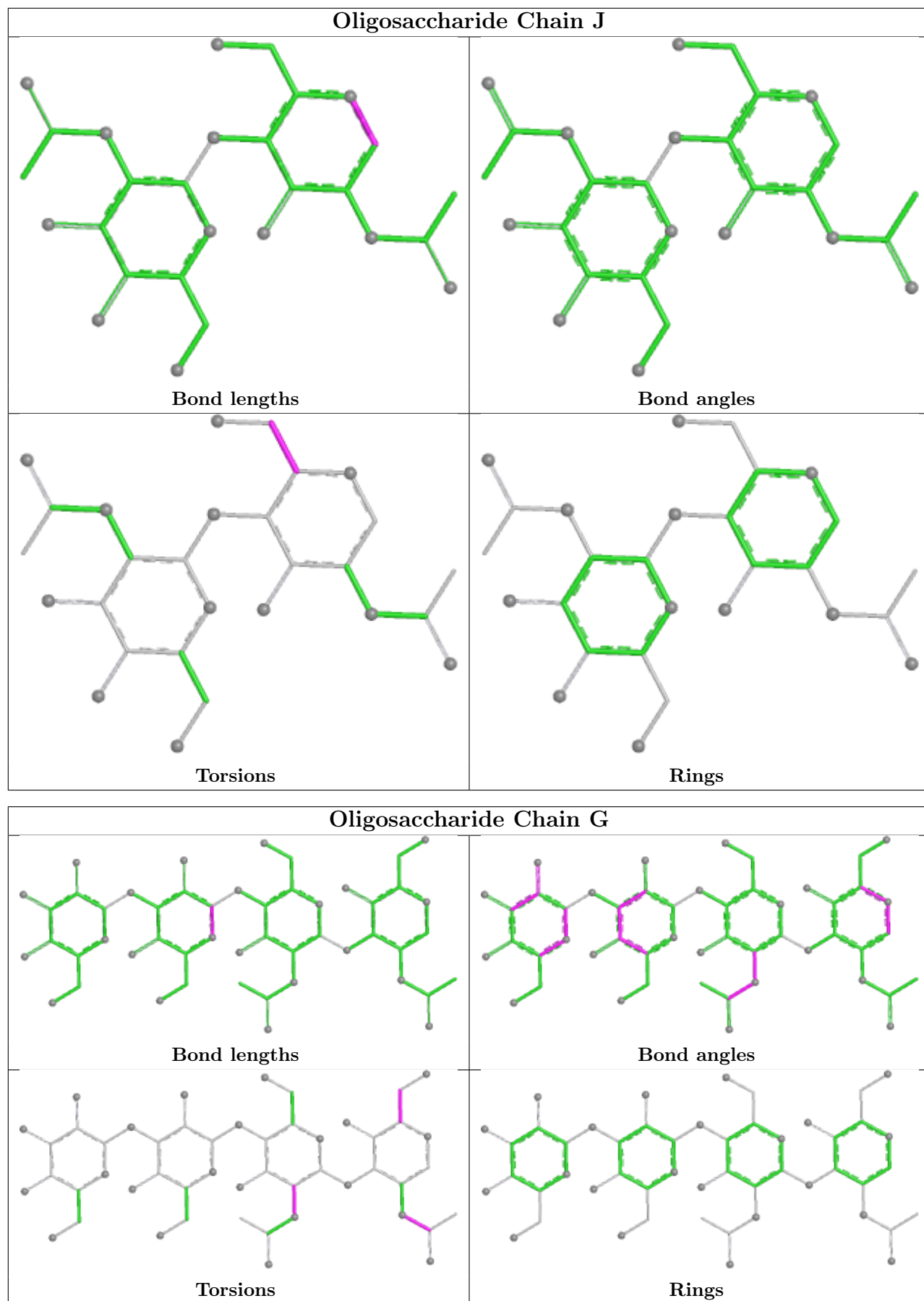












## 5.6 Ligand geometry

Of 32 ligands modelled in this entry, 11 are monoatomic - leaving 21 for Mogul analysis.

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
10	NAG	D	608	1	14,14,15	0.36	0	17,19,21	0.49	0
10	NAG	A	606	1	14,14,15	0.21	0	17,19,21	0.59	0
12	PO4	D	602	-	4,4,4	0.94	0	6,6,6	0.56	0
5	ATP	D	603	6	32,33,33	0.41	0	48,52,52	0.31	0
5	ATP	B	601	6	32,33,33	0.29	0	48,52,52	0.39	0
9	GOL	C	606	-	5,5,5	0.90	0	5,5,5	1.08	0
10	NAG	C	611	-	14,14,15	0.68	1 (7%)	17,19,21	0.49	0
9	GOL	D	607	-	5,5,5	0.79	0	5,5,5	1.20	1 (20%)
9	GOL	A	605	-	5,5,5	0.87	0	5,5,5	1.10	0
9	GOL	B	605	-	5,5,5	0.99	0	5,5,5	1.01	0
5	ATP	A	601	6	32,33,33	0.37	0	48,52,52	0.46	0
11	FLC	C	609	-	12,12,12	1.94	6 (50%)	17,17,17	2.18	6 (35%)
10	NAG	B	606	1	14,14,15	0.27	0	17,19,21	0.43	0
9	GOL	C	607	-	5,5,5	0.92	0	5,5,5	1.15	0
9	GOL	C	601	-	5,5,5	0.92	0	5,5,5	1.20	1 (20%)
9	GOL	D	606	-	5,5,5	0.88	0	5,5,5	1.09	0
5	ATP	C	602	6	32,33,33	0.31	0	48,52,52	0.49	0
9	GOL	C	608	-	5,5,5	0.90	0	5,5,5	1.36	1 (20%)
9	GOL	D	601	-	5,5,5	0.91	0	5,5,5	1.12	0
10	NAG	C	610	-	14,14,15	0.51	0	17,19,21	0.56	0
9	GOL	A	607	-	5,5,5	0.93	0	5,5,5	1.11	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
10	NAG	D	608	1	-	0/6/23/26	0/1/1/1
10	NAG	A	606	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	D	603	6	-	3/22/38/38	0/3/3/3
5	ATP	B	601	6	-	6/22/38/38	0/3/3/3
9	GOL	C	606	-	-	2/4/4/4	-
10	NAG	C	611	-	-	2/6/23/26	0/1/1/1
9	GOL	D	607	-	-	2/4/4/4	-
9	GOL	A	605	-	-	1/4/4/4	-
9	GOL	B	605	-	-	0/4/4/4	-
5	ATP	A	601	6	-	6/22/38/38	0/3/3/3
11	FLC	C	609	-	-	3/16/16/16	-
10	NAG	B	606	1	-	1/6/23/26	0/1/1/1
9	GOL	C	607	-	-	0/4/4/4	-
9	GOL	C	601	-	-	4/4/4/4	-
9	GOL	D	606	-	-	1/4/4/4	-
5	ATP	C	602	6	-	4/22/38/38	0/3/3/3
9	GOL	C	608	-	-	0/4/4/4	-
9	GOL	D	601	-	-	0/4/4/4	-
10	NAG	C	610	-	-	0/6/23/26	0/1/1/1
9	GOL	A	607	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	609	FLC	OB1-CBC	2.87	1.31	1.22
11	C	609	FLC	OA1-CAC	2.81	1.31	1.22
11	C	609	FLC	OA2-CAC	-2.79	1.21	1.30
11	C	609	FLC	OG1-CGC	2.70	1.30	1.22
11	C	609	FLC	OG2-CGC	-2.69	1.21	1.30
11	C	609	FLC	OB2-CBC	-2.54	1.21	1.30
10	C	611	NAG	O5-C1	-2.38	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	609	FLC	OB2-CBC-CB	4.76	122.27	113.14
11	C	609	FLC	OB1-CBC-CB	-4.53	113.32	122.09
11	C	609	FLC	OG1-CGC-CG	-3.42	113.28	122.95
11	C	609	FLC	OA1-CAC-CA	-3.21	113.87	122.95
11	C	609	FLC	OG2-CGC-CG	2.84	123.36	114.35
11	C	609	FLC	OA2-CAC-CA	2.62	122.64	114.35
9	C	608	GOL	C3-C2-C1	-2.29	103.39	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	601	GOL	C3-C2-C1	-2.20	103.71	111.80
9	D	607	GOL	C3-C2-C1	-2.11	104.06	111.80

