



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 10:24 PM EDT

PDB ID : 6PY9  
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with adenosine diphosphate metavanadate  
Authors : Feder, D.; Schenk, G.; Guddat, L.W.; McGeary, R.P.; Mitic, N.; Furtado, A.; Schulz, B.L.; Henry, R.J.; Schmidt, S.  
Deposited on : 2019-07-29  
Resolution : 2.20 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

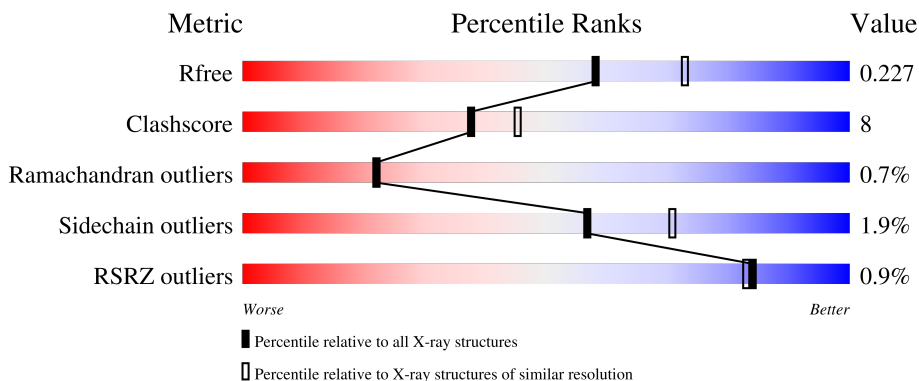
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



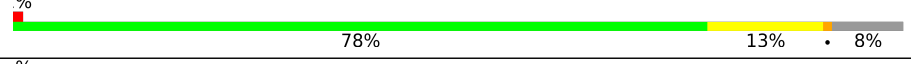
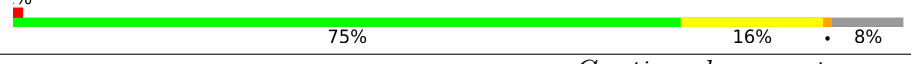
The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




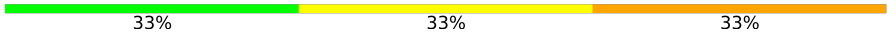
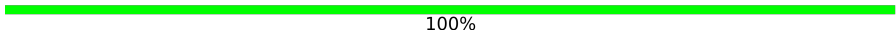
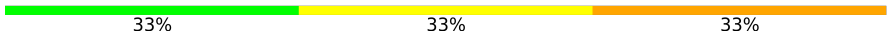
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	459	 78% 14% • 8%
1	B	459	 76% 15% • 7%
1	C	459	 78% 13% • 8%
1	D	459	 75% 16% • 8%

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Mol	Chain	Length	Quality of chain
2	E	3	 33% 67%
2	F	3	 33% 33% 33%
2	G	3	 100%
2	H	3	 33% 33% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	D	513	-	-	X	-
9	EDO	A	518	-	-	X	-
9	EDO	C	516	-	-	-	X

## 2 Entry composition [i](#)

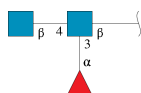
There are 15 unique types of molecules in this entry. The entry contains 16066 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fe(3+)-Zn(2+) purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	Total 3494	C 2243	N 607	O 634	S 10	0	0	0
1	B	425	Total 3532	C 2266	N 614	O 641	S 11	0	5	0
1	D	423	Total 3493	C 2245	N 606	O 632	S 10	0	1	0
1	C	423	Total 3504	C 2250	N 612	O 632	S 10	0	2	0

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[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			
2	E	3	Total 38	C 22	N 2	O 14	0	0	0
2	F	3	Total 38	C 22	N 2	O 14	0	0	0
2	G	3	Total 38	C 22	N 2	O 14	0	0	0
2	H	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

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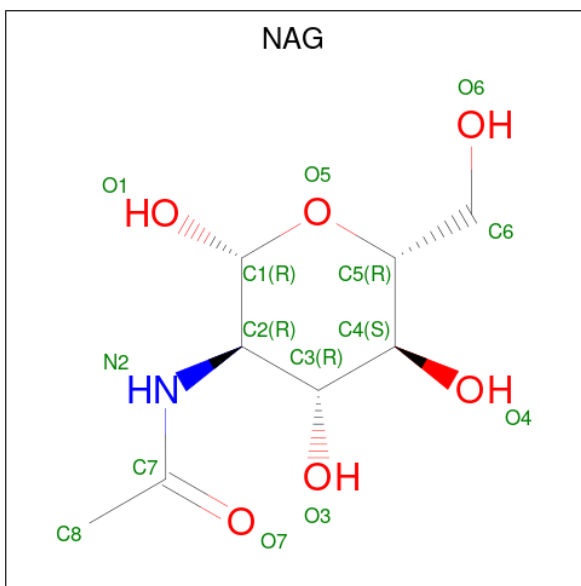
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0
4	B	1	Total Fe 1 1	0	0
4	D	1	Total Fe 1 1	0	0
4	C	1	Total Fe 1 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



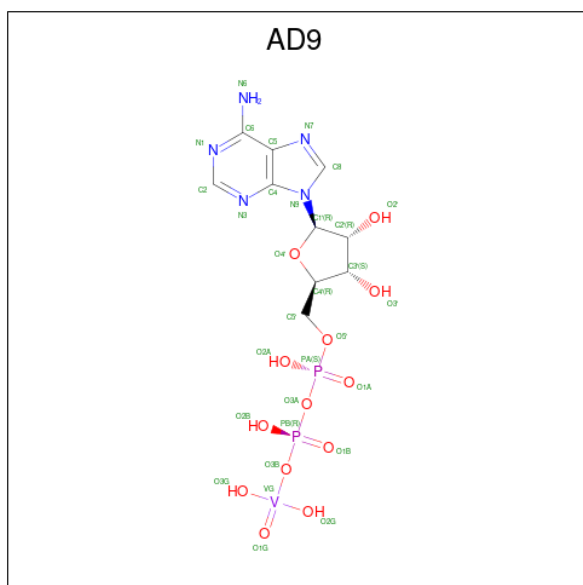
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

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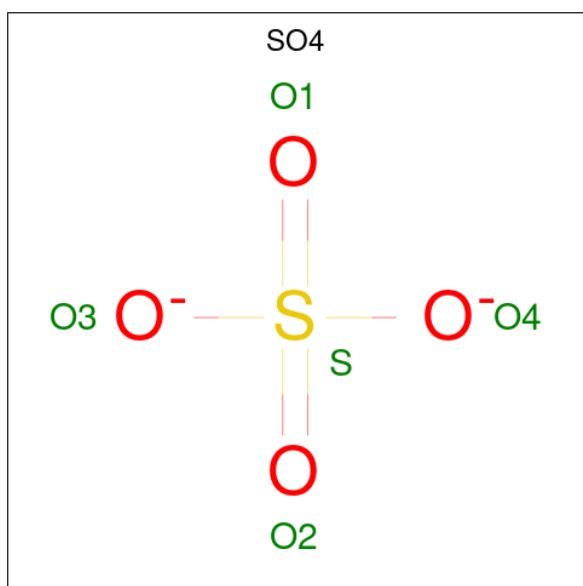
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	B	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	D	1	Total 14	C 8	N 1	O 5	0	0
5	C	1	Total 14	C 8	N 1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

- Molecule 6 is ADP METAVANADATE (three-letter code: AD9) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>2</sub>V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			V
6	A	1	Total 31	C 10	N 5	O 13	P 2	V 1	0	0
6	C	1	Total 31	C 10	N 5	O 13	P 2	V 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

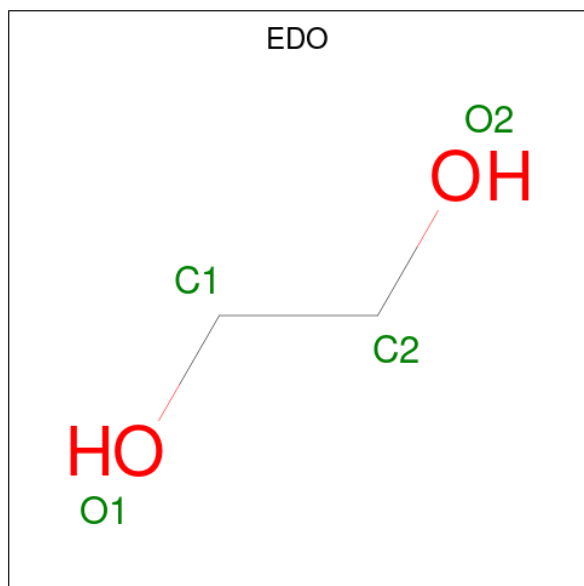


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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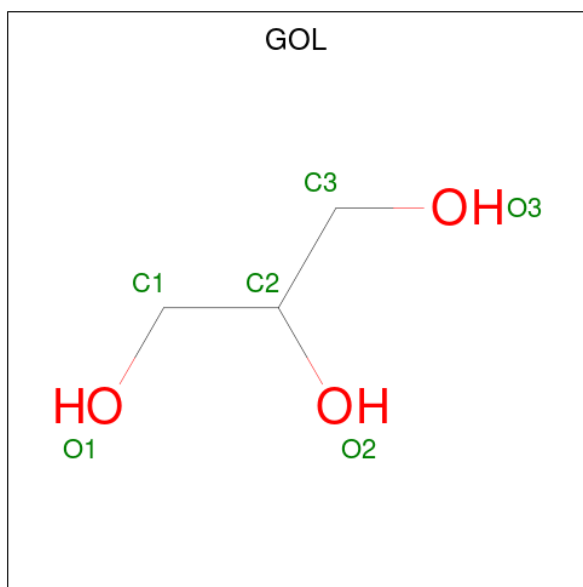
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	D	1	Total 4	C 2	O 2	0	0
9	D	1	Total 4	C 2	O 2	0	0
9	D	1	Total 4	C 2	O 2	0	0
9	D	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0
9	C	1	Total 4	C 2	O 2	0	0

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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



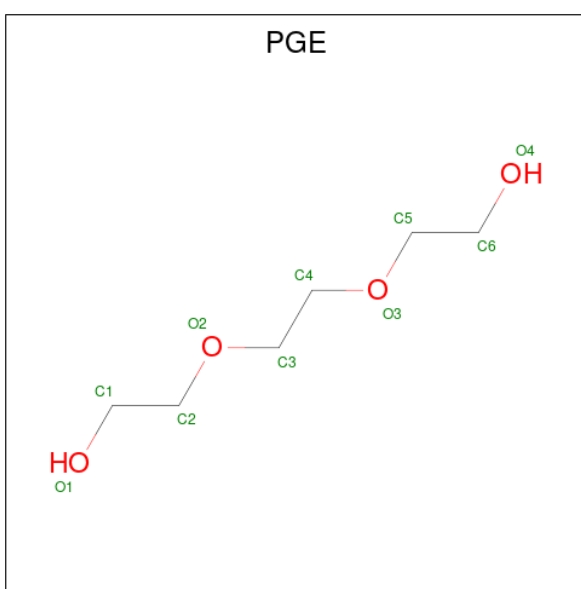
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 6 3 3	0	0
10	A	1	Total C O 12 6 6	0	1
10	B	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0
10	B	1	Total C O 6 3 3	0	0

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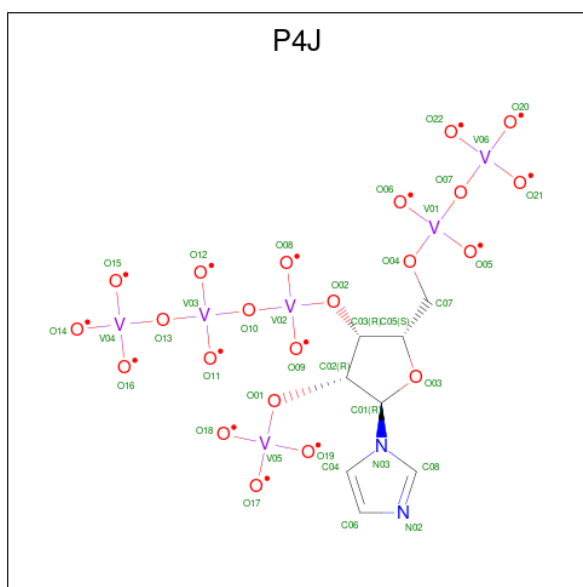
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			10	6	4		
11	A	1	Total	C	O	0	0
			7	4	3		
11	B	1	Total	C	O	0	0
			7	4	3		
11	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is [(2 {R},3 {R},4 {R},5 {S})-2-(5-azanylimidazol-1-yl)-4-[[bis(oxidanyl)-[tris(oxidanyl)vanadiooxy]vanadio]oxy-bis(oxidanyl)vanadio]oxy-5-[[bis(oxidanyl)-[tris(oxidanyl)vanadiooxy]vanadio]oxymethyl]oxolan-3-yl]oxy-tris(oxidanyl)vanadium (three-letter code: P4J) (formula: C<sub>8</sub>H<sub>9</sub>N<sub>2</sub>O<sub>22</sub>V<sub>6</sub>).

