



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 07:16 PM BST

PDB ID : 6Q4R  
Title : High-resolution crystal structure of ERAP1 with bound phosphinic transition-state analogue inhibitor  
Authors : Giastas, P.; Neu, M.; Rowland, P.; Stratikos, E.  
Deposited on : 2018-12-06  
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

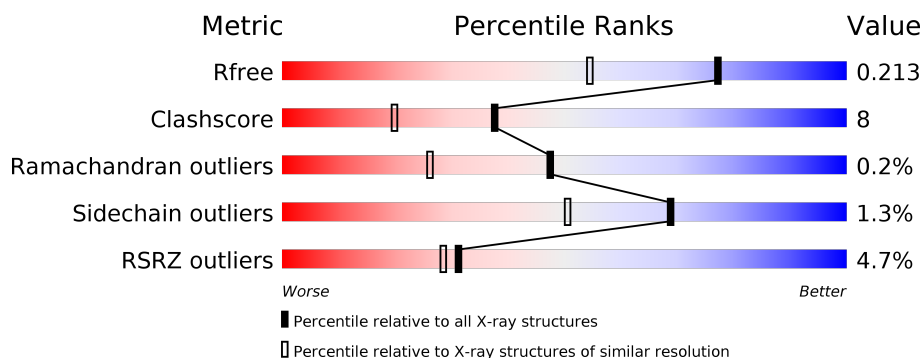
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	912	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
3	C	3	<div> <div>67%</div> <div>33%</div> </div>

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
11	PG4	A	1043	-	-	X	-
2	NAG	B	2	-	-	-	X
3	NAG	C	2	-	-	-	X
3	BMA	C	3	-	-	-	X
4	NAG	A	1006	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 8514 atoms, of which 285 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 Endoplasmic reticulum aminopeptidase 1, Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	855	Total	C	N	O	S	5	42	0
			7104	4594	1160	1310	40			

There are 3 discrepancies between the modelled and reference sequences:

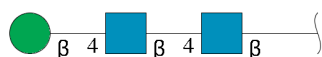
Chain	Residue	Modelled	Actual	Comment	Reference
A	511	GLY	-	linker	UNP Q9NZ08
A	512	SER	-	linker	UNP Q9NZ08
A	513	GLY	-	linker	UNP Q9NZ08

- Molecule 2 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
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