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	ATP	PB-O3B-PG-O3G
5	A	601	ATP	C5'-O5'-PA-O2A
5	A	601	ATP	C5'-O5'-PA-O3A
5	D	603	ATP	C5'-O5'-PA-O2A
5	D	603	ATP	C5'-O5'-PA-O3A
5	D	603	ATP	C4'-C5'-O5'-PA
9	C	601	GOL	C1-C2-C3-O3
9	D	607	GOL	C1-C2-C3-O3
10	A	606	NAG	C4-C5-C6-O6
10	A	606	NAG	O5-C5-C6-O6
10	C	611	NAG	O5-C5-C6-O6
5	A	601	ATP	O4'-C4'-C5'-O5'
10	C	611	NAG	C4-C5-C6-O6
5	B	601	ATP	O4'-C1'-N9-C8
9	C	601	GOL	O1-C1-C2-O2
5	B	601	ATP	O4'-C1'-N9-C4
11	C	609	FLC	CAC-CA-CB-OHB
5	A	601	ATP	C3'-C4'-C5'-O5'
9	A	607	GOL	O1-C1-C2-C3
9	C	601	GOL	O1-C1-C2-C3
9	C	606	GOL	C1-C2-C3-O3
9	D	606	GOL	O1-C1-C2-C3
9	C	601	GOL	O2-C2-C3-O3
9	C	606	GOL	O2-C2-C3-O3
11	C	609	FLC	CAC-CA-CB-CBC
9	A	607	GOL	O1-C1-C2-O2
5	B	601	ATP	O4'-C4'-C5'-O5'
9	D	607	GOL	O2-C2-C3-O3
5	C	602	ATP	C4'-C5'-O5'-PA
11	C	609	FLC	CAC-CA-CB-CG
5	C	602	ATP	PB-O3A-PA-O5'
9	A	605	GOL	O2-C2-C3-O3
5	B	601	ATP	C4'-C5'-O5'-PA
10	B	606	NAG	C4-C5-C6-O6
5	C	602	ATP	PA-O3A-PB-O2B

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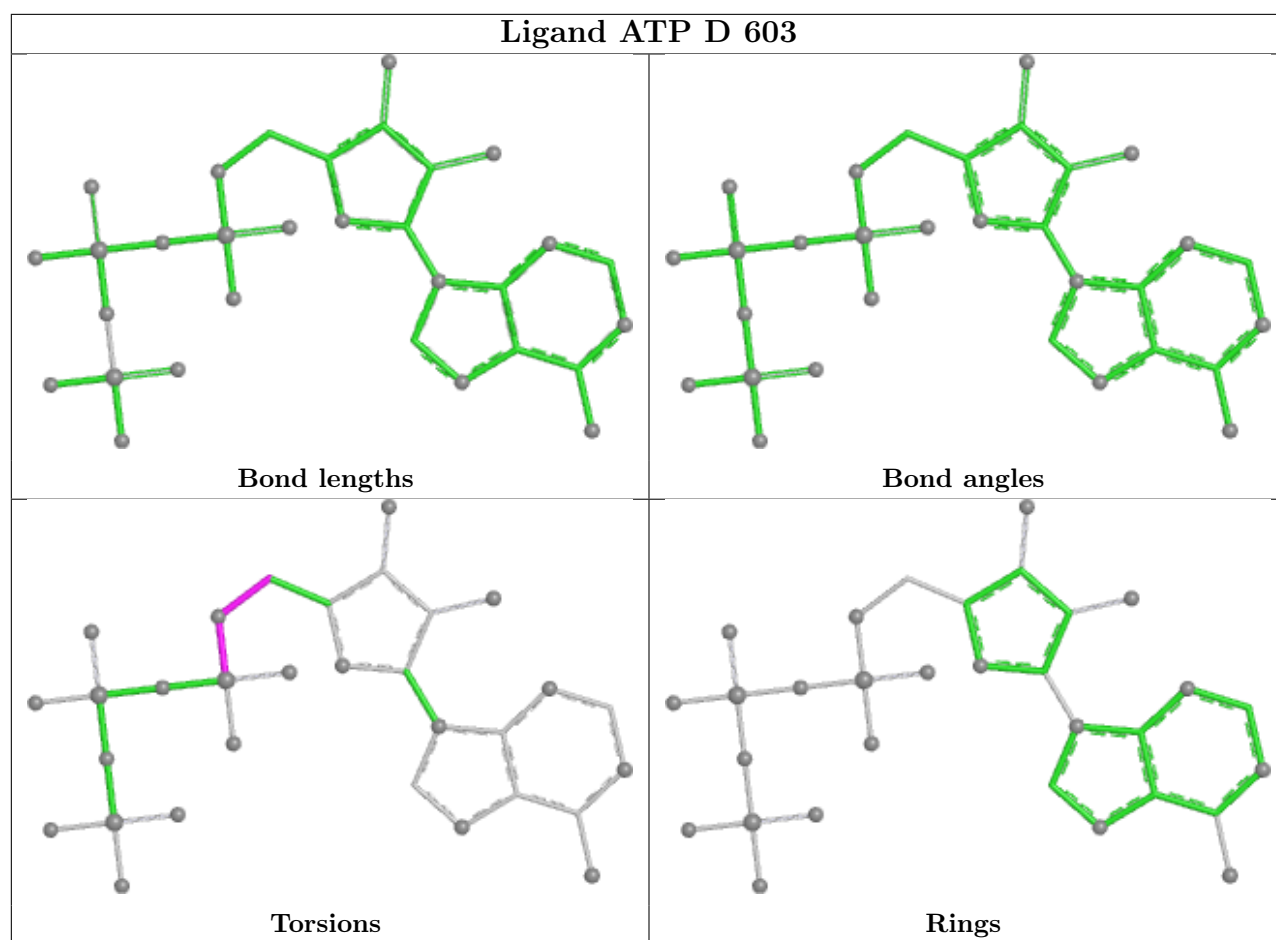
Mol	Chain	Res	Type	Atoms
5	B	601	ATP	PG-O3B-PB-O2B
5	C	602	ATP	O4'-C4'-C5'-O5'
5	A	601	ATP	O4'-C1'-N9-C8
5	B	601	ATP	PA-O3A-PB-O2B