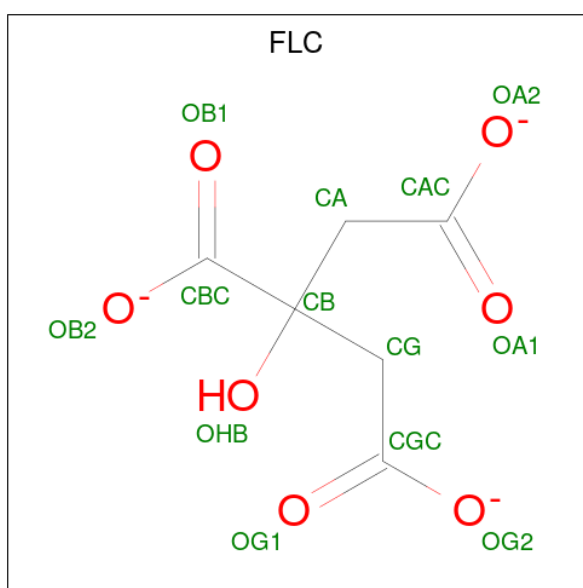


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
12	B	1	Total	C	N	O	V	0	0
			38	8	2	22	6		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Cl	0	0
			1	1		

- Molecule 14 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



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

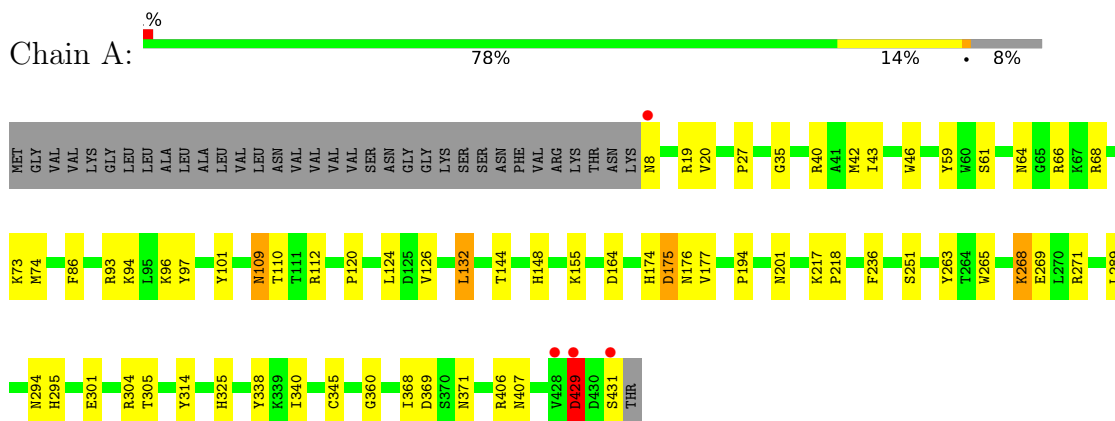
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	334	Total	O	0	0
			334	334		
15	B	301	Total	O	0	0
			301	301		
15	D	334	Total	O	0	0
			334	334		
15	C	332	Total	O	0	0
			332	332		

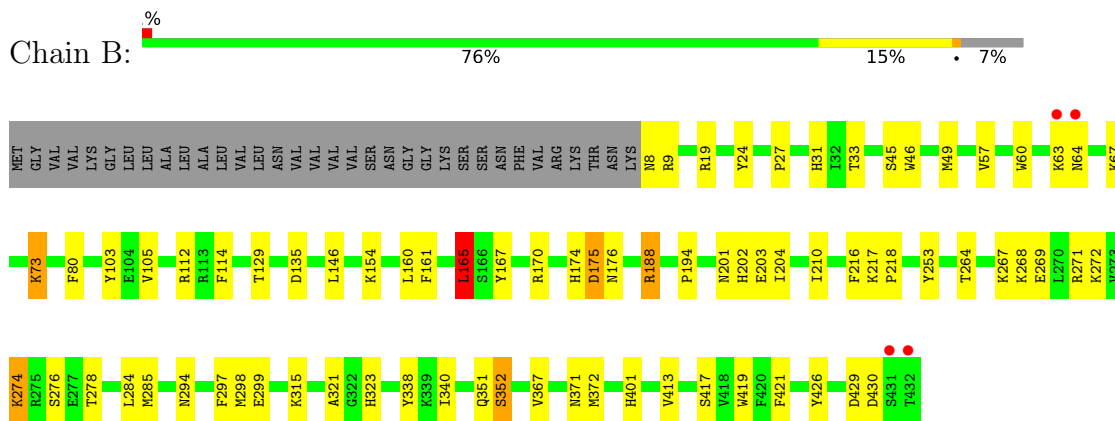
### 3 Residue-property plots [i](#)

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.

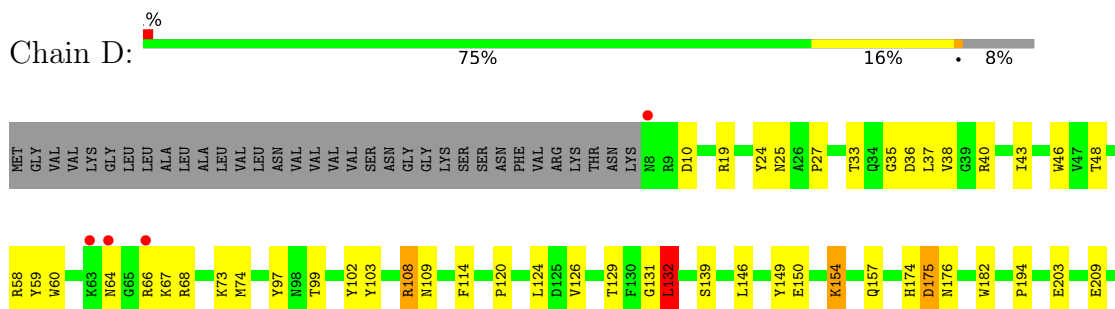
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

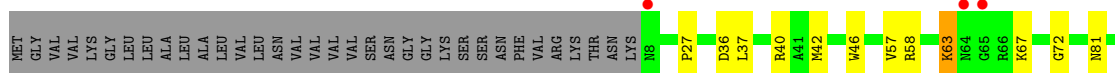
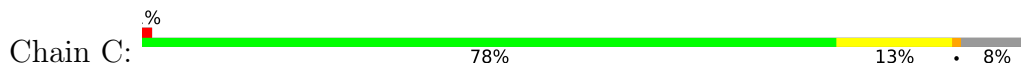