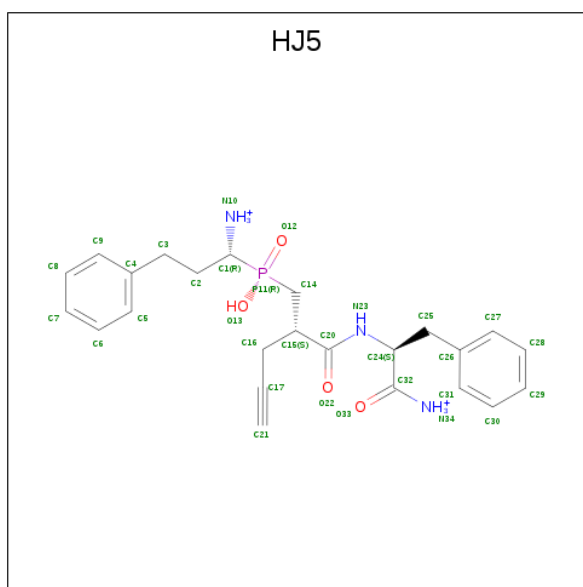


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

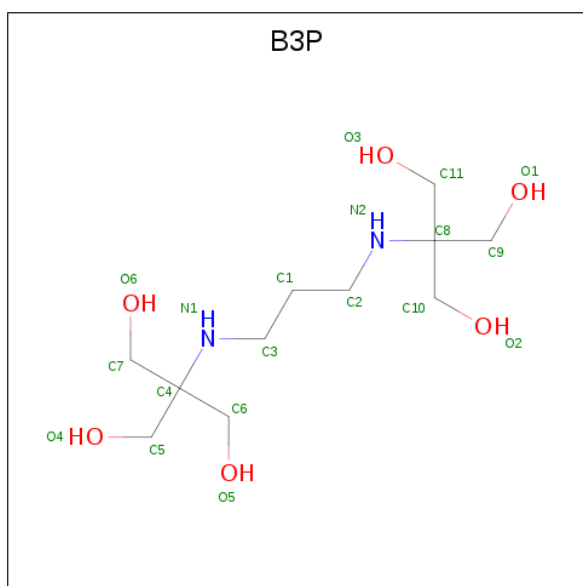
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is [(1 {R})-1-[(2 {S})-2-[(2 {S})-1-azaniumyl-1-oxidanylidene-3-phenyl-propa n-2-yl]carbamoyl]pent-4-ynyl]-oxidanyl-phosphoryl]-3-phenyl-propyl]azanium (three-letter code: HJ5) (formula:  $C_{24}H_{32}N_3O_4P$ ) (labeled as "Ligand of Interest" by author).



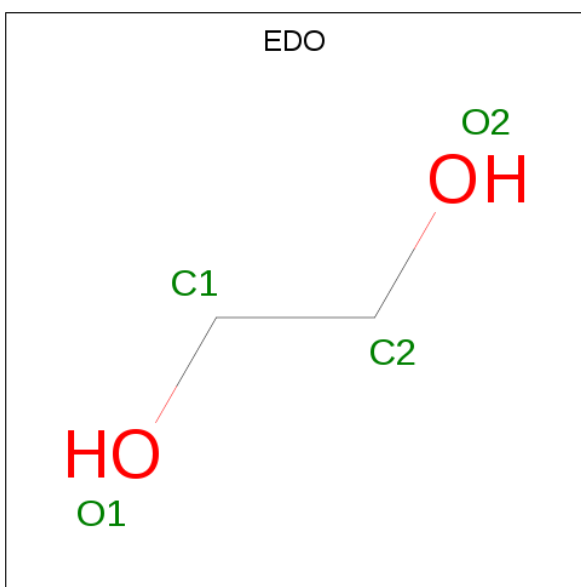
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	H	N	O	P	0	0
			63	24	31	3	4	1		

- Molecule 7 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O		
			45	11	26	2	6	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		

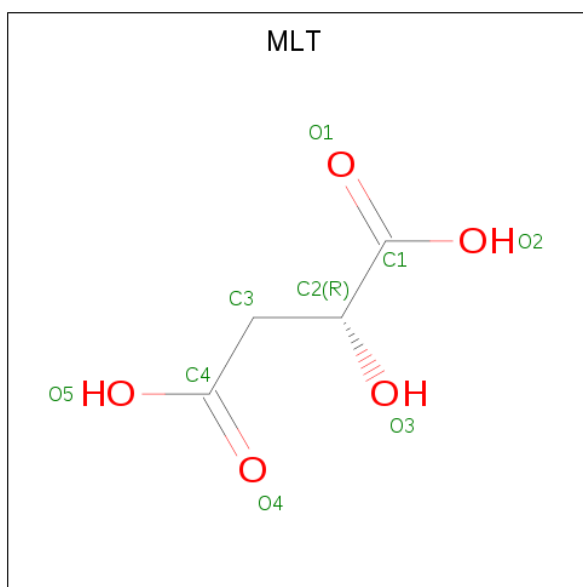
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		
8	A	1	Total	C	H	O	0	0
			10	2	6	2		