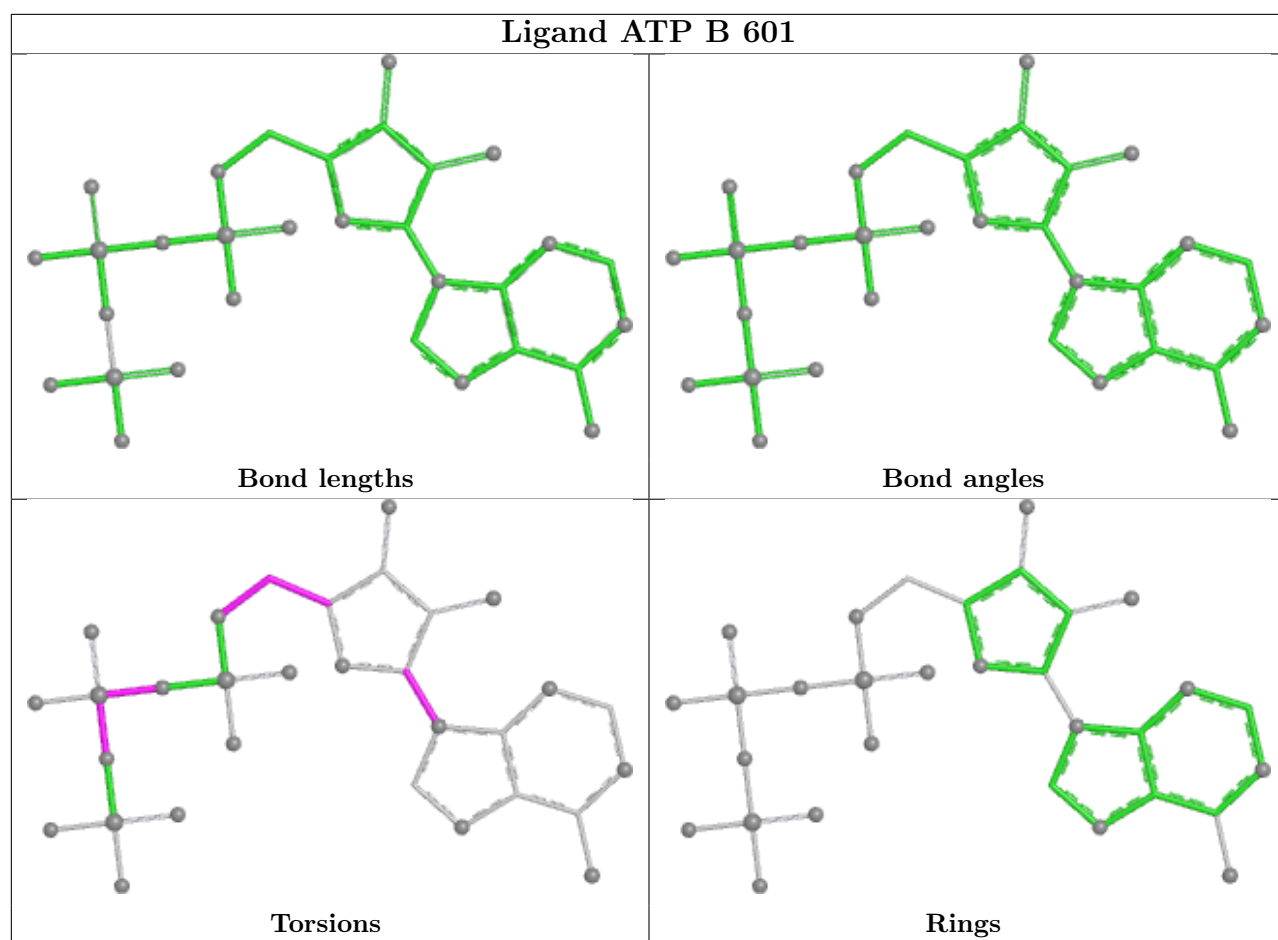
There are no ring outliers.

10 monomers are involved in 17 short contacts:

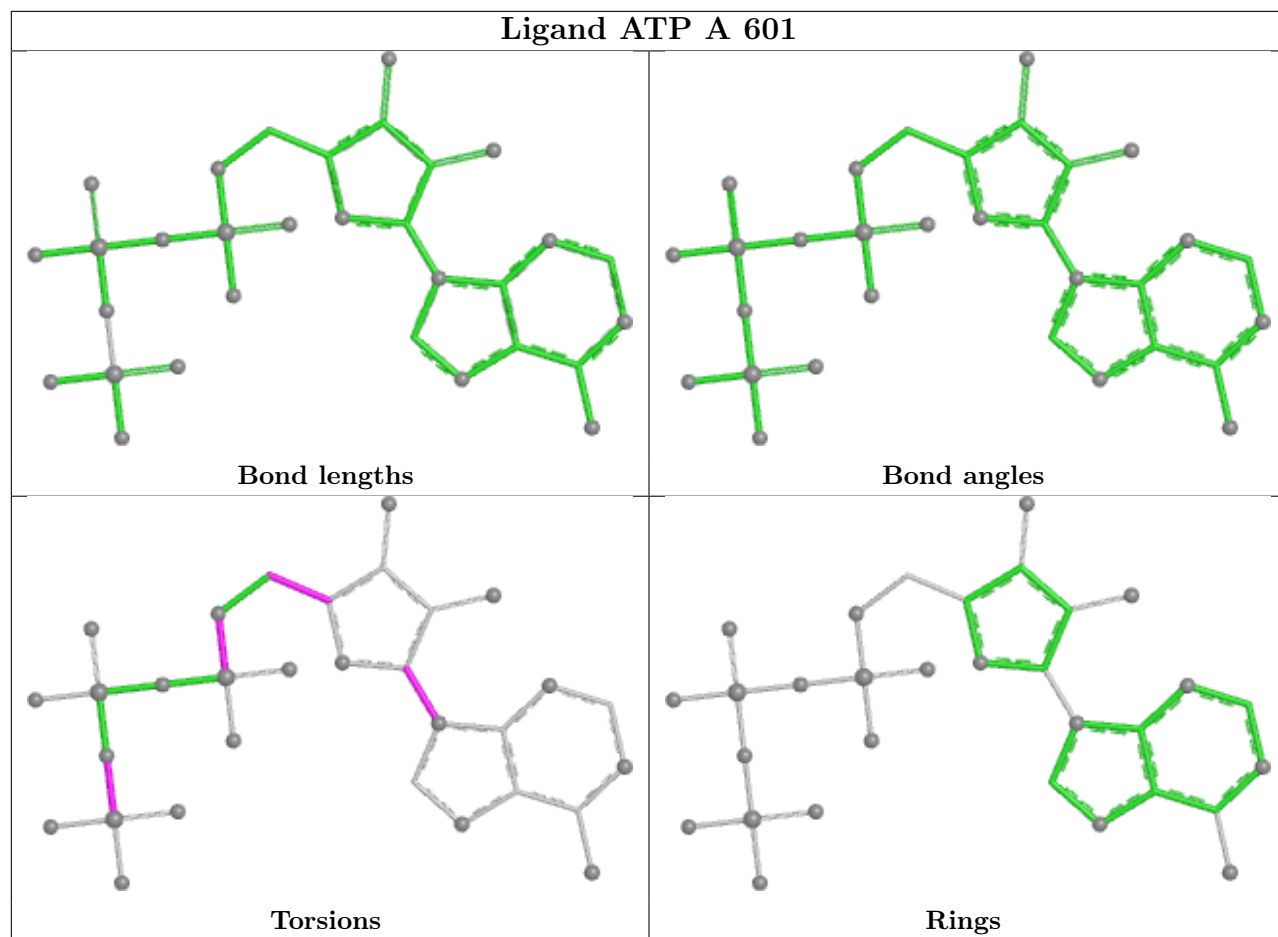
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	603	ATP	2	0
5	B	601	ATP	1	0
5	A	601	ATP	3	0
11	C	609	FLC	2	0
9	C	607	GOL	1	0
9	C	601	GOL	1	0
9	D	606	GOL	1	0
5	C	602	ATP	4	0
9	C	608	GOL	1	0
9	D	601	GOL	1	0