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase





- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



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



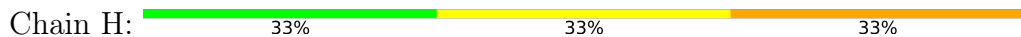
- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.05Å 126.05Å 295.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	81.1 (19.90-2.20) 81.1 (19.90-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.19Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.162 , 0.227 0.163 , 0.227	Depositor DCC
$R_{free}$ test set	5649 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtrriage
Anisotropy	0.095	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AD9, FUC, CL, FE, NAG, SO4, ZN, NA, FLC, EDO, P4J, PGE, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/3613	0.58	1/4913 (0.0%)
1	B	0.42	0/3661	0.56	1/4978 (0.0%)
1	C	0.42	0/3629	0.57	1/4933 (0.0%)
1	D	0.42	0/3615	0.56	1/4916 (0.0%)
All	All	0.42	0/14518	0.57	4/19740 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	LEU	CA-CB-CG	-7.32	98.46	115.30
1	B	165	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	132	LEU	CA-CB-CG	-5.91	101.70	115.30
1	C	132	LEU	CA-CB-CG	-5.58	102.48	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3309	53	0
1	B	3532	0	3347	49	0
1	C	3504	0	3329	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3493	0	3314	56	0
2	E	38	0	34	0	0
2	F	38	0	34	1	0
2	G	38	0	34	0	0
2	H	38	0	34	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	42	0	39	0	0
5	B	42	0	39	1	0
5	C	28	0	26	0	0
5	D	42	0	39	2	0
6	A	31	0	14	7	0
6	C	31	0	14	1	0
7	A	15	0	0	0	0
7	B	10	0	0	0	0
7	C	5	0	0	1	0
7	D	25	0	0	4	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	36	0	54	9	0
9	B	28	0	42	1	0
9	C	48	0	71	9	0
9	D	16	0	24	5	0
10	A	42	0	56	7	0
10	B	24	0	32	2	0
10	C	12	0	16	1	0
10	D	6	0	8	2	0
11	A	17	0	23	2	0
11	B	7	0	9	0	0
11	C	7	0	9	0	0
12	B	38	0	0	7	0
13	B	1	0	0	0	0
14	C	26	0	10	3	0
15	A	334	0	0	5	1
15	B	301	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	332	0	0	9	1
15	D	334	0	0	10	1
All	All	16066	0	13960	221	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ARG:HE	14:C:525:FLC:HG1	1.32	0.92
1:D:267:LYS:O	15:D:601:HOH:O	1.91	0.88
1:A:42:MET:SD	15:A:916:HOH:O	2.35	0.85
1:A:201:ASN:HD22	10:A:526:GOL:H12	1.41	0.84
1:C:414:GLU:H	9:C:520:EDO:H11	1.46	0.80
1:A:42:MET:HE1	1:A:194:PRO:HB3	1.64	0.80
1:C:63:LYS:HD3	1:C:99:THR:HG23	1.64	0.80
1:C:42:MET:HE1	1:C:194:PRO:HB3	1.65	0.79
6:A:509:AD9:O3G	15:A:601:HOH:O	2.00	0.78
1:C:154:LYS:NZ	15:C:602:HOH:O	2.17	0.78
1:A:40:ARG:HH12	9:A:518:EDO:H21	1.52	0.74
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.24	0.72
1:B:430:ASP:OD1	15:B:601:HOH:O	2.08	0.71
1:C:381:ALA:HB1	10:C:523:GOL:H11	1.74	0.70
1:B:315:LYS:NZ	1:B:352:SER:OG	2.24	0.70
1:A:371:ASN:HB2	10:A:527:GOL:H2	1.73	0.68
1:D:37:LEU:H	9:D:515:EDO:H11	1.58	0.68
1:D:109:ASN:OD1	15:D:602:HOH:O	2.11	0.67
1:D:150:GLU:OE2	15:D:603:HOH:O	2.13	0.67
1:D:157:GLN:NE2	15:D:606:HOH:O	2.24	0.66
1:A:263:TYR:HE2	9:A:519:EDO:H11	1.61	0.65
1:C:328:GLU:HG3	1:C:383:ARG:HB3	1.77	0.65
1:A:8:ASN:ND2	15:A:608:HOH:O	2.30	0.65
7:D:509:SO4:O1	15:D:604:HOH:O	2.15	0.64
1:C:37:LEU:H	9:C:510:EDO:H12	1.61	0.64
1:A:406:ARG:HH12	10:A:524:GOL:H2	1.63	0.63
1:A:73:LYS:HA	9:A:521:EDO:H22	1.80	0.63
1:A:265:TRP:CD1	1:A:268:LYS:HE2	2.34	0.63
1:D:33:THR:HA	1:D:194:PRO:HB3	1.80	0.62
1:B:264:THR:O	1:B:268:LYS:HG2	2.00	0.62
15:C:601:HOH:O	2:H:1:NAG:O6	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:HB3	1:A:46:TRP:CD1	2.34	0.62
6:A:509:AD9:O1A	10:A:526:GOL:O1	2.17	0.62
1:D:129:THR:HG22	1:D:391:MET:HE2	1.81	0.61
1:C:378:GLU:H	1:C:378:GLU:CD	2.04	0.60
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.36	0.60
12:B:509:P4J:O22	15:B:602:HOH:O	2.17	0.59
1:A:19:ARG:HE	1:A:20:VAL:H	1.50	0.59
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.38	0.59
1:A:295:HIS:CE1	6:A:509:AD9:H3'	2.37	0.59
1:C:27:PRO:HB3	1:C:46:TRP:CD1	2.36	0.59
1:A:301:GLU:O	1:A:305:THR:HG23	2.03	0.58
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.39	0.58
1:B:161:PHE:CE1	1:B:165:LEU:HD22	2.39	0.58
1:D:97:TYR:N	7:D:513:SO4:O4	2.37	0.57
1:D:36:ASP:HB2	9:D:515:EDO:H11	1.86	0.57
1:D:40:ARG:NH2	7:D:513:SO4:O3	2.33	0.57
1:D:10:ASP:HA	1:D:139:SER:HA	1.87	0.57
1:B:294:ASN:ND2	1:B:371[A]:ASN:OD1	2.38	0.56
1:A:66:ARG:NH1	15:A:618:HOH:O	2.37	0.56
6:A:509:AD9:O2'	15:A:603:HOH:O	2.18	0.55
1:D:369:ASP:HA	9:D:516:EDO:H12	1.87	0.55
1:B:188:ARG:HD3	15:B:739:HOH:O	2.07	0.55
1:D:275:ARG:NH1	1:D:317:ASP:OD2	2.39	0.55
1:B:274:LYS:HE3	1:B:276:SER:H	1.70	0.55
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.40	0.55
1:C:383:ARG:HG2	14:C:525:FLC:HA2	1.89	0.55
1:D:40:ARG:HG3	1:D:97:TYR:CZ	2.42	0.54
1:B:267:LYS:NZ	15:B:617:HOH:O	2.39	0.54
1:A:109:ASN:HD22	1:A:110:THR:H	1.54	0.54
1:D:296:HIS:ND1	1:D:299:GLU:OE1	2.33	0.53
1:A:64:ASN:HD21	1:A:96:LYS:HE3	1.72	0.53
1:D:124:LEU:HD12	1:D:279:PRO:HG3	1.89	0.53
1:C:58:ARG:HD3	1:C:67:LYS:HD3	1.90	0.53
1:C:263:TYR:OH	9:C:513:EDO:H22	2.10	0.52
1:C:285:MET:O	1:C:321:ALA:HA	2.10	0.52
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.92	0.52
1:D:267:LYS:HZ1	10:D:519:GOL:H11	1.74	0.52
1:C:178:ARG:HA	1:C:181:THR:HG22	1.91	0.52
1:B:33:THR:HA	1:B:194:PRO:HB3	1.91	0.51
1:D:271:ARG:N	15:D:601:HOH:O	2.17	0.51
1:B:73:LYS:NZ	15:B:612:HOH:O	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:PHE:CD2	1:C:428:VAL:HG23	2.46	0.51
1:A:66:ARG:NE	1:A:66:ARG:HA	2.26	0.51
1:B:271:ARG:NH2	15:B:607:HOH:O	2.25	0.51
1:B:367:VAL:HA	9:B:519:EDO:H12	1.92	0.51
1:D:182:TRP:HZ3	1:D:223:TYR:HH	1.56	0.51
1:A:429:ASP:OD1	1:A:431:SER:OG	2.26	0.50
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.92	0.50
1:C:203:GLU:O	1:C:216:PHE:HA	2.11	0.50
1:C:258[B]:ARG:NH1	15:C:629:HOH:O	2.44	0.50
1:B:8:ASN:N	15:B:624:HOH:O	2.43	0.50
1:A:295:HIS:HD2	1:A:369:ASP:OD2	1.95	0.49
1:B:351:GLN:OE1	1:B:429:ASP:HA	2.12	0.49
1:C:36:ASP:HB2	9:C:510:EDO:H12	1.95	0.49
1:A:74:MET:H	9:A:521:EDO:H11	1.76	0.49
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.47	0.49
1:D:27:PRO:HB3	1:D:46:TRP:CD1	2.47	0.49
1:D:315:LYS:HB3	1:D:423:ARG:HB3	1.93	0.49
1:A:86:PHE:HZ	1:C:81:ASN:HA	1.78	0.48
1:D:203:GLU:O	1:D:216:PHE:HA	2.13	0.48
1:B:323:HIS:O	12:B:509:P4J:O15	2.31	0.48
1:A:271:ARG:HG2	1:A:314:TYR:OH	2.13	0.48
1:D:60:TRP:CD2	1:D:67:LYS:HE2	2.48	0.48
1:D:371:ASN:ND2	9:D:516:EDO:H22	2.29	0.48
1:A:109:ASN:ND2	1:A:110:THR:H	2.12	0.47
1:A:265:TRP:O	1:A:268:LYS:HG3	2.13	0.47
1:A:345:CYS:HB2	1:D:338:TYR:CE1	2.49	0.47
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.49	0.47
6:A:509:AD9:O2'	11:A:530:PGE:O1	2.28	0.47
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.96	0.47
1:C:154:LYS:HE2	1:C:391:MET:HG3	1.97	0.47
1:A:175:ASP:OD1	1:A:177:VAL:HG12	2.15	0.47
1:D:146:LEU:O	1:D:150:GLU:HG3	2.14	0.47
1:B:338:TYR:CZ	1:B:340:ILE:HA	2.49	0.47
1:D:214:GLU:HG3	15:D:903:HOH:O	2.15	0.47
1:C:413:VAL:HG21	9:C:518:EDO:H11	1.95	0.47
1:D:60:TRP:HB3	1:D:67:LYS:HA	1.97	0.47
1:D:267:LYS:HZ1	10:D:519:GOL:H31	1.80	0.47
1:D:370:SER:H	9:D:516:EDO:H21	1.80	0.47
1:C:285:MET:HE3	1:C:287:SER:O	2.15	0.47
1:D:38:VAL:HB	15:D:678:HOH:O	2.14	0.46
1:D:108:ARG:NH2	5:D:507:NAG:H5	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:GLY:HA3	1:D:149:TYR:CE1	2.50	0.46
1:A:112:ARG:HE	10:A:523:GOL:H2	1.80	0.46
1:A:268:LYS:HE3	1:A:269:GLU:HB2	1.97	0.46
1:D:73:LYS:HD2	1:D:74:MET:H	1.80	0.46
1:B:135:ASP:HB3	1:B:167:TYR:OH	2.16	0.46
9:C:519:EDO:H21	15:C:823:HOH:O	2.15	0.46
1:B:160:LEU:HD13	1:B:284:LEU:HD21	1.97	0.46
1:B:161:PHE:HE1	1:B:165:LEU:HD22	1.79	0.46
10:B:522:GOL:H2	15:B:756:HOH:O	2.16	0.46
1:C:285:MET:HE2	1:C:289:LEU:HG	1.98	0.46
1:B:170:ARG:NH2	12:B:509:P4J:O01	2.45	0.46
1:C:371:ASN:HA	7:C:509:SO4:O3	2.16	0.46
6:A:509:AD9:H8	1:D:258:ARG:NH2	2.31	0.46
1:A:19:ARG:HE	1:A:20:VAL:N	2.12	0.45
1:D:97:TYR:O	1:D:99:THR:HG23	2.16	0.45
1:D:35:GLY:HA2	1:D:43:ILE:HG13	1.98	0.45
1:A:263:TYR:CE2	9:A:519:EDO:H11	2.46	0.45
1:B:285:MET:O	1:B:321:ALA:HA	2.16	0.45
11:A:529:PGE:H5	11:A:529:PGE:H32	1.66	0.45
1:C:85:GLY:HA2	9:C:515:EDO:H22	1.99	0.45
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.51	0.45
1:A:35:GLY:HA2	1:A:43:ILE:HG13	1.99	0.45
1:A:40:ARG:HH12	9:A:518:EDO:C2	2.27	0.45
1:A:112:ARG:HG2	10:A:523:GOL:H32	1.99	0.45
12:B:509:P4J:O11	12:B:509:P4J:O14	2.33	0.45
1:A:97:TYR:H	9:A:518:EDO:H22	1.81	0.44
1:C:178:ARG:HD3	1:C:181:THR:HG21	1.98	0.44
1:C:301:GLU:O	1:C:305:THR:HG23	2.18	0.44
1:A:295:HIS:HE1	6:A:509:AD9:C5'	2.30	0.44
1:A:338:TYR:CZ	1:A:340:ILE:HA	2.52	0.44
1:B:269:GLU:OE2	1:B:272:LYS:NZ	2.51	0.44
12:B:509:P4J:O20	12:B:509:P4J:O06	2.35	0.44
1:A:325:HIS:HA	1:A:360:GLY:O	2.18	0.44
1:C:325:HIS:HA	1:C:360:GLY:O	2.17	0.44
1:D:40:ARG:NH1	7:D:511:SO4:O3	2.51	0.44
1:D:25:ASN:OD1	1:D:48:THR:HB	2.18	0.44
1:C:209:GLU:HG2	1:C:210:ILE:N	2.31	0.44
1:C:409:ASP:HB3	1:C:413:VAL:HB	1.99	0.44
1:A:148:HIS:CE1	1:A:407:ASN:HA	2.53	0.44
1:D:73:LYS:HD2	1:D:73:LYS:HA	1.67	0.44
14:C:524:FLC:OB2	15:C:603:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:PRO:HB2	1:D:126:VAL:HG11	1.99	0.44
1:D:154:LYS:HE2	1:D:414:GLU:OE2	2.18	0.44
1:C:63:LYS:N	1:C:63:LYS:HD2	2.33	0.44
1:A:97:TYR:H	9:A:518:EDO:C2	2.31	0.43
1:B:80:PHE:HB2	1:B:210:ILE:HD12	2.00	0.43
1:B:217:LYS:HB3	1:B:218:PRO:HD3	2.00	0.43
1:B:299:GLU:HG2	9:C:513:EDO:H12	1.99	0.43
1:A:236:PHE:O	1:A:251:SER:HB2	2.17	0.43
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.85	0.43
1:B:297:PHE:CD2	1:B:298:MET:HG3	2.53	0.43
1:D:395:LYS:HE3	1:D:395:LYS:HB3	1.82	0.43
1:B:19:ARG:NH2	15:B:632:HOH:O	2.46	0.43
1:B:112:ARG:HE	10:B:520:GOL:H31	1.83	0.43
1:D:103:TYR:CE2	1:D:114:PHE:HB2	2.54	0.43
1:B:80:PHE:CD2	1:B:210:ILE:HB	2.53	0.43
1:D:132:LEU:HD22	1:D:320:PHE:CD1	2.54	0.43
1:C:63:LYS:HD2	1:C:63:LYS:H	1.83	0.43
1:C:72:GLY:HA3	1:C:90:THR:OG1	2.18	0.43
1:D:174:HIS:O	1:D:175:ASP:C	2.56	0.43
1:C:174:HIS:O	1:C:175:ASP:C	2.56	0.43
1:D:24:TYR:CD2	5:D:507:NAG:H82	2.53	0.43
1:B:33:THR:HA	1:B:194:PRO:CB	2.48	0.42
1:B:57:VAL:HG22	1:B:105:VAL:HG12	2.00	0.42
1:A:97:TYR:HB2	9:A:518:EDO:H22	2.01	0.42
1:C:93:ARG:NH2	15:C:639:HOH:O	2.52	0.42
1:C:291:ASN:HB3	15:C:793:HOH:O	2.19	0.42
1:A:175:ASP:CG	1:A:177:VAL:HG12	2.40	0.42
1:A:93:ARG:O	1:A:94:LYS:HG2	2.18	0.42
1:A:120:PRO:HB2	1:A:126:VAL:HG11	2.00	0.42
1:B:401:HIS:HB2	1:B:419:TRP:CZ3	2.53	0.42
1:C:274:LYS:HA	1:C:274:LYS:HD3	1.86	0.42
1:B:202:HIS:NE2	12:B:509:P4J:O16	2.53	0.42
1:A:368:ILE:HD12	1:A:368:ILE:HA	1.95	0.42
1:B:203:GLU:O	1:B:216:PHE:HA	2.20	0.42
1:A:289:LEU:HD13	1:A:304:ARG:HA	2.01	0.42
1:D:209:GLU:OE1	1:D:209:GLU:N	2.32	0.42
1:A:59:TYR:CZ	1:A:68:ARG:HB2	2.55	0.41
12:B:509:P4J:O12	1:C:258[B]:ARG:NH2	2.44	0.41
1:D:270:LEU:N	15:D:601:HOH:O	2.53	0.41
1:D:59:TYR:HA	1:D:102:TYR:O	2.20	0.41
1:B:204:ILE:HD11	1:B:253:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ARG:NH1	15:D:629:HOH:O	2.50	0.41
1:C:398:THR:OG1	1:C:399:HIS:ND1	2.34	0.41
1:B:24:TYR:CG	5:B:503:NAG:H82	2.55	0.41
1:B:421:PHE:HB3	1:B:426:TYR:O	2.21	0.41
1:B:49:MET:HE1	15:B:751:HOH:O	2.19	0.41
1:B:201[B]:ASN:HB3	1:B:253:TYR:CZ	2.56	0.41
1:D:66:ARG:HD3	1:D:68:ARG:CZ	2.51	0.41
1:C:40:ARG:HD2	9:C:512:EDO:H12	2.02	0.41
1:C:57:VAL:HG22	1:C:105:VAL:HG12	2.01	0.41
6:C:508:AD9:H8	15:C:804:HOH:O	2.21	0.41
1:A:61:SER:HB3	1:A:101:TYR:CE2	2.56	0.41
1:A:64:ASN:ND2	1:A:96:LYS:HE3	2.36	0.41
1:A:305:THR:HB	10:A:525:GOL:O3	2.21	0.41
1:B:129:THR:HG21	1:B:154:LYS:HG3	2.03	0.41
1:B:174:HIS:O	1:B:175:ASP:C	2.58	0.41
1:C:398:THR:HG1	1:C:399:HIS:CE1	2.31	0.41
1:B:60:TRP:HB3	1:B:67:LYS:HA	2.03	0.41
1:B:274:LYS:HA	1:B:274:LYS:HD2	1.58	0.41
2:F:1:NAG:O4	2:F:2:FUC:H5	2.21	0.40
1:C:109:ASN:HB2	15:C:622:HOH:O	2.22	0.40
1:B:31:HIS:CE1	1:B:45:SER:HB2	2.56	0.40
1:B:146:LEU:HD12	1:B:146:LEU:HA	1.91	0.40
1:B:278:THR:HG23	1:B:278:THR:O	2.21	0.40
1:D:58:ARG:O	1:D:103:TYR:HA	2.21	0.40
1:B:73:LYS:HA	1:B:73:LYS:HD2	1.37	0.40
1:C:96:LYS:HE3	1:C:96:LYS:HB3	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:772:HOH:O	15:A:852:HOH:O[5_554]	2.12	0.08
15:D:860:HOH:O	15:C:916:HOH:O[5_564]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/459 (92%)	398 (94%)	20 (5%)	4 (1%)	17	16
1	B	428/459 (93%)	408 (95%)	17 (4%)	3 (1%)	22	22
1	C	423/459 (92%)	404 (96%)	16 (4%)	3 (1%)	22	22
1	D	422/459 (92%)	397 (94%)	24 (6%)	1 (0%)	47	55
All	All	1695/1836 (92%)	1607 (95%)	77 (4%)	11 (1%)	22	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	A	109	ASN
1	A	175	ASP
1	A	429	ASP
1	B	63	LYS
1	B	175	ASP
1	D	175	ASP
1	C	63	LYS
1	C	175	ASP
1	C	155	LYS
1	A	164	ASP

### 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	373/402 (93%)	365 (98%)	8 (2%)	53	67
1	B	379/402 (94%)	369 (97%)	10 (3%)	46	58
1	C	374/402 (93%)	372 (100%)	2 (0%)	88	94
1	D	373/402 (93%)	364 (98%)	9 (2%)	49	62
All	All	1499/1608 (93%)	1470 (98%)	29 (2%)	57	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	144	THR
1	A	155	LYS
1	A	174	HIS
1	A	176	ASN
1	A	268	LYS
1	A	294	ASN
1	A	429	ASP
1	B	9	ARG
1	B	73	LYS
1	B	165	LEU
1	B	176	ASN
1	B	188	ARG
1	B	274	LYS
1	B	352	SER
1	B	372	MET
1	B	413	VAL
1	B	417	SER
1	D	64	ASN
1	D	108	ARG
1	D	132	LEU
1	D	154	LYS
1	D	176	ASN
1	D	231	GLN
1	D	318	VAL
1	D	348	VAL
1	D	391	MET
1	C	176	ASN
1	C	428	VAL

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

Mol	Chain	Res	Type
1	A	295	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

12 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	2,1	14,14,15	0.26	0	17,19,21	0.76	1 (5%)
2	FUC	E	2	2	10,10,11	0.50	0	14,14,16	1.02	1 (7%)
2	NAG	E	3	2	14,14,15	0.48	0	17,19,21	0.43	0
2	NAG	F	1	2,1	14,14,15	0.33	0	17,19,21	0.42	0
2	FUC	F	2	2	10,10,11	0.78	0	14,14,16	1.31	3 (21%)
2	NAG	F	3	2	14,14,15	0.36	0	17,19,21	0.46	0
2	NAG	G	1	2,1	14,14,15	0.55	0	17,19,21	0.48	0
2	FUC	G	2	2	10,10,11	0.78	0	14,14,16	0.91	0
2	NAG	G	3	2	14,14,15	0.45	0	17,19,21	0.41	0
2	NAG	H	1	2,1	14,14,15	0.75	1 (7%)	17,19,21	0.63	0
2	FUC	H	2	2	10,10,11	0.82	0	14,14,16	1.13	2 (14%)
2	NAG	H	3	2	14,14,15	0.23	0	17,19,21	0.41	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	2,1	-	0/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1
2	NAG	F	3	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	H	2	2	-	-	0/1/1/1
2	NAG	H	3	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O5-C1	-2.71	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	FUC	C1-O5-C5	3.04	119.67	112.78
2	F	2	FUC	C1-O5-C5	2.56	118.57	112.78
2	F	2	FUC	C1-C2-C3	-2.43	106.68	109.67
2	E	1	NAG	C1-O5-C5	2.25	115.24	112.19
2	F	2	FUC	O5-C5-C4	2.21	113.49	109.52
2	H	2	FUC	O5-C5-C4	2.02	113.15	109.52
2	E	2	FUC	C1-O5-C5	2.01	117.32	112.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