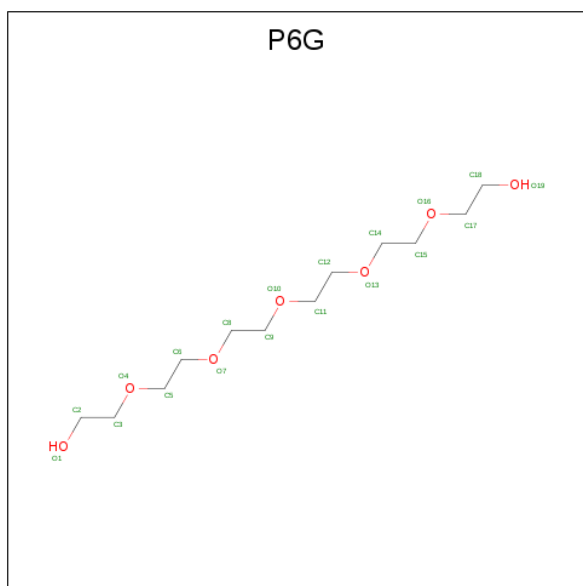
- Molecule 9 is D-MALATE (three-letter code: MLT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).





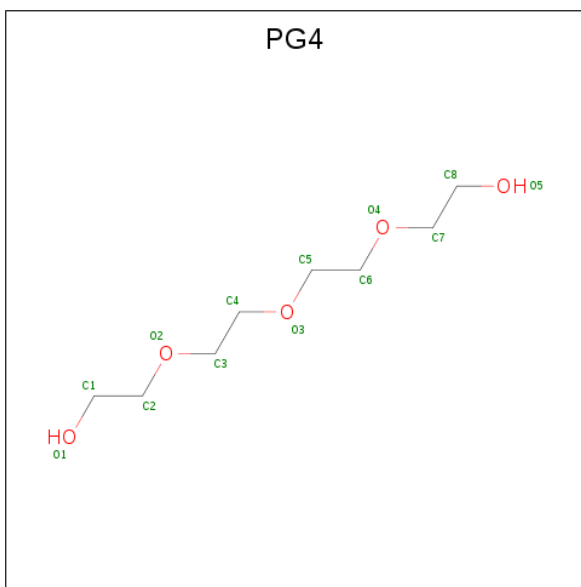
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			13	4	4	5		

- Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			45	12	26	7		

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	3	Total	Na	0	0
			3	3		

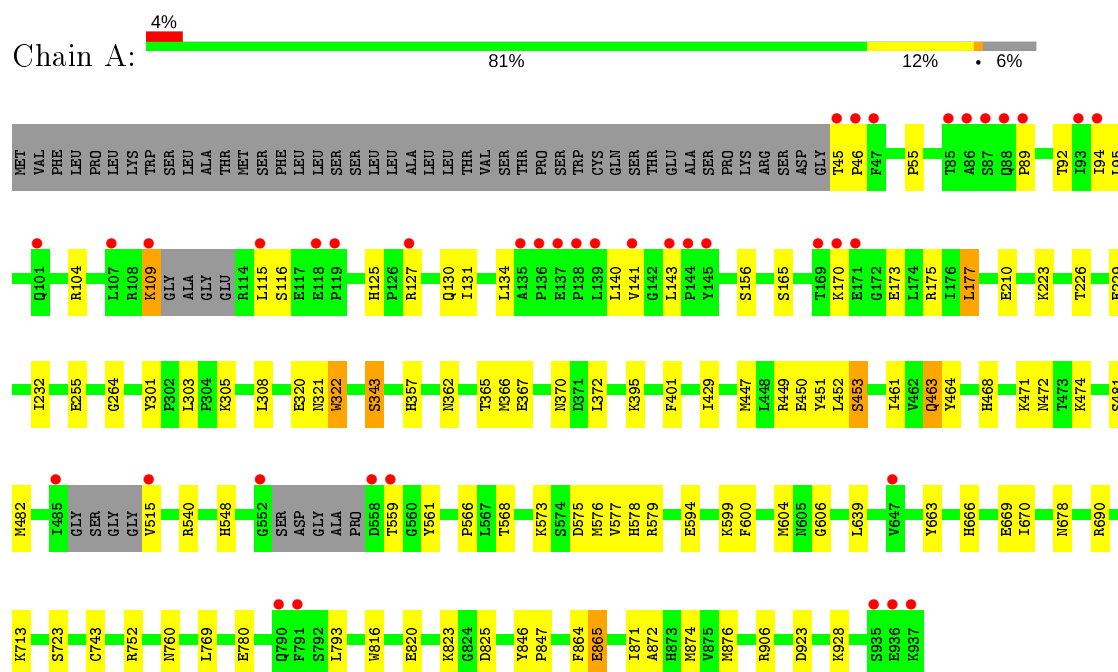
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	814	Total	O	0	0
			814	814		