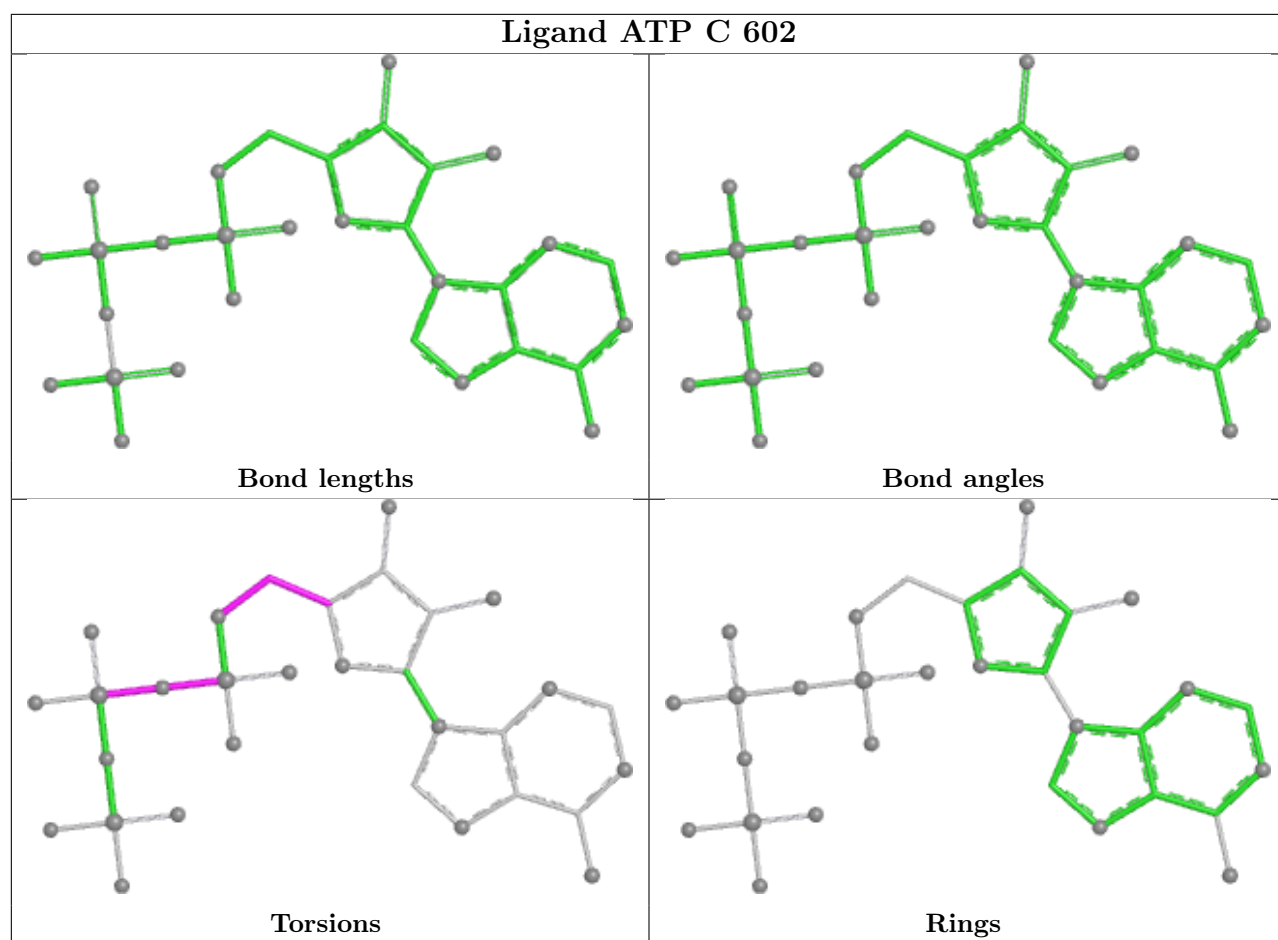
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	484/493 (98%)	1.05	49 (10%)	12 11	28, 46, 63, 81	0
1	B	481/493 (97%)	1.12	58 (12%)	8 8	27, 46, 65, 84	0
1	C	482/493 (97%)	1.31	92 (19%)	3 3	25, 50, 70, 86	0
1	D	481/493 (97%)	1.08	55 (11%)	10 9	29, 46, 62, 78	0
All	All	1928/1972 (97%)	1.14	254 (13%)	7 6	25, 47, 66, 86	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	ALA	6.2
1	A	500	ALA	4.9
1	A	499	TRP	4.6
1	C	238	LEU	4.2
1	A	17	SER	4.2
1	B	433	MET	4.0
1	B	498	ALA	3.9
1	A	18	PHE	3.8
1	B	18	PHE	3.8
1	C	433	MET	3.8
1	B	19	VAL	3.8
1	C	230	ASN	3.7
1	A	86	ARG	3.7
1	C	324	LEU	3.6
1	C	187	TYR	3.5
1	C	245	THR	3.4
1	B	435	ASP	3.4
1	C	183	ASP	3.4
1	C	241	LYS	3.4
1	D	425	ASP	3.4
1	C	263	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	320	LEU	3.3
1	A	19	VAL	3.3
1	B	241	LYS	3.3
1	C	303	ASN	3.3
1	B	24	ARG	3.2
1	C	229	LYS	3.2
1	A	242	ALA	3.2
1	C	145	ASN	3.1
1	D	140	ASN	3.1
1	B	26	PRO	3.1
1	C	171	HIS	3.1
1	C	193	PRO	3.1
1	A	468	ALA	3.1
1	B	33	ALA	3.1
1	B	282	ARG	3.1
1	D	433	MET	3.1
1	C	180	HIS	3.1
1	C	195	GLU	3.1
1	C	194	PRO	3.1
1	D	326	GLY	3.1
1	A	125	GLU	3.0
1	B	263	HIS	3.0
1	C	199	GLN	3.0
1	B	238	LEU	3.0
1	C	212	ILE	3.0
1	A	132	ALA	3.0
1	C	172	ALA	3.0
1	D	182	ALA	3.0
1	D	424	VAL	3.0
1	C	490	ILE	3.0
1	A	424	VAL	3.0
1	B	439	ASN	2.9
1	D	136	ARG	2.9
1	C	144	GLY	2.9
1	B	412	ALA	2.9
1	A	262	ARG	2.9
1	C	186	TRP	2.9
1	C	130	VAL	2.9
1	B	21	GLU	2.8
1	C	133	ALA	2.8
1	A	267	HIS	2.8
1	C	237	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	29	TRP	2.8
1	C	244	GLY	2.8
1	A	278	LEU	2.8
1	C	232	THR	2.8
1	D	263	HIS	2.8
1	B	438	HIS	2.8
1	C	163	ILE	2.8
1	C	198	SER	2.8
1	C	170	ASN	2.8
1	A	137	THR	2.8
1	B	110	ALA	2.8
1	C	182	ALA	2.8
1	C	450	ARG	2.8
1	B	82	GLY	2.7
1	C	265	HIS	2.7
1	A	277	ALA	2.7
1	C	269	VAL	2.7
1	D	235	GLU	2.7
1	B	262	ARG	2.7
1	A	388	TYR	2.7
1	A	81	THR	2.7
1	D	316	ALA	2.7
1	A	435	ASP	2.7
1	B	270	TRP	2.7
1	D	186	TRP	2.7
1	D	266	SER	2.7
1	C	234	VAL	2.7
1	D	238	LEU	2.6
1	B	297	TYR	2.6
1	C	227	TYR	2.6
1	B	446	ALA	2.6
1	C	273	THR	2.6
1	C	290	PHE	2.6
1	D	103	THR	2.6
1	D	148	THR	2.6
1	D	228	PRO	2.6
1	C	106	GLN	2.6
1	C	438	HIS	2.6
1	A	245	THR	2.6
1	C	184	ARG	2.6
1	B	288	GLY	2.6
1	B	139	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	132	ALA	2.6
1	D	242	ALA	2.6
1	A	241	LYS	2.5
1	B	422	LYS	2.5
1	B	60	ASP	2.5
1	C	435	ASP	2.5
1	D	171	HIS	2.5
1	D	75	GLY	2.5
1	C	18	PHE	2.5
1	C	181	SER	2.5
1	B	404	ASP	2.5
1	A	261	PRO	2.5
1	C	434	VAL	2.5
1	D	142	THR	2.5
1	D	478	ASN	2.5
1	A	138	ARG	2.5
1	A	238	LEU	2.5
1	B	395	ILE	2.5
1	C	138	ARG	2.5
1	B	370	ASP	2.5
1	D	332	GLU	2.5
1	C	143	GLN	2.5
1	C	485	ALA	2.5
1	A	190	ASN	2.4
1	C	140	ASN	2.4
1	D	404	ASP	2.4
1	C	387	GLY	2.4
1	A	290	PHE	2.4
1	A	247	LEU	2.4
1	D	145	ASN	2.4
1	B	171	HIS	2.4
1	C	325	LYS	2.4
1	A	51	ALA	2.4
1	D	114	ALA	2.4
1	D	412	ALA	2.4
1	C	49	ASN	2.4
1	B	332	GLU	2.4
1	B	432	SER	2.4
1	B	105	ALA	2.4
1	A	187	TYR	2.3
1	B	142	THR	2.3
1	C	430	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	2.3
1	B	234	VAL	2.3
1	B	474	VAL	2.3
1	D	132	ALA	2.3
1	B	85	THR	2.3
1	C	66	THR	2.3
1	A	198	SER	2.3
1	C	483	VAL	2.3
1	A	412	ALA	2.3
1	D	110	ALA	2.3
1	B	388	TYR	2.3
1	D	407	LYS	2.3
1	C	24	ARG	2.3
1	B	293	GLY	2.3
1	B	410	PHE	2.3
1	C	316	ALA	2.3
1	C	210	HIS	2.3
1	C	134	THR	2.3
1	D	237	GLU	2.3
1	B	27	SER	2.3
1	D	450	ARG	2.3
1	A	263	HIS	2.2
1	D	479	TYR	2.2
1	B	281	SER	2.2
1	C	251	ASP	2.2
1	C	495	ASP	2.2
1	D	149	SER	2.2
1	B	491	GLY	2.2
1	A	431	VAL	2.2
1	B	423	VAL	2.2
1	C	147	VAL	2.2
1	A	350	HIS	2.2
1	B	182	ALA	2.2
1	D	411	THR	2.2
1	B	307	PRO	2.2
1	C	307	PRO	2.2
1	D	185	ASP	2.2
1	C	115	THR	2.2
1	C	137	THR	2.2
1	B	25	ASP	2.2
1	A	186	TRP	2.2
1	B	475	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	204	ILE	2.2
1	B	36	THR	2.2
1	B	232	THR	2.2
1	A	184	ARG	2.2
1	B	140	ASN	2.2
1	C	117	TYR	2.2
1	D	104	ASN	2.2
1	D	257	LYS	2.2
1	A	126	GLY	2.2
1	A	250	LEU	2.2
1	C	112	GLY	2.2
1	D	120	GLY	2.2
1	D	188	SER	2.2
1	D	474	VAL	2.2
1	D	475	HIS	2.2
1	C	487	ALA	2.1
1	C	231	ARG	2.1
1	D	138	ARG	2.1
1	A	349	LEU	2.1
1	C	59	GLY	2.1
1	C	249	GLY	2.1
1	A	265	HIS	2.1
1	C	255	ILE	2.1
1	D	269	VAL	2.1
1	A	492	ALA	2.1
1	C	123	ALA	2.1
1	D	193	PRO	2.1
1	D	369	LYS	2.1
1	A	236	TYR	2.1
1	C	225	TYR	2.1
1	B	424	VAL	2.1
1	C	185	ASP	2.1
1	D	239	ASP	2.1
1	C	131	SER	2.1
1	B	240	GLU	2.1
1	D	197	LEU	2.1
1	C	102	ASN	2.1
1	C	190	ASN	2.1
1	C	323	ASN	2.1
1	C	338	HIS	2.1
1	A	255	ILE	2.1
1	D	184	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	241	LYS	2.1
1	D	143	GLN	2.1
1	C	197	LEU	2.1
1	B	268	TYR	2.1
1	A	22	LYS	2.0
1	C	142	THR	2.0
1	C	173	THR	2.0
1	C	261	PRO	2.0
1	C	448	PRO	2.0
1	B	278	LEU	2.0
1	D	324	LEU	2.0
1	A	243	ARG	2.0
1	A	96	ALA	2.0
1	B	239	ASP	2.0
1	D	314	GLU	2.0
1	D	364	ALA	2.0
1	D	463	ALA	2.0
1	C	228	PRO	2.0
1	D	453	THR	2.0
1	A	249	GLY	2.0
1	C	136	ARG	2.0
1	C	382	VAL	2.0
1	C	178	TYR	2.0