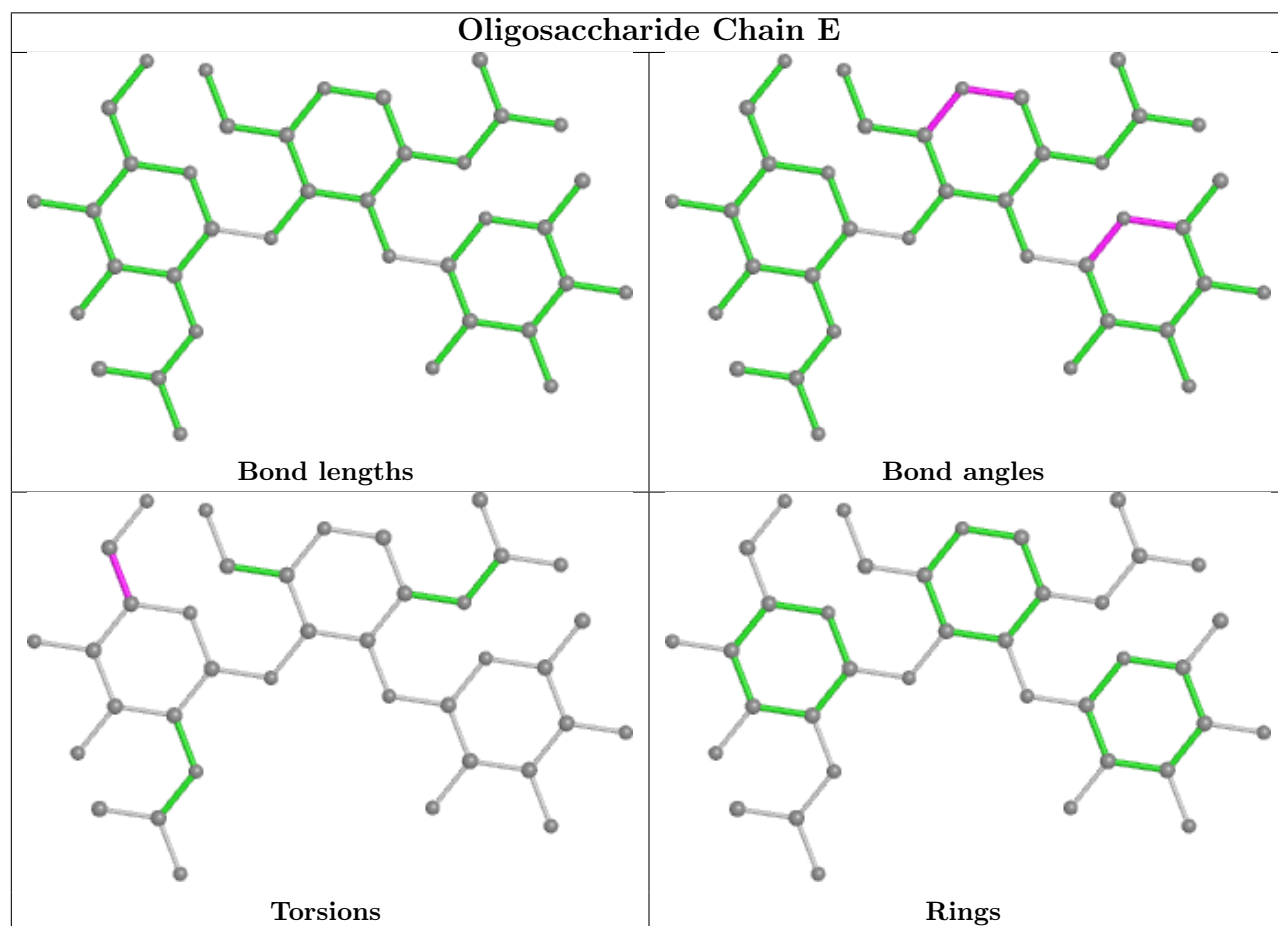
Mol	Chain	Res	Type	Atoms
2	F	3	NAG	O5-C5-C6-O6
2	F	3	NAG	C4-C5-C6-O6
2	H	3	NAG	C4-C5-C6-O6
2	H	3	NAG	O5-C5-C6-O6
2	E	3	NAG	C4-C5-C6-O6

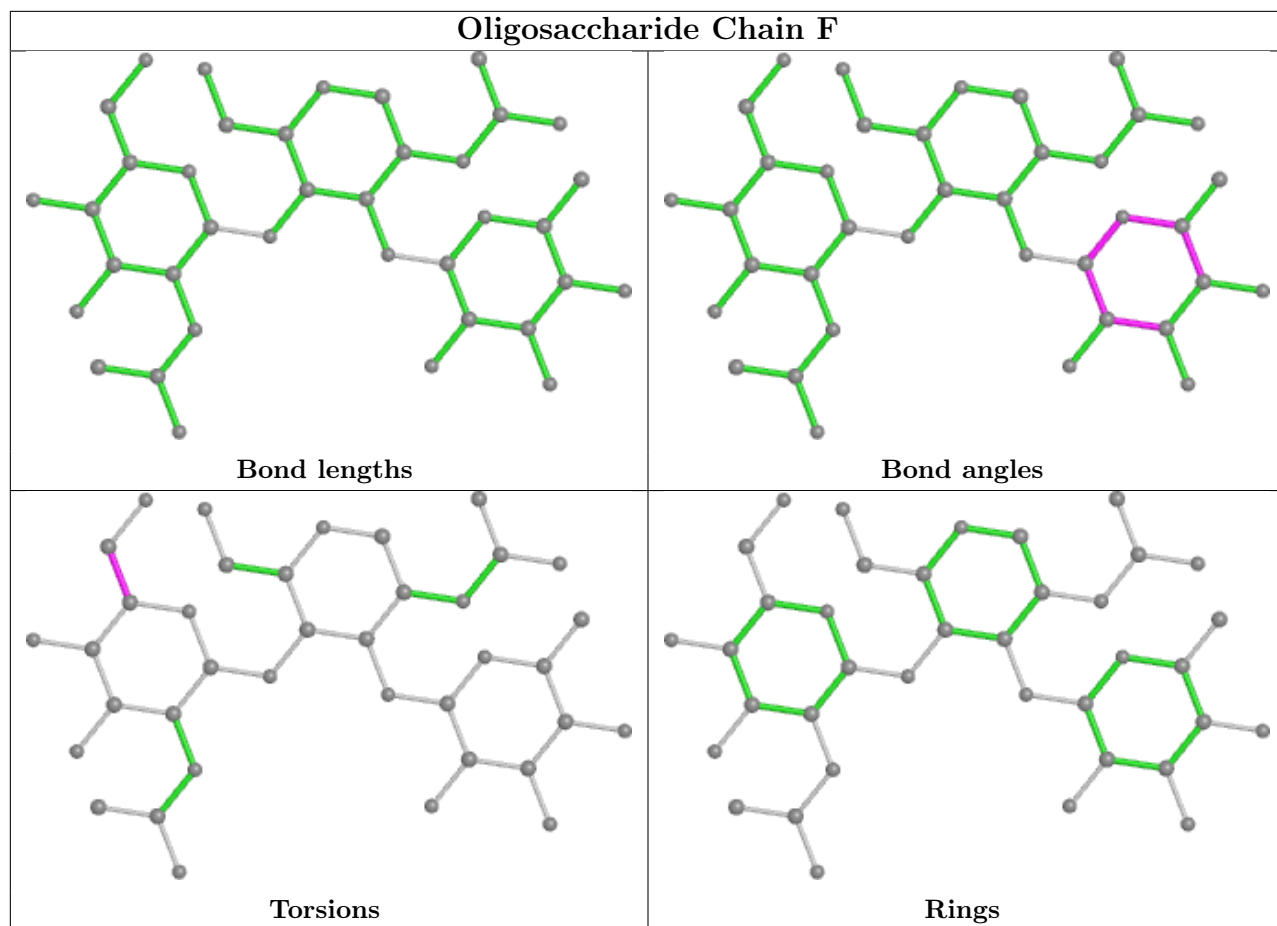
There are no ring outliers.

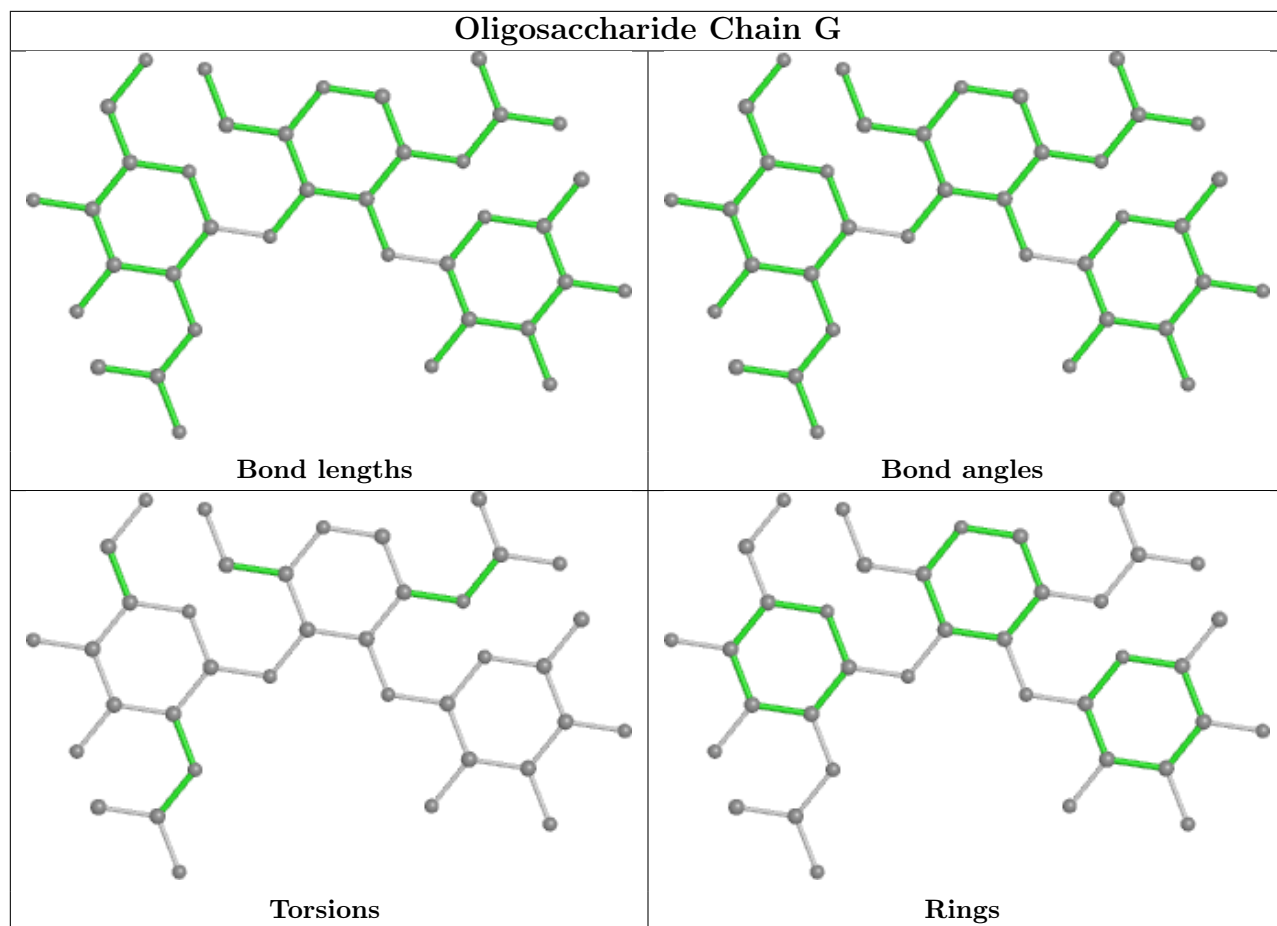
3 monomers are involved in 2 short contacts:

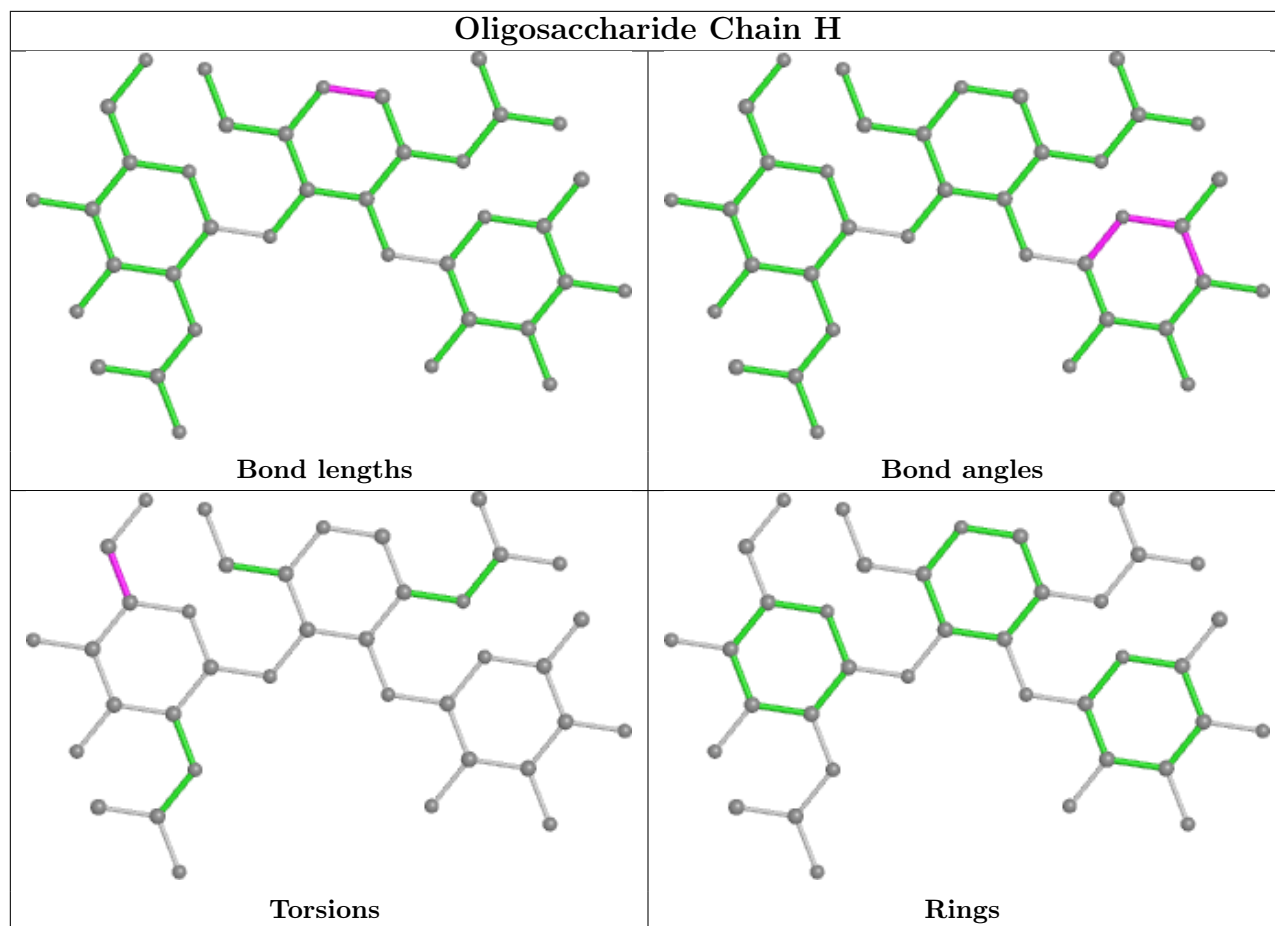
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	F	2	FUC	1	0
2	H	1	NAG	1	0

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](#)

Of 89 ligands modelled in this entry, 12 are monoatomic - leaving 77 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	$\# Z  > 2$
9	EDO	C	510	-	3,3,3	0.40	0	2,2,2	0.24	0
9	EDO	B	514	-	3,3,3	0.57	0	2,2,2	0.16	0
9	EDO	D	515	-	3,3,3	0.43	0	2,2,2	0.32	0
9	EDO	B	517	-	3,3,3	0.51	0	2,2,2	0.37	0
10	GOL	A	528[B]	-	5,5,5	0.98	0	5,5,5	0.91	0
10	GOL	B	520	-	5,5,5	0.99	0	5,5,5	0.83	0
5	NAG	C	503	1	14,14,15	0.78	1 (7%)	17,19,21	0.46	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	A	511	-	4,4,4	0.13	0	6,6,6	0.24	0
9	EDO	C	516	-	3,3,3	0.46	0	2,2,2	0.40	0
5	NAG	A	504	1	14,14,15	0.91	1 (7%)	17,19,21	0.68	1 (5%)
10	GOL	A	525	-	5,5,5	0.85	0	5,5,5	1.08	0
10	GOL	A	526	-	5,5,5	1.04	0	5,5,5	0.83	0
11	PGE	A	529	-	9,9,9	0.31	0	8,8,8	0.60	0
7	SO4	D	513	-	4,4,4	0.17	0	6,6,6	0.15	0
7	SO4	C	509	-	4,4,4	0.19	0	6,6,6	0.23	0
9	EDO	B	518	-	3,3,3	0.49	0	2,2,2	0.28	0
10	GOL	B	523	-	5,5,5	0.78	0	5,5,5	1.11	1 (20%)
9	EDO	D	516	-	3,3,3	0.47	0	2,2,2	0.28	0
9	EDO	C	512	-	3,3,3	0.41	0	2,2,2	0.48	0
9	EDO	A	518	-	3,3,3	0.34	0	2,2,2	0.76	0
14	FLC	C	525	-	12,12,12	1.10	1 (8%)	17,17,17	1.87	5 (29%)
9	EDO	A	517	-	3,3,3	0.52	0	2,2,2	0.23	0
5	NAG	D	508	1	14,14,15	0.92	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	B	504	1	14,14,15	0.40	0	17,19,21	0.47	0
9	EDO	A	519	-	3,3,3	0.44	0	2,2,2	0.40	0
9	EDO	C	518	-	3,3,3	0.49	0	2,2,2	0.33	0
7	SO4	B	511	-	4,4,4	0.14	0	6,6,6	0.28	0
9	EDO	A	516	-	3,3,3	0.53	0	2,2,2	0.23	0
7	SO4	D	512	-	4,4,4	0.14	0	6,6,6	0.16	0
7	SO4	D	509	-	4,4,4	0.16	0	6,6,6	0.26	0
7	SO4	D	511	-	4,4,4	0.16	0	6,6,6	0.13	0
14	FLC	C	524	-	12,12,12	1.06	0	17,17,17	1.61	4 (23%)
9	EDO	C	511	-	3,3,3	0.52	0	2,2,2	0.30	0
9	EDO	B	516	-	3,3,3	0.41	0	2,2,2	0.57	0
9	EDO	D	518	-	3,3,3	0.54	0	2,2,2	0.21	0
9	EDO	D	517	-	3,3,3	0.45	0	2,2,2	0.40	0
10	GOL	B	522	-	5,5,5	0.71	0	5,5,5	1.04	0
10	GOL	A	524	-	5,5,5	0.86	0	5,5,5	0.97	0
9	EDO	C	513	-	3,3,3	0.36	0	2,2,2	0.61	0
10	GOL	A	527	-	5,5,5	0.72	0	5,5,5	1.00	0
9	EDO	A	520	-	3,3,3	0.49	0	2,2,2	0.33	0
5	NAG	B	503	1	14,14,15	0.51	0	17,19,21	0.66	1 (5%)
9	EDO	B	513	-	3,3,3	0.44	0	2,2,2	0.67	0
11	PGE	A	530	-	6,6,9	0.28	0	5,5,8	0.38	0
7	SO4	A	510	-	4,4,4	0.09	0	6,6,6	0.22	0
9	EDO	C	519	-	3,3,3	0.46	0	2,2,2	0.43	0
9	EDO	A	521	-	3,3,3	0.43	0	2,2,2	0.51	0
10	GOL	C	522	-	5,5,5	0.95	0	5,5,5	1.04	0
9	EDO	C	517	-	3,3,3	0.44	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	PGE	C	526	-	6,6,9	0.32	0	5,5,8	0.38	0
6	AD9	C	508	15	24,33,33	1.42	2 (8%)	26,52,52	1.37	4 (15%)
9	EDO	C	515	-	3,3,3	0.45	0	2,2,2	0.46	0
9	EDO	B	519	-	3,3,3	0.50	0	2,2,2	0.36	0
7	SO4	D	510	-	4,4,4	0.13	0	6,6,6	0.32	0
5	NAG	A	503	1	14,14,15	0.37	0	17,19,21	0.53	0
10	GOL	C	523	-	5,5,5	0.77	0	5,5,5	1.02	0
10	GOL	A	523	-	5,5,5	0.92	0	5,5,5	1.00	0
5	NAG	B	505	1	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
10	GOL	A	528[A]	-	5,5,5	0.98	0	5,5,5	0.90	0
9	EDO	B	515	-	3,3,3	0.39	0	2,2,2	0.74	0
10	GOL	D	519	-	5,5,5	0.94	0	5,5,5	0.95	0
12	P4J	B	509	3,4,8	14,39,39	3.94	7 (50%)	12,63,63	1.91	3 (25%)
9	EDO	A	514	-	3,3,3	0.50	0	2,2,2	0.32	0
11	PGE	B	524	-	6,6,9	0.30	0	5,5,8	0.31	0
10	GOL	B	521	-	5,5,5	0.96	0	5,5,5	0.99	0
9	EDO	A	515	-	3,3,3	0.45	0	2,2,2	0.45	0
9	EDO	A	522	-	3,3,3	0.48	0	2,2,2	0.33	0
5	NAG	C	507	1	14,14,15	0.35	0	17,19,21	0.71	0
5	NAG	D	503	1	14,14,15	0.35	0	17,19,21	0.56	0
9	EDO	C	521	-	3,3,3	0.48	0	2,2,2	0.29	0
6	AD9	A	509	15,4	24,33,33	1.51	3 (12%)	26,52,52	1.56	5 (19%)
7	SO4	B	510	-	4,4,4	0.15	0	6,6,6	0.09	0
7	SO4	A	512	-	4,4,4	0.13	0	6,6,6	0.17	0
9	EDO	C	514	-	3,3,3	0.55	0	2,2,2	0.28	0
5	NAG	D	507	1	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
5	NAG	A	508	-	14,14,15	0.43	0	17,19,21	1.71	2 (11%)
9	EDO	C	520	-	3,3,3	0.49	0	2,2,2	0.35	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	GOL	A	523	-	-	2/4/4/4	-
9	EDO	C	510	-	-	0/1/1/1	-
5	NAG	B	505	1	-	0/6/23/26	0/1/1/1
9	EDO	C	512	-	-	0/1/1/1	-
9	EDO	B	514	-	-	0/1/1/1	-
9	EDO	C	513	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	B	515	-	-	1/1/1/1	-
10	GOL	A	524	-	-	2/4/4/4	-
10	GOL	A	527	-	-	4/4/4/4	-
9	EDO	A	520	-	-	1/1/1/1	-
5	NAG	B	503	1	-	2/6/23/26	0/1/1/1
9	EDO	B	513	-	-	1/1/1/1	-
9	EDO	B	517	-	-	1/1/1/1	-
9	EDO	D	515	-	-	0/1/1/1	-
9	EDO	A	518	-	-	1/1/1/1	-
10	GOL	D	519	-	-	0/4/4/4	-
14	FLC	C	525	-	-	1/16/16/16	-
9	EDO	A	517	-	-	1/1/1/1	-
10	GOL	A	528[B]	-	-	0/4/4/4	-
10	GOL	B	520	-	-	2/4/4/4	-
5	NAG	D	508	1	-	0/6/23/26	0/1/1/1
5	NAG	B	504	1	-	0/6/23/26	0/1/1/1
5	NAG	C	503	1	-	2/6/23/26	0/1/1/1
9	EDO	A	519	-	-	1/1/1/1	-
12	P4J	B	509	3,4,8	-	2/2/54/54	0/2/2/2
9	EDO	C	518	-	-	1/1/1/1	-
9	EDO	A	514	-	-	1/1/1/1	-
9	EDO	C	516	-	-	0/1/1/1	-
11	PGE	A	530	-	-	2/4/4/7	-
10	GOL	B	521	-	-	2/4/4/4	-
9	EDO	A	515	-	-	0/1/1/1	-
11	PGE	B	524	-	-	2/4/4/7	-
5	NAG	A	504	1	-	1/6/23/26	0/1/1/1
9	EDO	C	519	-	-	1/1/1/1	-
9	EDO	A	516	-	-	0/1/1/1	-
10	GOL	A	525	-	-	0/4/4/4	-
9	EDO	A	522	-	-	0/1/1/1	-
5	NAG	C	507	1	-	0/6/23/26	0/1/1/1
9	EDO	A	521	-	-	1/1/1/1	-
10	GOL	A	526	-	-	2/4/4/4	-
5	NAG	D	503	1	-	1/6/23/26	0/1/1/1
14	FLC	C	524	-	-	6/16/16/16	-
9	EDO	C	521	-	-	0/1/1/1	-
10	GOL	C	522	-	-	0/4/4/4	-
11	PGE	A	529	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AD9	A	509	15,4	-	5/12/38/38	0/3/3/3
9	EDO	C	517	-	-	0/1/1/1	-
9	EDO	C	511	-	-	0/1/1/1	-
11	PGE	C	526	-	-	2/4/4/7	-
9	EDO	C	514	-	-	0/1/1/1	-
9	EDO	B	516	-	-	0/1/1/1	-
6	AD9	C	508	15	-	5/12/38/38	0/3/3/3
9	EDO	C	515	-	-	0/1/1/1	-
9	EDO	B	518	-	-	0/1/1/1	-
9	EDO	B	519	-	-	0/1/1/1	-
9	EDO	D	518	-	-	1/1/1/1	-
10	GOL	B	523	-	-	1/4/4/4	-
5	NAG	D	507	1	-	0/6/23/26	0/1/1/1
9	EDO	D	516	-	-	1/1/1/1	-
9	EDO	D	517	-	-	1/1/1/1	-
10	GOL	A	528[A]	-	-	2/4/4/4	-
10	GOL	B	522	-	-	2/4/4/4	-
5	NAG	A	508	-	-	4/6/23/26	0/1/1/1
5	NAG	A	503	1	-	0/6/23/26	0/1/1/1
9	EDO	C	520	-	-	1/1/1/1	-
10	GOL	C	523	-	-	3/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	509	P4J	O03-C01	-9.63	1.27	1.41
12	B	509	P4J	O03-C05	7.93	1.62	1.45
6	A	509	AD9	O4'-C1'	4.63	1.47	1.41
12	B	509	P4J	C03-C05	-4.62	1.40	1.52
6	C	508	AD9	O4'-C1'	4.42	1.47	1.41
12	B	509	P4J	O04-V01	-3.61	1.64	1.81
5	D	508	NAG	O5-C1	3.33	1.49	1.43
12	B	509	P4J	O02-C03	3.15	1.54	1.44
5	A	504	NAG	O5-C1	2.89	1.48	1.43
6	A	509	AD9	C2-N3	2.62	1.36	1.32
12	B	509	P4J	O02-V02	2.55	1.93	1.81
6	C	508	AD9	C2-N3	2.46	1.36	1.32
6	A	509	AD9	C2'-C1'	2.40	1.57	1.53
5	C	503	NAG	O5-C1	2.27	1.47	1.43
12	B	509	P4J	O01-C02	-2.14	1.36	1.44
14	C	525	FLC	OB1-CBC	2.09	1.28	1.22