## 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, 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.

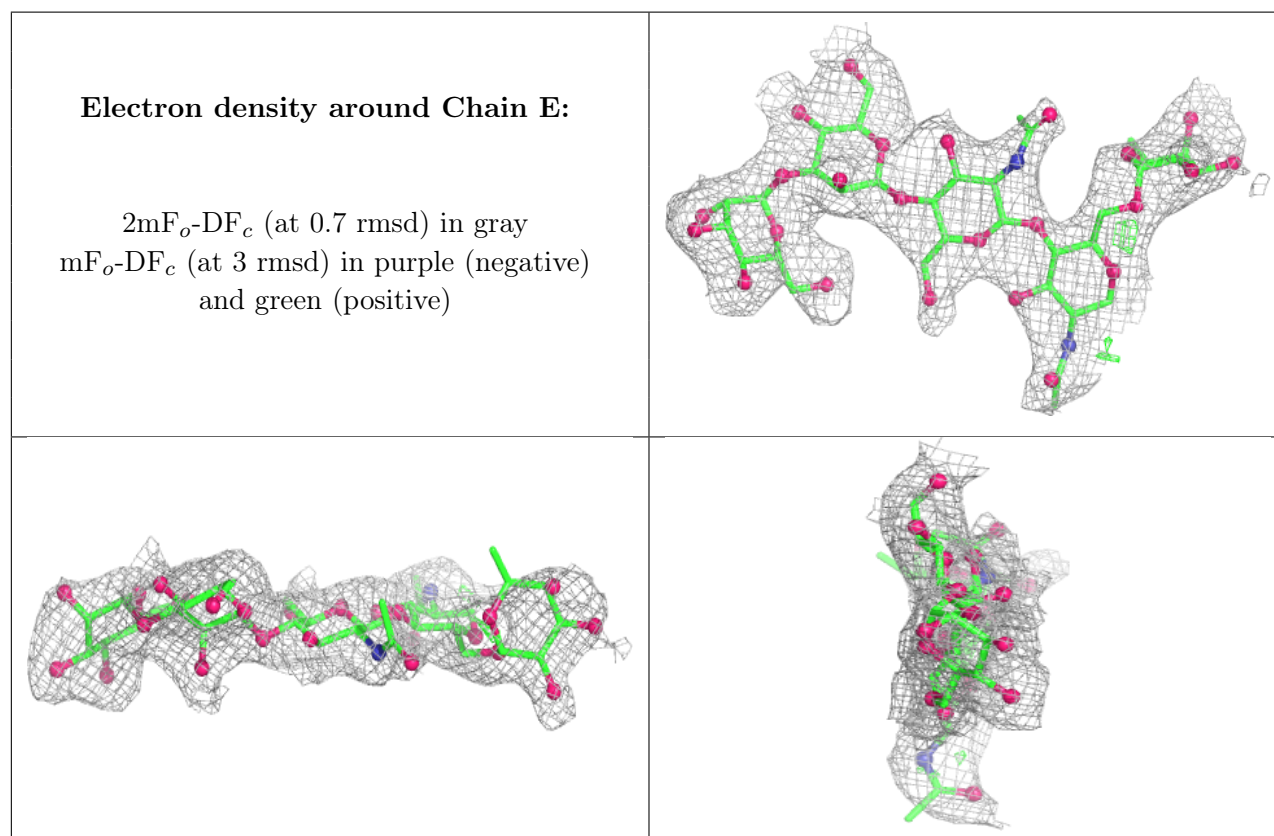
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	F	2	14/15	0.51	0.26	67,84,94,95	0
3	NAG	H	2	14/15	0.53	0.24	74,86,101,104	0
3	NAG	I	2	14/15	0.54	0.21	73,87,97,100	0
3	NAG	J	2	14/15	0.66	0.17	76,86,94,100	0
4	MAN	G	4	11/12	0.69	0.20	53,61,65,67	0