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	508	NAG	C1-O5-C5	6.23	120.63	112.19
14	C	525	FLC	OB1-CBC-CB	-4.44	115.97	122.25
6	A	509	AD9	O3B-PB-O1B	-4.27	95.02	110.99
6	C	508	AD9	O3B-PB-O1B	-3.99	96.05	110.99
12	B	509	P4J	O02-C03-C02	3.97	120.48	110.88
14	C	525	FLC	OB2-CBC-CB	3.46	119.06	113.05
6	A	509	AD9	O2B-PB-O3B	3.38	119.33	107.52
12	B	509	P4J	O01-C02-C03	3.23	118.69	110.88
14	C	524	FLC	OB2-CBC-CB	3.03	118.31	113.05
5	D	508	NAG	C1-O5-C5	3.02	116.28	112.19
5	B	505	NAG	C1-O5-C5	2.82	116.01	112.19
6	C	508	AD9	O2B-PB-O3B	2.61	116.65	107.52
5	D	507	NAG	C1-O5-C5	2.60	115.72	112.19
12	B	509	P4J	O01-C02-C01	2.49	115.61	110.37
5	A	508	NAG	C3-C4-C5	2.47	114.65	110.24
6	A	509	AD9	O5'-PA-O1A	2.40	118.43	109.07
14	C	525	FLC	OA2-CAC-CA	2.34	121.86	114.35
6	A	509	AD9	C3'-C2'-C1'	2.33	104.49	100.98
5	A	504	NAG	C1-O5-C5	2.31	115.33	112.19
6	C	508	AD9	O4'-C1'-C2'	-2.27	103.61	106.93
14	C	524	FLC	OA2-CAC-CA	2.23	121.51	114.35
5	B	503	NAG	C1-O5-C5	2.16	115.12	112.19
6	A	509	AD9	C2'-C3'-C4'	2.15	106.81	102.64
6	C	508	AD9	O5'-PA-O1A	2.13	117.40	109.07
14	C	525	FLC	CG-CB-CBC	-2.11	105.58	110.11
14	C	525	FLC	OHB-CB-CG	2.09	114.28	109.40
14	C	524	FLC	CB-CG-CGC	2.07	118.83	113.81
14	C	524	FLC	OB1-CBC-CB	-2.03	119.37	122.25
10	B	523	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	509	AD9	C5'-O5'-PA-O3A
10	A	523	GOL	O1-C1-C2-C3
10	A	526	GOL	O1-C1-C2-C3
10	A	527	GOL	C1-C2-C3-O3
10	A	528[A]	GOL	O1-C1-C2-C3
10	B	520	GOL	C1-C2-C3-O3
10	B	521	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	B	522	GOL	O1-C1-C2-C3
12	B	509	P4J	O03-C05-C07-O04
14	C	524	FLC	CG-CB-CBC-OB1
14	C	524	FLC	CG-CB-CBC-OB2
14	C	524	FLC	OHB-CB-CBC-OB1
14	C	524	FLC	OHB-CB-CBC-OB2
11	C	526	PGE	C3-C4-O3-C5
6	C	508	AD9	O4'-C4'-C5'-O5'
6	C	508	AD9	C3'-C4'-C5'-O5'
5	C	503	NAG	O5-C5-C6-O6
5	A	508	NAG	C4-C5-C6-O6
5	C	503	NAG	C4-C5-C6-O6
5	A	508	NAG	C8-C7-N2-C2
5	A	508	NAG	O7-C7-N2-C2
10	A	524	GOL	O2-C2-C3-O3
10	A	528[A]	GOL	O1-C1-C2-O2
10	B	521	GOL	O2-C2-C3-O3
11	A	530	PGE	O1-C1-C2-O2
12	B	509	P4J	C03-C05-C07-O04
5	B	503	NAG	O5-C5-C6-O6
11	A	529	PGE	O1-C1-C2-O2
10	A	524	GOL	C1-C2-C3-O3
10	C	523	GOL	O1-C1-C2-C3
10	C	523	GOL	C1-C2-C3-O3
5	B	503	NAG	C4-C5-C6-O6
5	A	508	NAG	O5-C5-C6-O6
10	A	526	GOL	O1-C1-C2-O2
10	B	522	GOL	O1-C1-C2-O2
11	C	526	PGE	O2-C3-C4-O3
5	A	504	NAG	O5-C5-C6-O6
11	A	529	PGE	C3-C4-O3-C5
10	A	527	GOL	O2-C2-C3-O3
10	B	520	GOL	O2-C2-C3-O3
11	A	530	PGE	C4-C3-O2-C2
9	C	520	EDO	O1-C1-C2-O2
11	B	524	PGE	O2-C3-C4-O3
10	C	523	GOL	O1-C1-C2-O2
9	A	514	EDO	O1-C1-C2-O2
9	D	516	EDO	O1-C1-C2-O2
11	A	529	PGE	C4-C3-O2-C2
10	A	527	GOL	O1-C1-C2-O2
6	A	509	AD9	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	C	508	AD9	C5'-O5'-PA-O2A
10	A	523	GOL	O1-C1-C2-O2
9	A	519	EDO	O1-C1-C2-O2
6	C	508	AD9	PA-O3A-PB-O2B
9	B	513	EDO	O1-C1-C2-O2
11	A	529	PGE	C1-C2-O2-C3
6	A	509	AD9	C3'-C4'-C5'-O5'
9	A	520	EDO	O1-C1-C2-O2
9	D	517	EDO	O1-C1-C2-O2
5	D	503	NAG	C4-C5-C6-O6
6	A	509	AD9	O4'-C4'-C5'-O5'
9	A	517	EDO	O1-C1-C2-O2
9	A	518	EDO	O1-C1-C2-O2
9	A	521	EDO	O1-C1-C2-O2
9	B	517	EDO	O1-C1-C2-O2
9	D	518	EDO	O1-C1-C2-O2
6	A	509	AD9	PB-O3A-PA-O1A
10	A	527	GOL	O1-C1-C2-C3
10	B	523	GOL	C1-C2-C3-O3
14	C	524	FLC	CBC-CB-CG-CGC
14	C	524	FLC	OHB-CB-CG-CGC
11	B	524	PGE	C1-C2-O2-C3
6	C	508	AD9	C4'-C5'-O5'-PA
9	B	515	EDO	O1-C1-C2-O2
9	C	518	EDO	O1-C1-C2-O2
9	C	519	EDO	O1-C1-C2-O2
14	C	525	FLC	CAC-CA-CB-CG

There are no ring outliers.

35 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	510	EDO	2	0
9	D	515	EDO	2	0
10	B	520	GOL	1	0
10	A	525	GOL	1	0
10	A	526	GOL	2	0
11	A	529	PGE	1	0
7	D	513	SO4	2	0
7	C	509	SO4	1	0
9	D	516	EDO	3	0
9	C	512	EDO	1	0

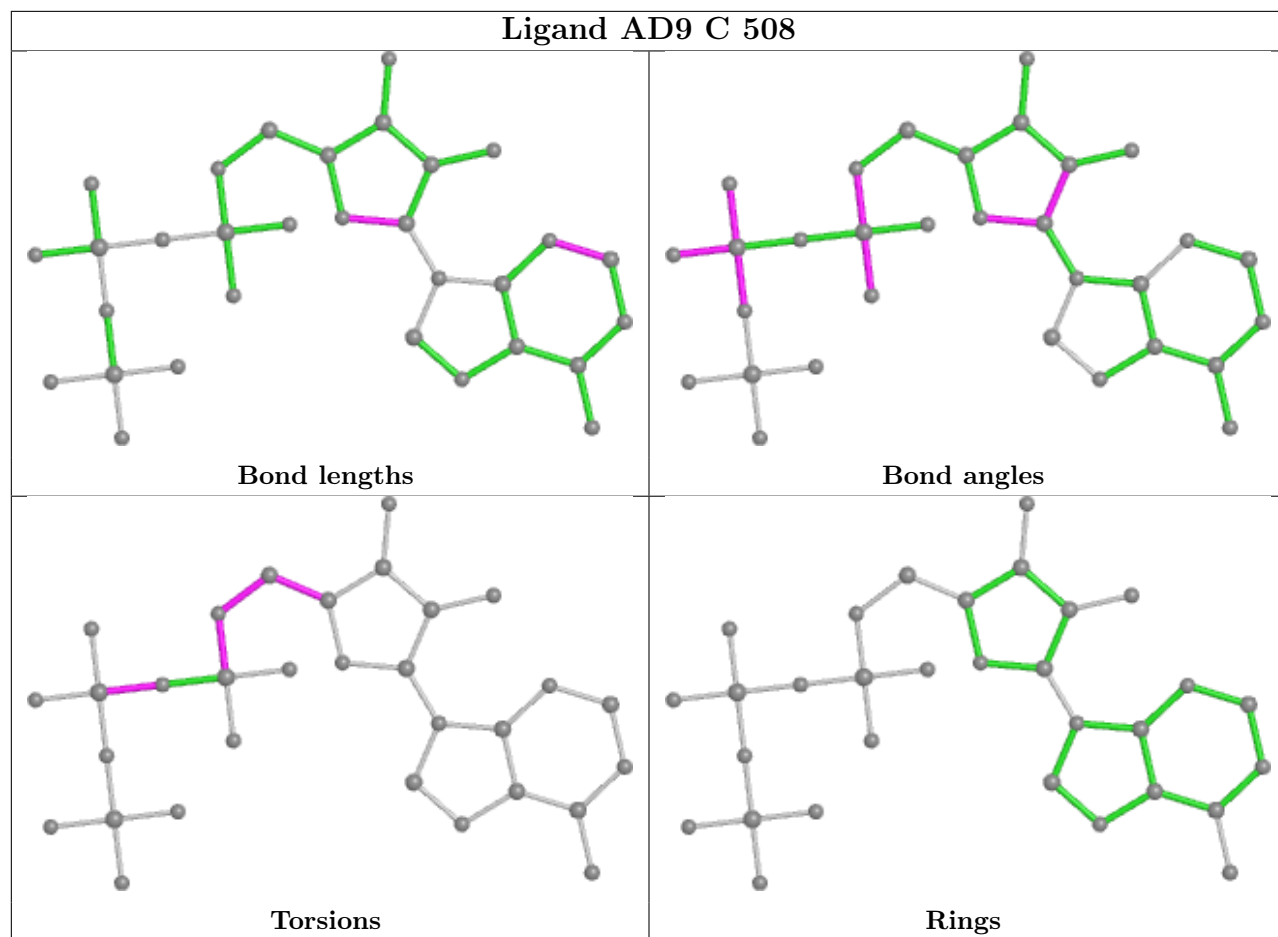
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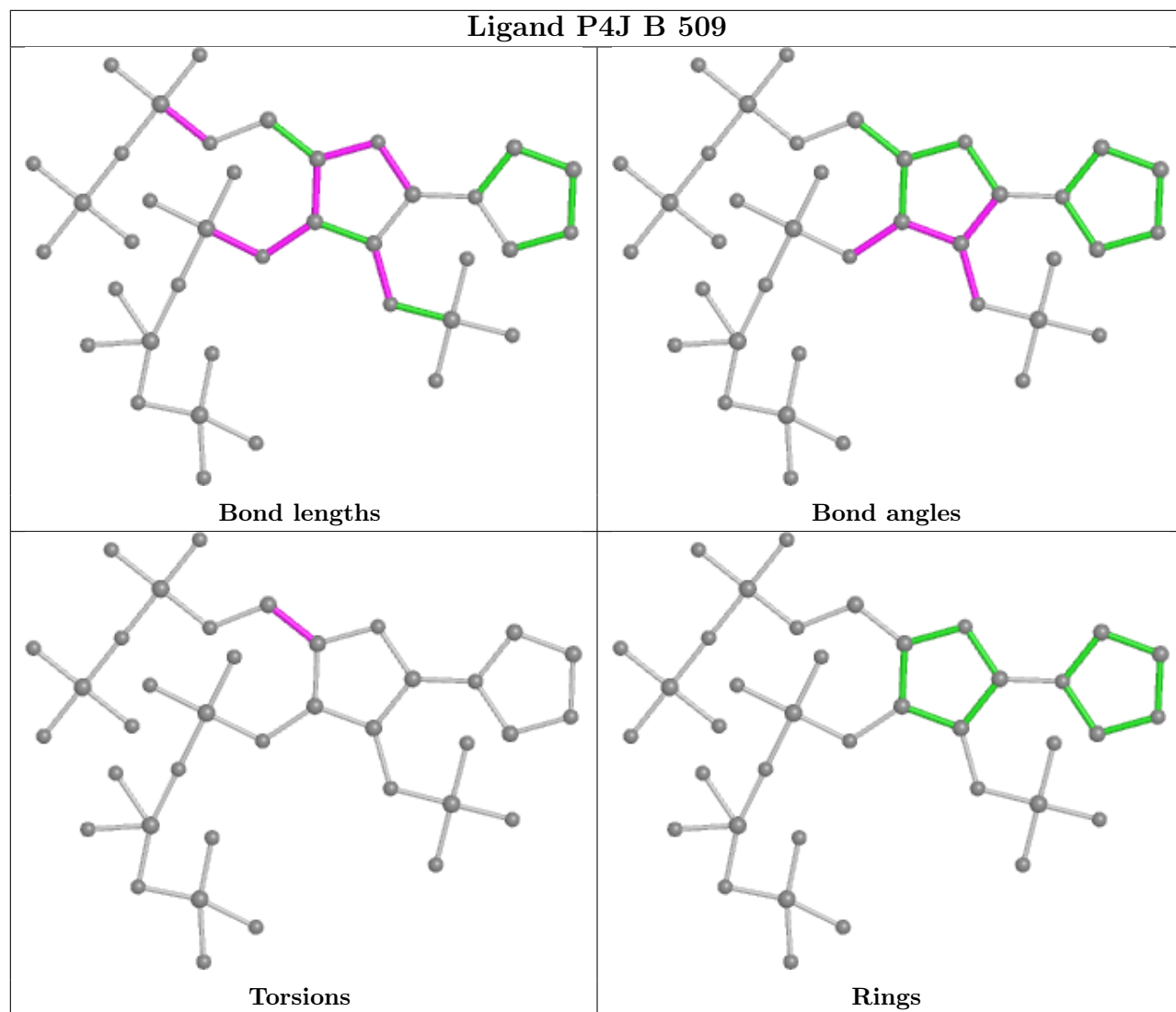
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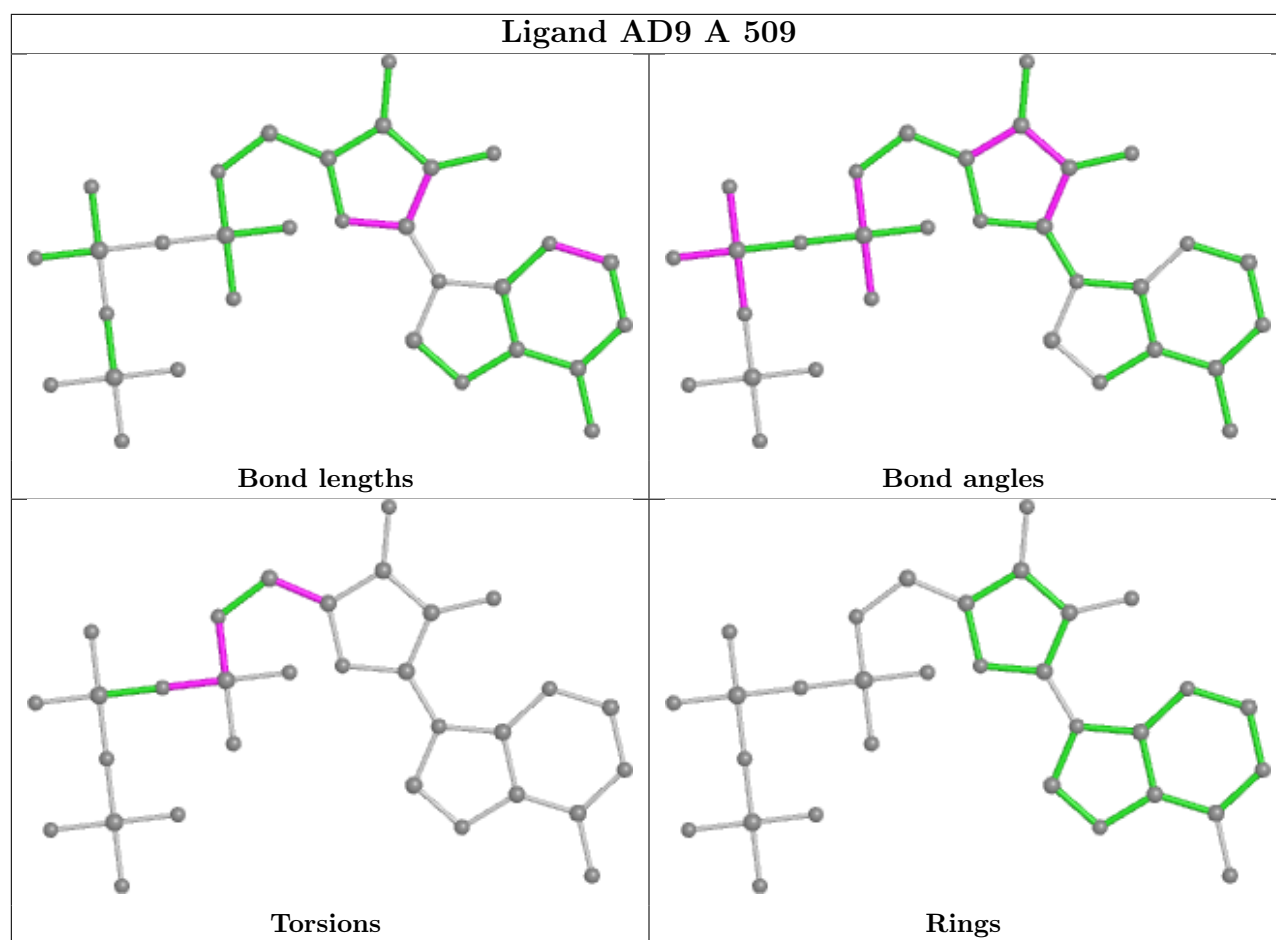
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	518	EDO	5	0
14	C	525	FLC	2	0
9	A	519	EDO	2	0
9	C	518	EDO	1	0
7	D	509	SO4	1	0
7	D	511	SO4	1	0
14	C	524	FLC	1	0
10	B	522	GOL	1	0
10	A	524	GOL	1	0
9	C	513	EDO	2	0
10	A	527	GOL	1	0
5	B	503	NAG	1	0
11	A	530	PGE	1	0
9	C	519	EDO	1	0
9	A	521	EDO	2	0
6	C	508	AD9	1	0
9	C	515	EDO	1	0
9	B	519	EDO	1	0
10	C	523	GOL	1	0
10	A	523	GOL	2	0
10	D	519	GOL	2	0
12	B	509	P4J	7	0
6	A	509	AD9	7	0
5	D	507	NAG	2	0
9	C	520	EDO	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 [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	424/459 (92%)	-0.86	4 (0%) 84 83	17, 25, 38, 70	0
1	B	425/459 (92%)	-0.68	4 (0%) 84 83	19, 30, 44, 70	0
1	C	423/459 (92%)	-0.79	3 (0%) 87 86	17, 26, 42, 73	0
1	D	423/459 (92%)	-0.75	4 (0%) 84 83	17, 26, 41, 64	0
All	All	1695/1836 (92%)	-0.77	15 (0%) 84 83	17, 27, 42, 73	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	432	THR	4.1
1	A	431	SER	3.8
1	C	64	ASN	3.7
1	B	64	ASN	3.3
1	A	8	ASN	3.2
1	C	65	GLY	3.1
1	B	431	SER	2.9
1	C	8	ASN	2.8
1	B	63	LYS	2.6
1	D	8	ASN	2.6
1	D	66	ARG	2.6
1	A	429	ASP	2.5
1	D	64	ASN	2.5
1	A	428	VAL	2.4
1	D	63	LYS	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