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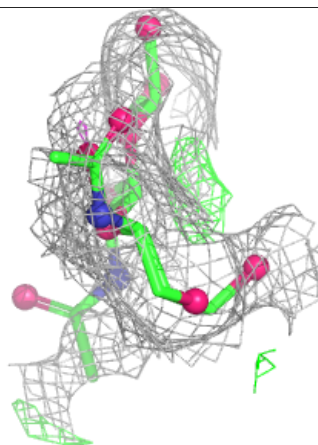
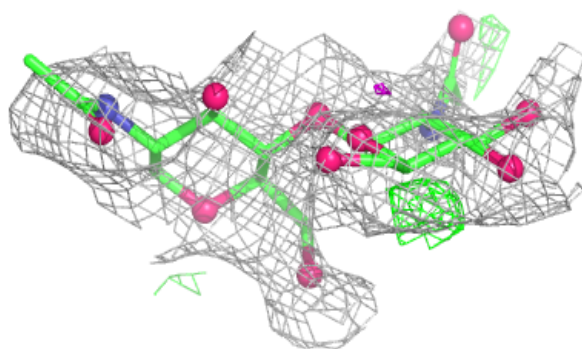
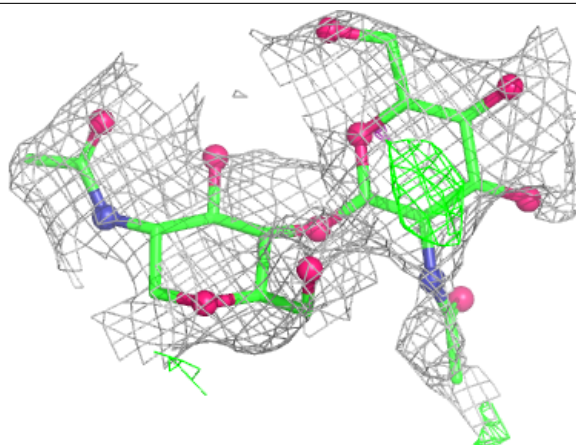
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	F	1	14/15	0.77	0.19	61,70,80,82	0
2	FUC	E	5	10/11	0.77	0.20	56,64,74,76	0
4	NAG	G	2	14/15	0.78	0.18	56,63,70,75	0
4	NAG	G	1	14/15	0.78	0.18	50,63,71,72	0
4	BMA	G	3	11/12	0.79	0.15	52,56,68,68	0
3	NAG	I	1	14/15	0.81	0.17	62,75,87,90	0
3	NAG	H	1	14/15	0.83	0.15	65,71,82,84	0
3	NAG	J	1	14/15	0.84	0.16	55,67,78,82	0
2	MAN	E	4	11/12	0.85	0.13	36,49,61,63	0
2	NAG	E	2	14/15	0.85	0.15	50,57,70,73	0
2	BMA	E	3	11/12	0.87	0.11	37,47,58,58	0
2	NAG	E	1	14/15	0.88	0.16	45,56,67,73	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.

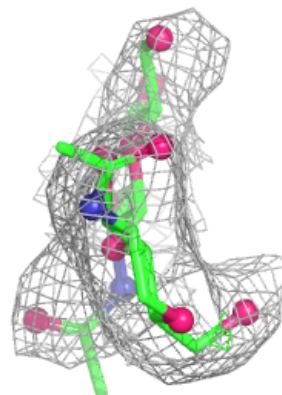
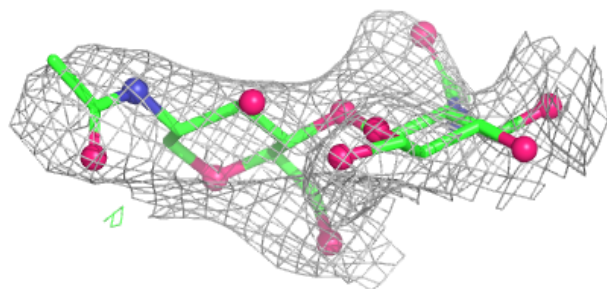
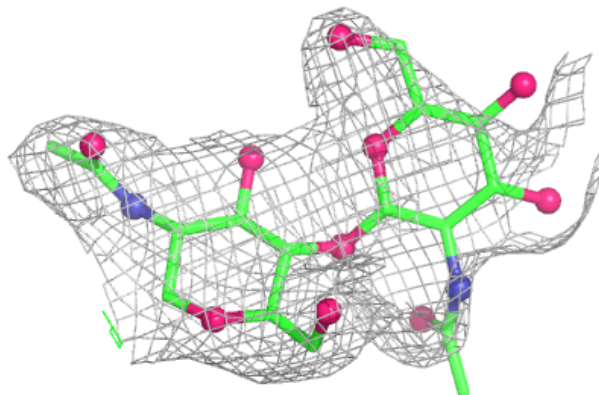


**Electron density around Chain F:**

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

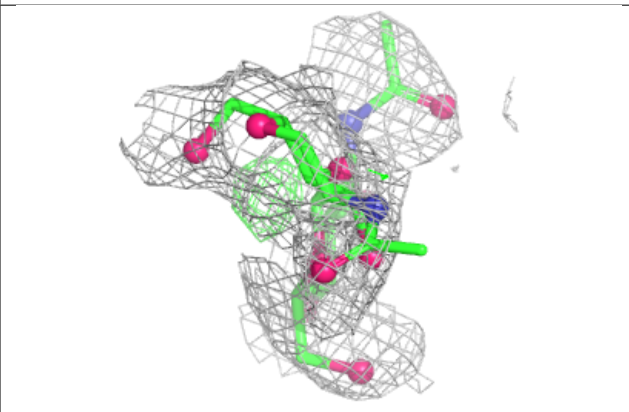
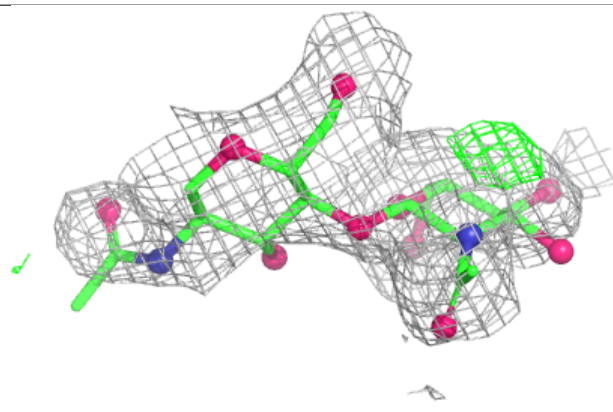
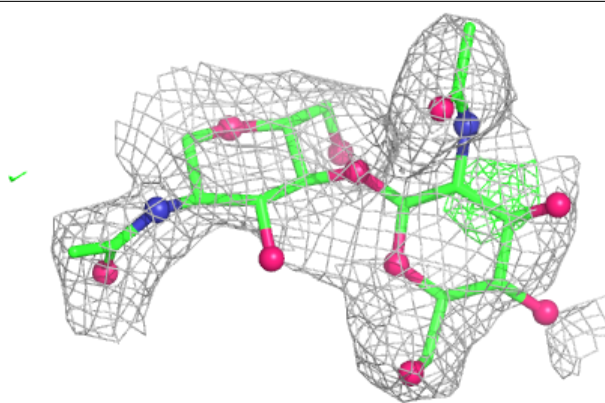
**Electron density around Chain H:**

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

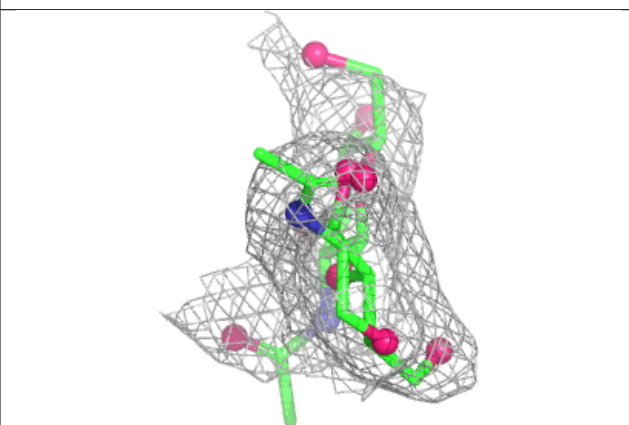
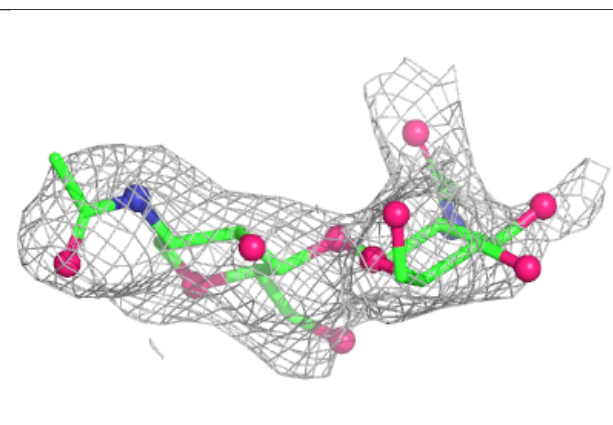
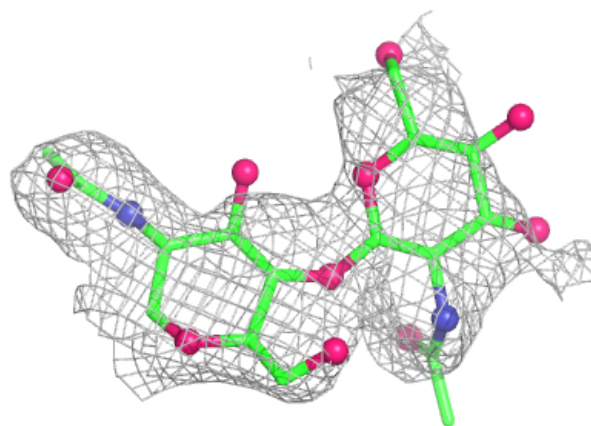


**Electron density around Chain I:**

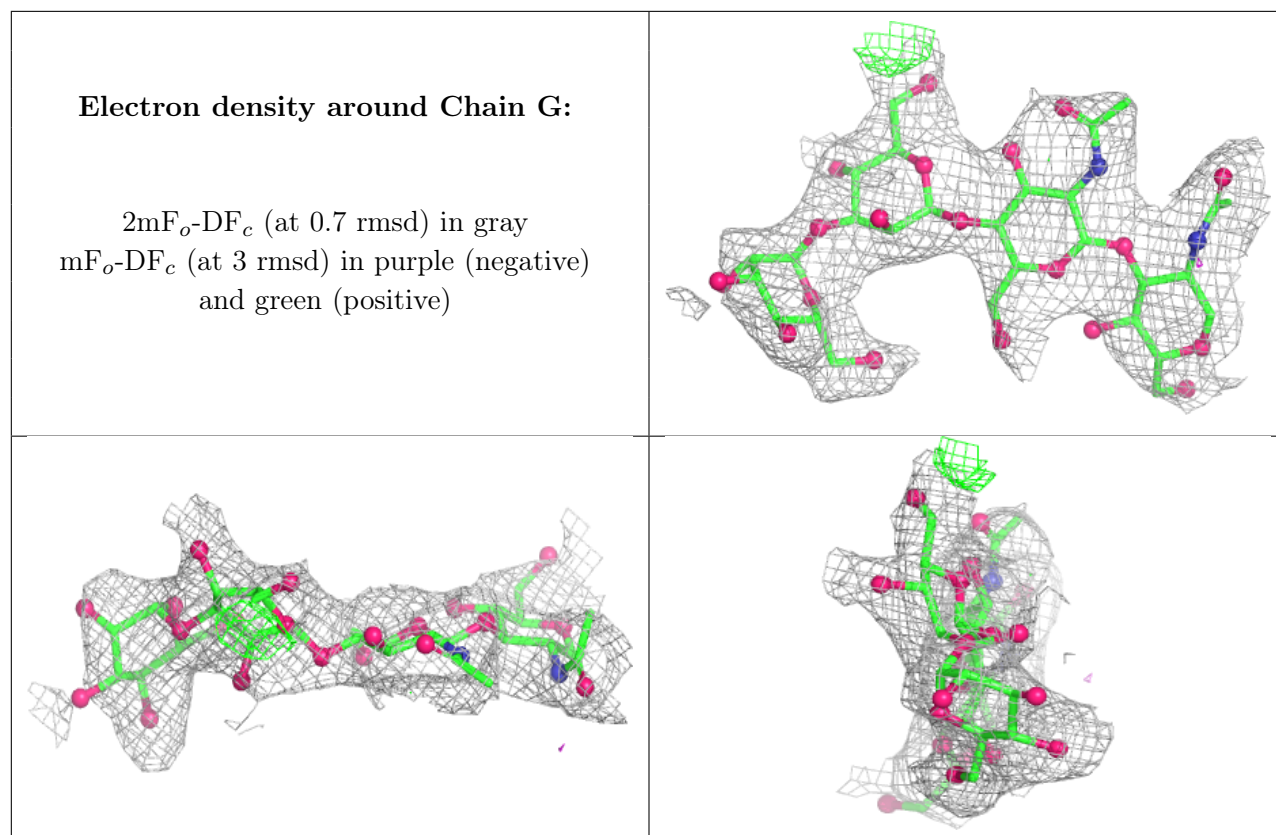
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain J:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
10	NAG	D	608	14/15	0.56	0.19	75,92,97,102	0
10	NAG	C	611	14/15	0.57	0.24	48,67,73,81	0
10	NAG	C	610	14/15	0.64	0.23	53,74,88,92	0
10	NAG	B	606	14/15	0.66	0.20	62,79,86,91	0
10	NAG	A	606	14/15	0.66	0.20	77,84,89,90	0
9	GOL	B	605	6/6	0.68	0.24	41,56,63,64	0
5	ATP	B	601	31/31	0.72	0.31	39,54,61,68	31
11	FLC	C	609	13/13	0.73	0.22	56,71,76,85	0
8	CA	A	604	1/1	0.74	0.19	75,75,75,75	0
8	CA	B	604	1/1	0.75	0.22	81,81,81,81	0
5	ATP	A	601	31/31	0.76	0.26	44,58,65,67	31
9	GOL	A	605	6/6	0.77	0.20	56,60,69,72	0
5	ATP	D	603	31/31	0.77	0.21	51,56,66,70	20
7	MG	B	603	1/1	0.77	0.24	57,57,57,57	0