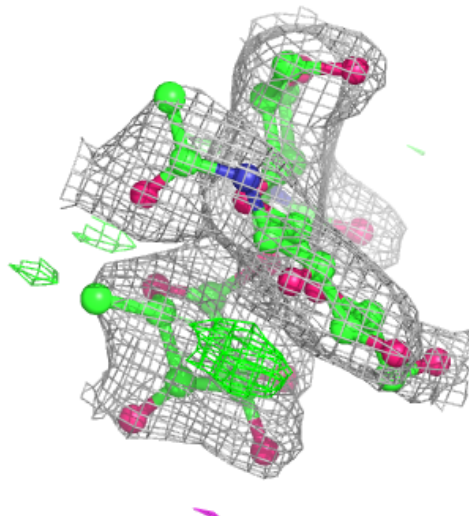
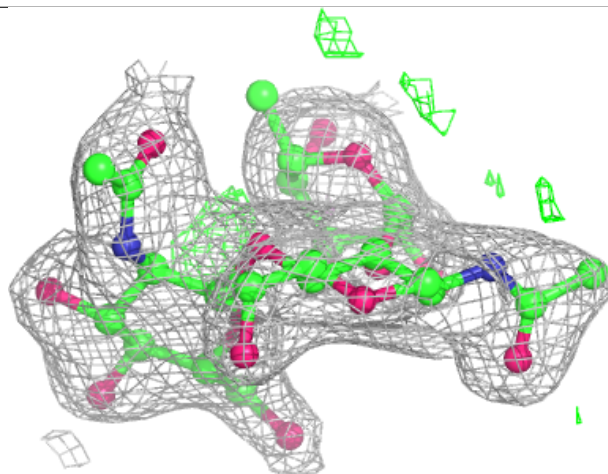
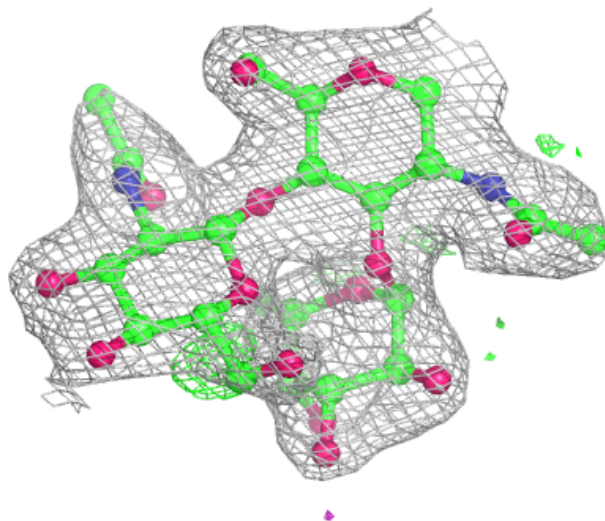
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	FUC	H	2	10/11	0.87	0.20	35,43,47,48	10
2	NAG	H	3	14/15	0.88	0.28	30,41,50,54	14
2	FUC	G	2	10/11	0.92	0.24	42,49,52,65	10
2	NAG	G	3	14/15	0.94	0.25	28,40,51,54	14
2	FUC	F	2	10/11	0.94	0.18	36,46,54,58	0
2	FUC	E	2	10/11	0.94	0.27	42,47,52,52	10
2	NAG	E	3	14/15	0.95	0.22	31,45,50,54	14
2	NAG	F	3	14/15	0.95	0.20	39,44,52,57	0
2	NAG	E	1	14/15	0.96	0.13	30,36,45,46	0
2	NAG	H	1	14/15	0.97	0.10	25,35,42,44	0
2	NAG	F	1	14/15	0.97	0.10	34,39,44,46	0
2	NAG	G	1	14/15	0.97	0.09	28,36,45,45	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.

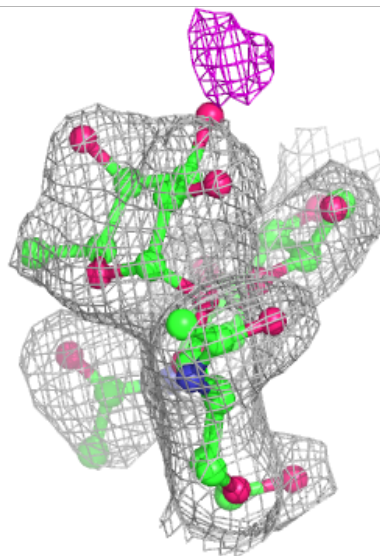
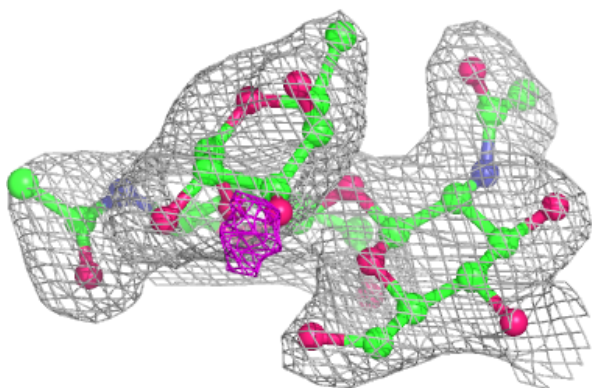
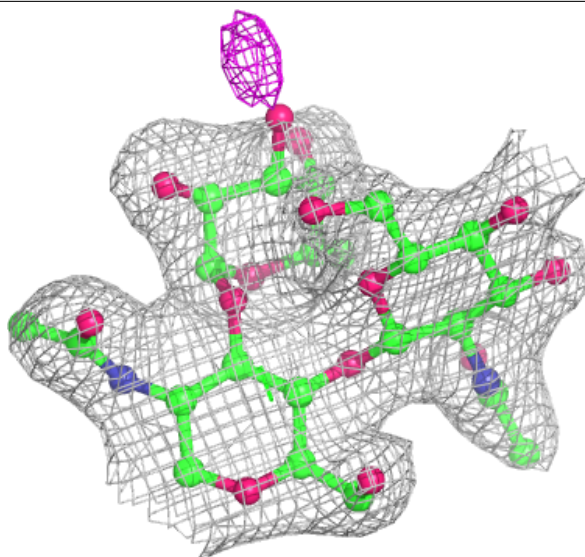
**Electron density around Chain E:**

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



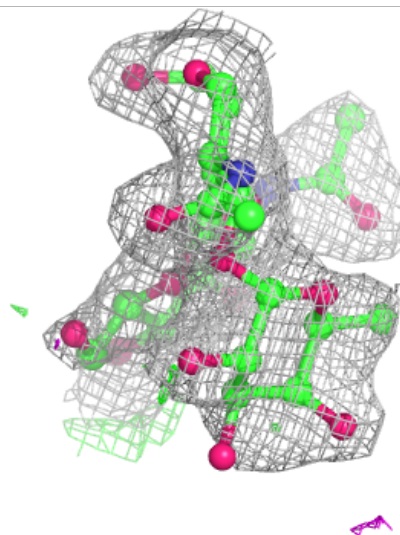
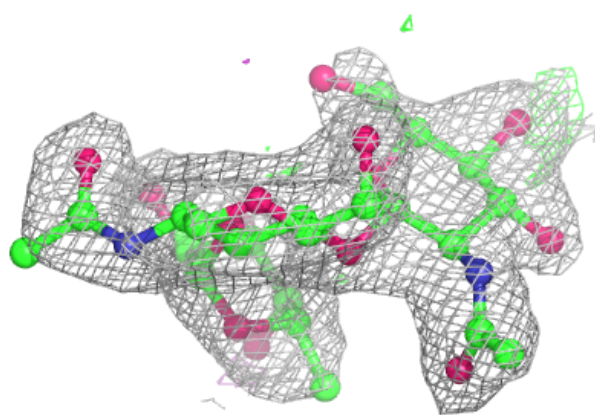
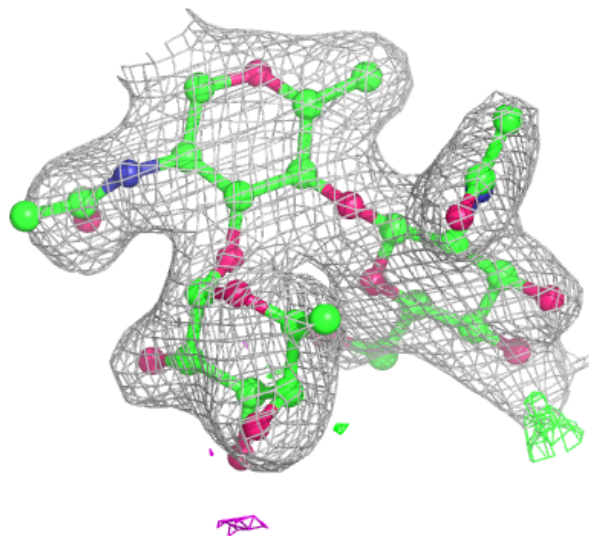
**Electron density around Chain F:**