*Continued on next page...*

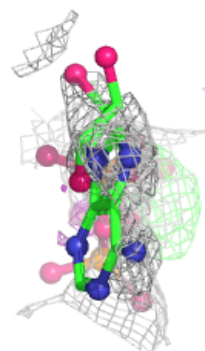
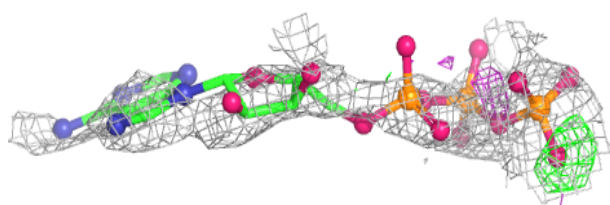
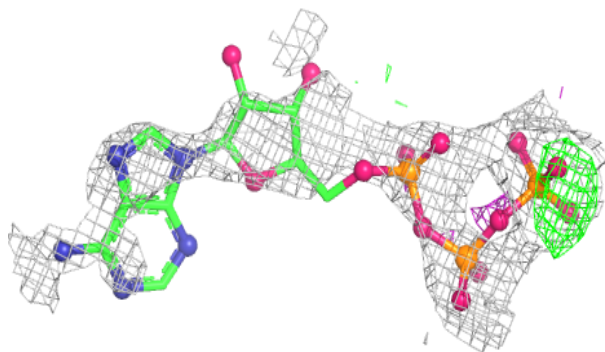
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CA	C	605	1/1	0.77	0.19	74,74,74,74	0
9	GOL	C	608	6/6	0.78	0.24	52,61,64,81	0
7	MG	A	603	1/1	0.80	0.25	65,65,65,65	0
9	GOL	A	607	6/6	0.80	0.18	38,50,54,55	0
9	GOL	C	601	6/6	0.81	0.19	48,55,69,76	0
5	ATP	C	602	31/31	0.81	0.25	42,64,72,76	31
9	GOL	D	607	6/6	0.85	0.18	39,48,54,56	0
9	GOL	C	607	6/6	0.86	0.24	50,61,67,71	0
9	GOL	D	601	6/6	0.87	0.18	55,63,65,66	0
9	GOL	C	606	6/6	0.87	0.15	38,45,47,48	0
8	CA	D	605	1/1	0.89	0.17	75,75,75,75	0
7	MG	C	604	1/1	0.89	0.17	65,65,65,65	0
12	PO4	D	602	5/5	0.89	0.19	56,64,74,77	0
9	GOL	D	606	6/6	0.91	0.11	32,38,40,40	0
6	ZN	D	604	1/1	0.94	0.07	52,52,52,52	0
6	ZN	B	602	1/1	0.95	0.06	55,55,55,55	0
6	ZN	A	602	1/1	0.95	0.06	49,49,49,49	0
6	ZN	C	603	1/1	0.96	0.06	54,54,54,54	0

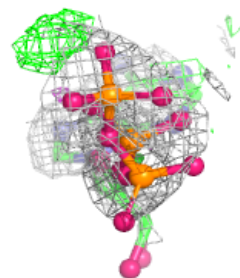
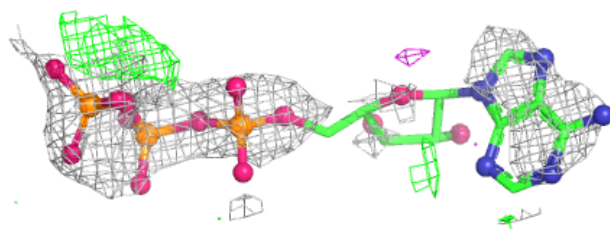
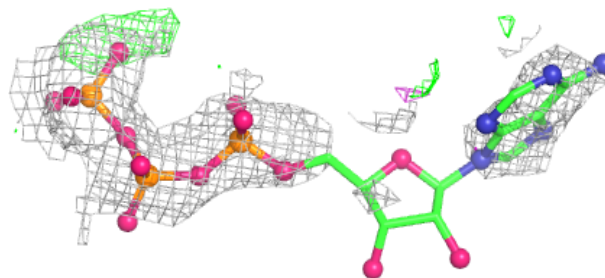
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ATP B 601:**

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

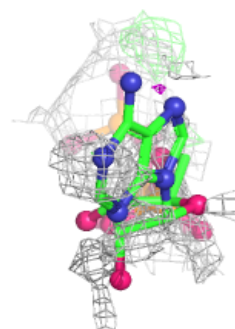
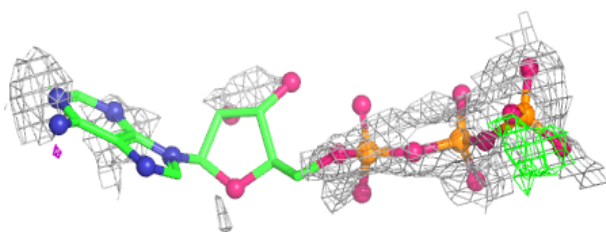
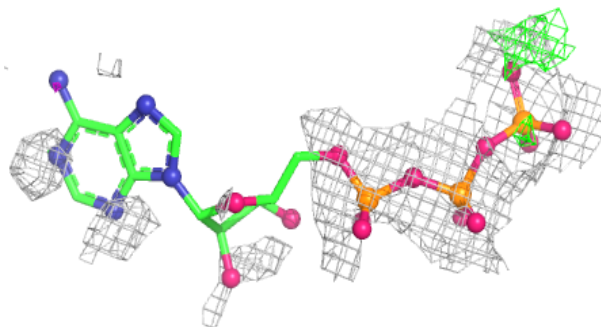
**Electron density around ATP A 601:**

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

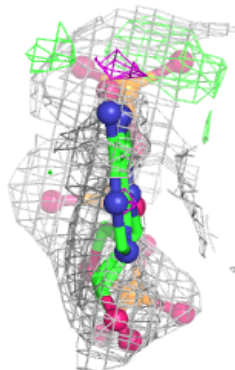
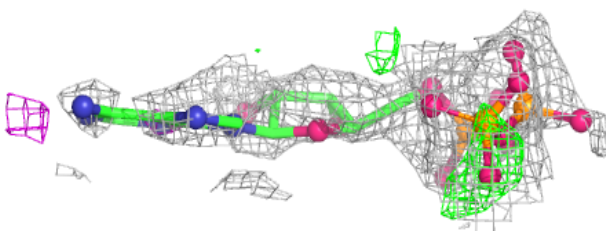
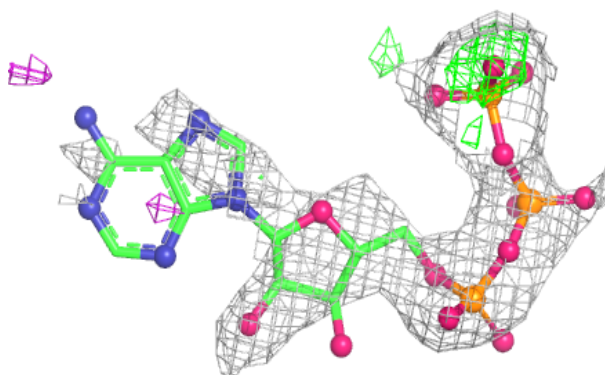


**Electron density around ATP D 603:**

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

**Electron density around ATP C 602:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.