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

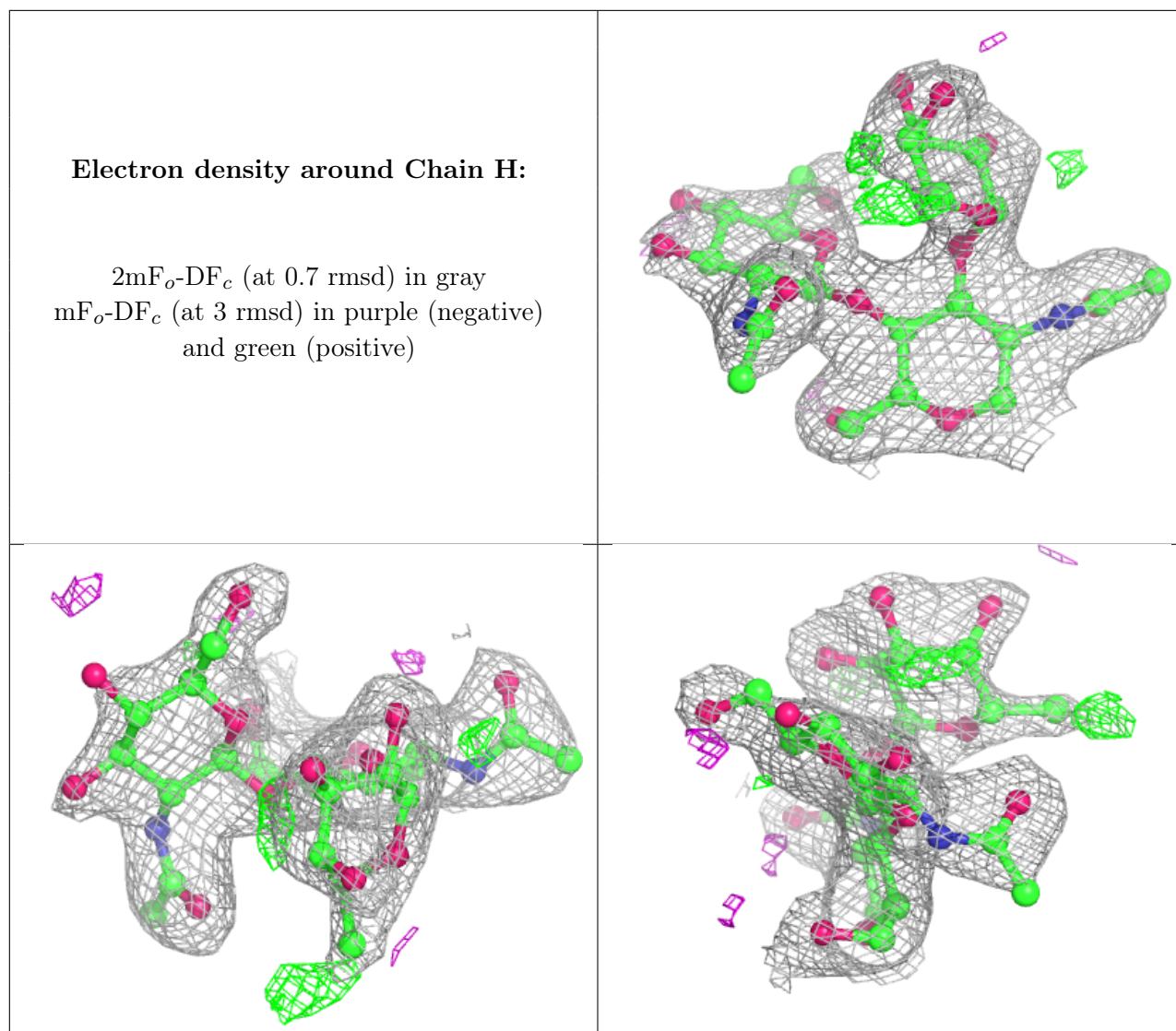


**Electron density around Chain G:**

$2mF_o-DF_c$  (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
11	PGE	A	530	7/10	0.71	0.38	45,49,51,59	7
9	EDO	C	516	4/4	0.78	0.65	59,60,67,68	4
9	EDO	C	514	4/4	0.79	0.27	41,44,49,50	4
10	GOL	B	521	6/6	0.82	0.39	61,64,69,70	6
14	FLC	C	524	13/13	0.82	0.25	38,47,53,71	13
10	GOL	C	522	6/6	0.83	0.14	51,51,54,61	0
9	EDO	A	520	4/4	0.83	0.25	40,42,45,49	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	508	14/15	0.83	0.24	48,62,69,75	0
6	AD9	A	509	31/31	0.85	0.29	28,43,48,49	31
6	AD9	C	508	31/31	0.85	0.29	35,55,62,63	31
12	P4J	B	509	38/38	0.85	0.27	24,44,55,70	38
10	GOL	B	523	6/6	0.85	0.15	46,50,51,53	6
5	NAG	D	507	14/15	0.86	0.29	37,45,52,53	14
9	EDO	B	518	4/4	0.86	0.25	46,49,50,59	4
9	EDO	C	511	4/4	0.87	0.21	37,39,49,55	4
10	GOL	D	519	6/6	0.87	0.25	58,64,67,68	6
14	FLC	C	525	13/13	0.87	0.25	27,39,43,46	13
5	NAG	B	503	14/15	0.88	0.22	43,55,66,67	14
11	PGE	A	529	10/10	0.88	0.24	28,30,40,41	10
9	EDO	A	516	4/4	0.88	0.17	29,44,47,48	0
8	NA	B	512	1/1	0.89	0.24	66,66,66,66	0
9	EDO	B	517	4/4	0.89	0.35	58,58,61,61	0
9	EDO	C	520	4/4	0.89	0.27	25,42,48,55	4
10	GOL	C	523	6/6	0.90	0.15	39,47,51,52	0
9	EDO	C	512	4/4	0.91	0.21	41,42,48,57	0
5	NAG	B	504	14/15	0.91	0.17	36,41,48,53	14
9	EDO	C	521	4/4	0.92	0.31	52,52,54,59	0
11	PGE	C	526	7/10	0.92	0.19	34,38,45,46	7
10	GOL	A	523	6/6	0.92	0.16	32,41,45,51	0
9	EDO	D	515	4/4	0.92	0.18	27,36,46,47	0
9	EDO	A	514	4/4	0.92	0.17	35,39,42,42	4
10	GOL	A	526	6/6	0.93	0.17	31,32,35,44	6
9	EDO	C	517	4/4	0.93	0.29	41,47,48,68	0
5	NAG	C	503	14/15	0.93	0.16	36,40,49,49	14
9	EDO	A	521	4/4	0.93	0.30	30,34,47,52	4
5	NAG	A	504	14/15	0.93	0.15	36,41,50,57	0
10	GOL	A	524	6/6	0.93	0.18	39,45,48,52	0
9	EDO	D	517	4/4	0.94	0.15	30,32,35,36	4
9	EDO	B	516	4/4	0.94	0.11	38,41,44,49	0
9	EDO	A	519	4/4	0.94	0.14	25,30,32,45	4
5	NAG	D	503	14/15	0.94	0.14	27,34,43,43	0
9	EDO	B	519	4/4	0.94	0.29	49,55,61,68	0
10	GOL	A	527	6/6	0.94	0.13	24,36,40,49	6
5	NAG	B	505	14/15	0.94	0.17	33,36,49,56	0
10	GOL	B	522	6/6	0.94	0.12	29,34,35,37	6
9	EDO	C	519	4/4	0.94	0.17	44,48,52,56	0
9	EDO	C	510	4/4	0.95	0.11	28,33,37,40	4
9	EDO	C	518	4/4	0.95	0.39	34,37,44,62	0
9	EDO	A	518	4/4	0.95	0.12	29,34,40,42	0

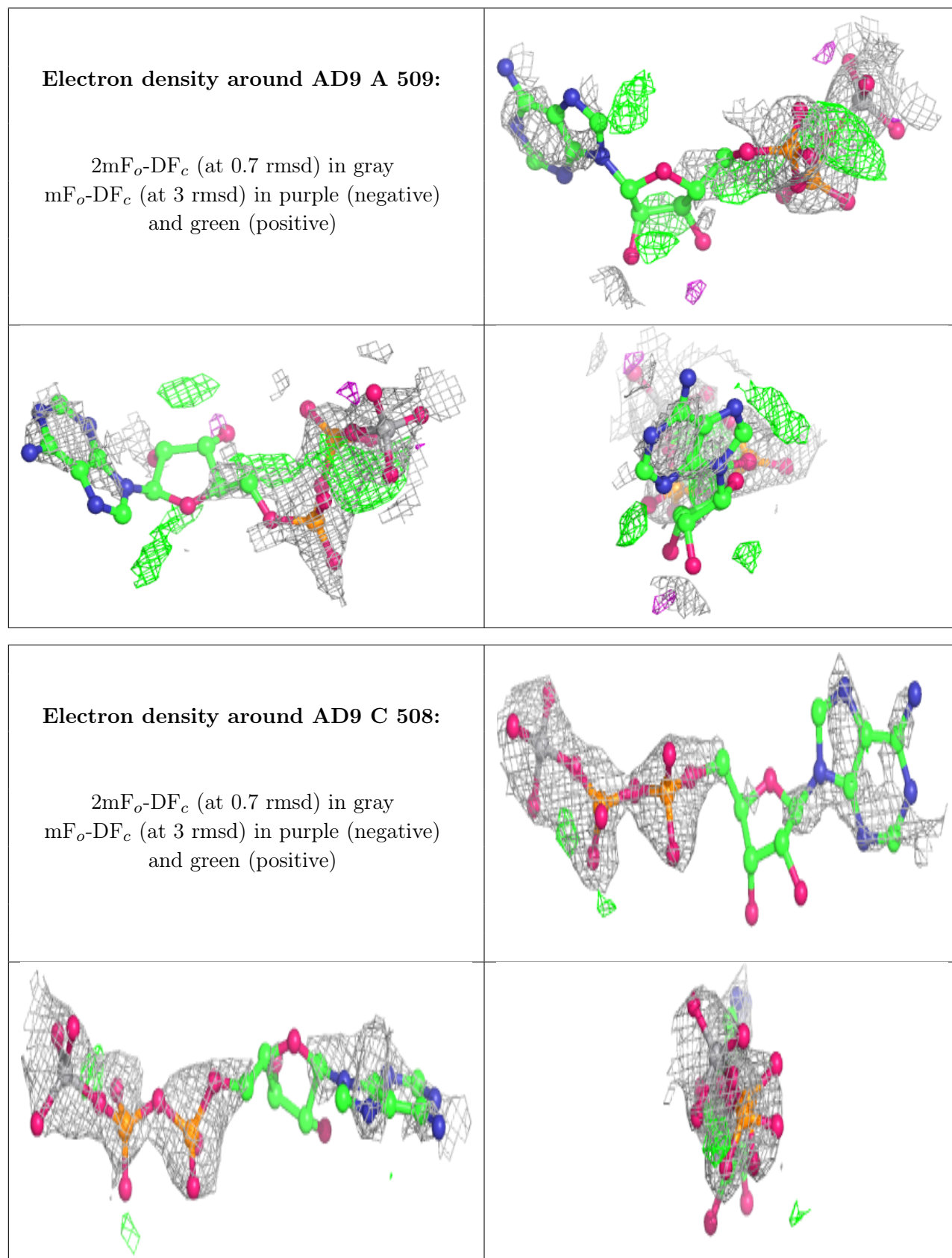
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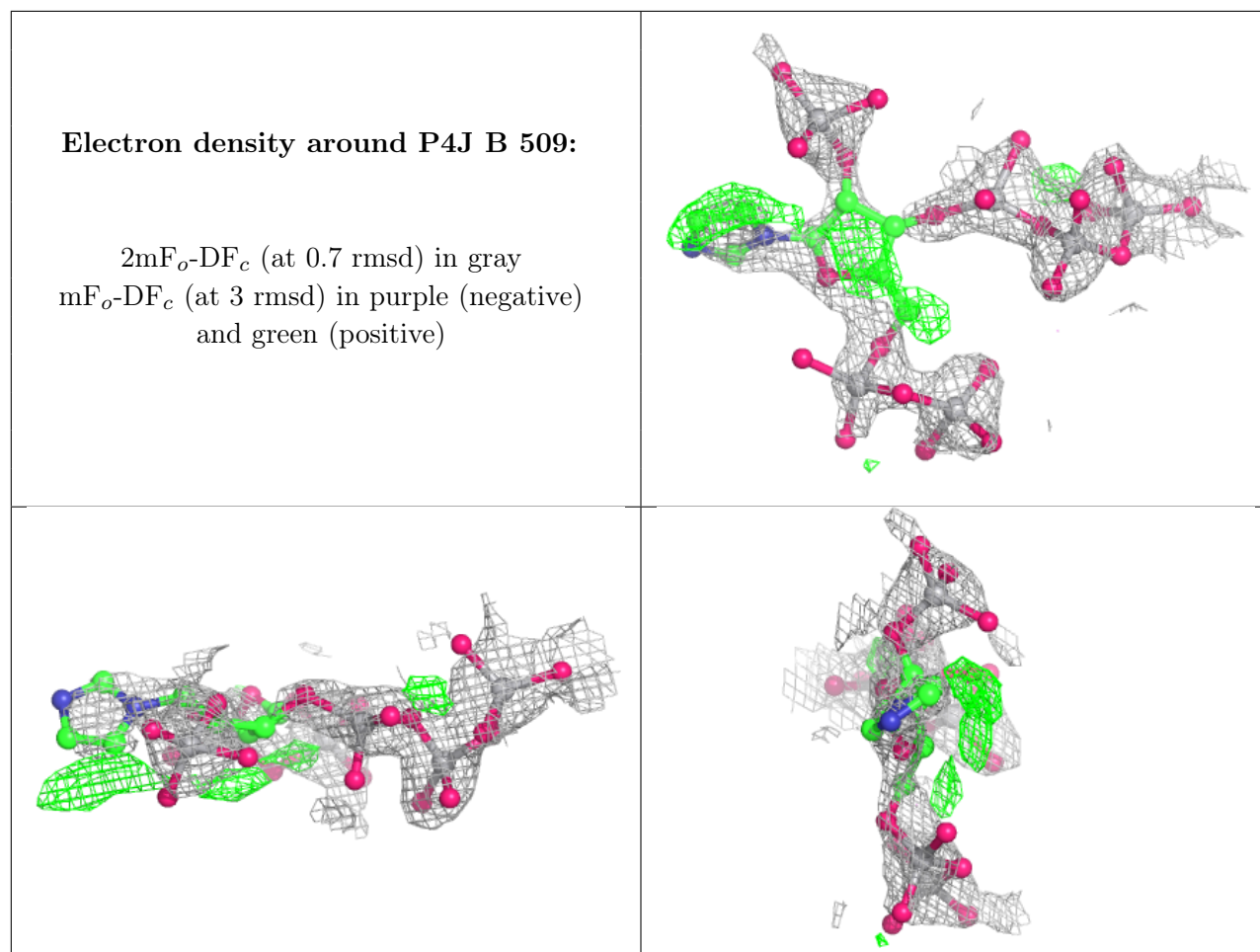
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	GOL	A	528[A]	6/6	0.95	0.17	32,34,37,38	6
10	GOL	A	528[B]	6/6	0.95	0.17	30,34,38,38	6
10	GOL	B	520	6/6	0.95	0.17	45,49,56,59	0
9	EDO	D	516	4/4	0.95	0.22	31,32,38,54	0
9	EDO	B	514	4/4	0.95	0.09	38,39,45,47	0
9	EDO	D	518	4/4	0.95	0.12	36,39,45,45	0
9	EDO	A	522	4/4	0.96	0.23	57,57,59,62	0
9	EDO	A	517	4/4	0.96	0.19	30,42,52,53	0
9	EDO	C	515	4/4	0.96	0.11	36,37,39,41	0
11	PGE	B	524	7/10	0.96	0.14	47,54,59,61	1
7	SO4	D	511	5/5	0.96	0.22	48,59,61,63	5
5	NAG	D	508	14/15	0.96	0.15	35,45,52,55	0
7	SO4	B	510	5/5	0.96	0.20	40,45,53,55	5
7	SO4	D	510	5/5	0.96	0.11	28,36,53,63	5
5	NAG	C	507	14/15	0.97	0.11	29,33,41,43	0
5	NAG	A	503	14/15	0.97	0.10	29,35,44,44	0
9	EDO	A	515	4/4	0.97	0.08	22,25,31,44	0
9	EDO	C	513	4/4	0.97	0.10	22,22,25,45	0
7	SO4	D	512	5/5	0.97	0.16	35,36,46,47	5
9	EDO	B	513	4/4	0.97	0.18	39,42,47,49	0
7	SO4	D	513	5/5	0.97	0.19	43,43,49,51	5
7	SO4	C	509	5/5	0.97	0.28	40,40,43,49	5
7	SO4	A	511	5/5	0.98	0.21	36,40,50,52	5
9	EDO	B	515	4/4	0.98	0.17	35,40,42,47	0
10	GOL	A	525	6/6	0.98	0.08	23,25,28,30	0
7	SO4	B	511	5/5	0.99	0.09	37,38,45,49	5
8	NA	A	513	1/1	0.99	0.05	17,17,17,17	0
7	SO4	D	509	5/5	0.99	0.12	22,24,29,33	5
7	SO4	A	510	5/5	0.99	0.06	31,33,35,41	0
4	FE	D	502	1/1	0.99	0.03	36,36,36,36	1
7	SO4	A	512	5/5	0.99	0.09	27,37,42,45	5
4	FE	B	502	1/1	0.99	0.04	27,27,27,27	1
3	ZN	D	501	1/1	1.00	0.01	25,25,25,25	1
3	ZN	C	501	1/1	1.00	0.03	30,30,30,30	0
8	NA	D	514	1/1	1.00	0.07	15,15,15,15	0
4	FE	A	502	1/1	1.00	0.02	26,26,26,26	1
3	ZN	A	501	1/1	1.00	0.03	27,27,27,27	1
13	CL	B	525	1/1	1.00	0.03	21,21,21,21	1
3	ZN	B	501	1/1	1.00	0.03	29,29,29,29	0
4	FE	C	502	1/1	1.00	0.03	25,25,25,25	1

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.