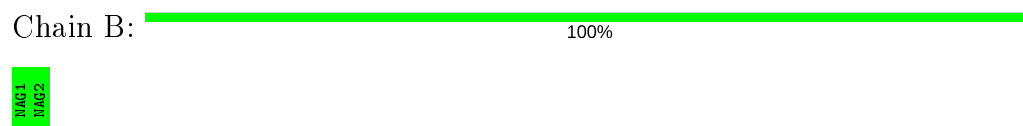
### 3 Residue-property plots

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.

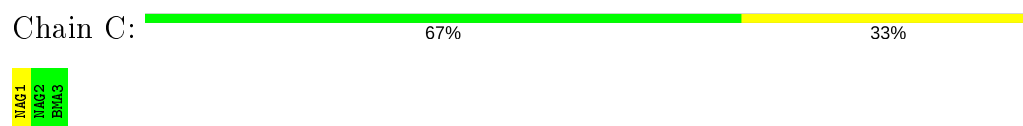
- Molecule 1: Endoplasmic reticulum aminopeptidase 1,Endoplasmic reticulum aminopeptidase 1



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



- Molecule 3: beta-D-mannopyranose-(1-4)-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 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.68Å 116.67Å 147.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.45 – 1.60 91.45 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (91.45-1.60) 99.5 (91.45-1.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.180 , 0.213 0.180 , 0.213	Depositor DCC
$R_{free}$ test set	6495 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: HJ5, ZN, BMA, NAG, NA, B3P, EDO, PG4, P6G, MLT

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	0.37	2/7401 (0.0%)	0.53	0/10020

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	743[A]	CYS	CB-SG	5.94	1.92	1.82
1	A	743[B]	CYS	CB-SG	5.94	1.92	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7104	0	7156	107	0
2	B	28	0	25	0	0
3	C	39	0	34	1	0
4	A	28	0	26	1	0
5	A	1	0	0	0	0
6	A	32	31	0	0	0
7	A	19	26	26	0	0
8	A	120	180	180	23	0
9	A	9	4	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	19	26	26	7	0
11	A	13	18	18	11	0
12	A	3	0	0	0	0
13	A	814	0	0	22	0
All	All	8229	285	7495	115	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 8.

The worst 5 of 115 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:578:HIS:HB3	10:A:1042:P6G:H111	1.50	0.92
1:A:559:THR:HG23	1:A:561:TYR:H	1.35	0.91
1:A:669:GLU:HA	8:A:1021:EDO:H21	1.64	0.80
1:A:760:ASN:OD1	13:A:1101:HOH:O	1.99	0.80
1:A:579[A]:ARG:HB3	11:A:1043:PG4:H72	1.64	0.78

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	889/912 (98%)	864 (97%)	23 (3%)	2 (0%)	47 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	SER
1	A	865	GLU

### 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	807/811 (100%)	796 (99%)	11 (1%)	67 47

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	LYS
1	A	322	TRP
1	A	663	TYR
1	A	177	LEU
1	A	463	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	GLN
1	A	321	ASN
1	A	446	ASN
1	A	463	GLN
1	A	628	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	B	1	1,2	14,14,15	0.33	0	17,19,21	0.42	0
2	NAG	B	2	2	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	C	1	1,3	14,14,15	0.41	0	17,19,21	0.43	0
3	NAG	C	2	3	14,14,15	0.27	0	17,19,21	0.42	0
3	BMA	C	3	3	11,11,12	0.61	0	15,15,17	0.74	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

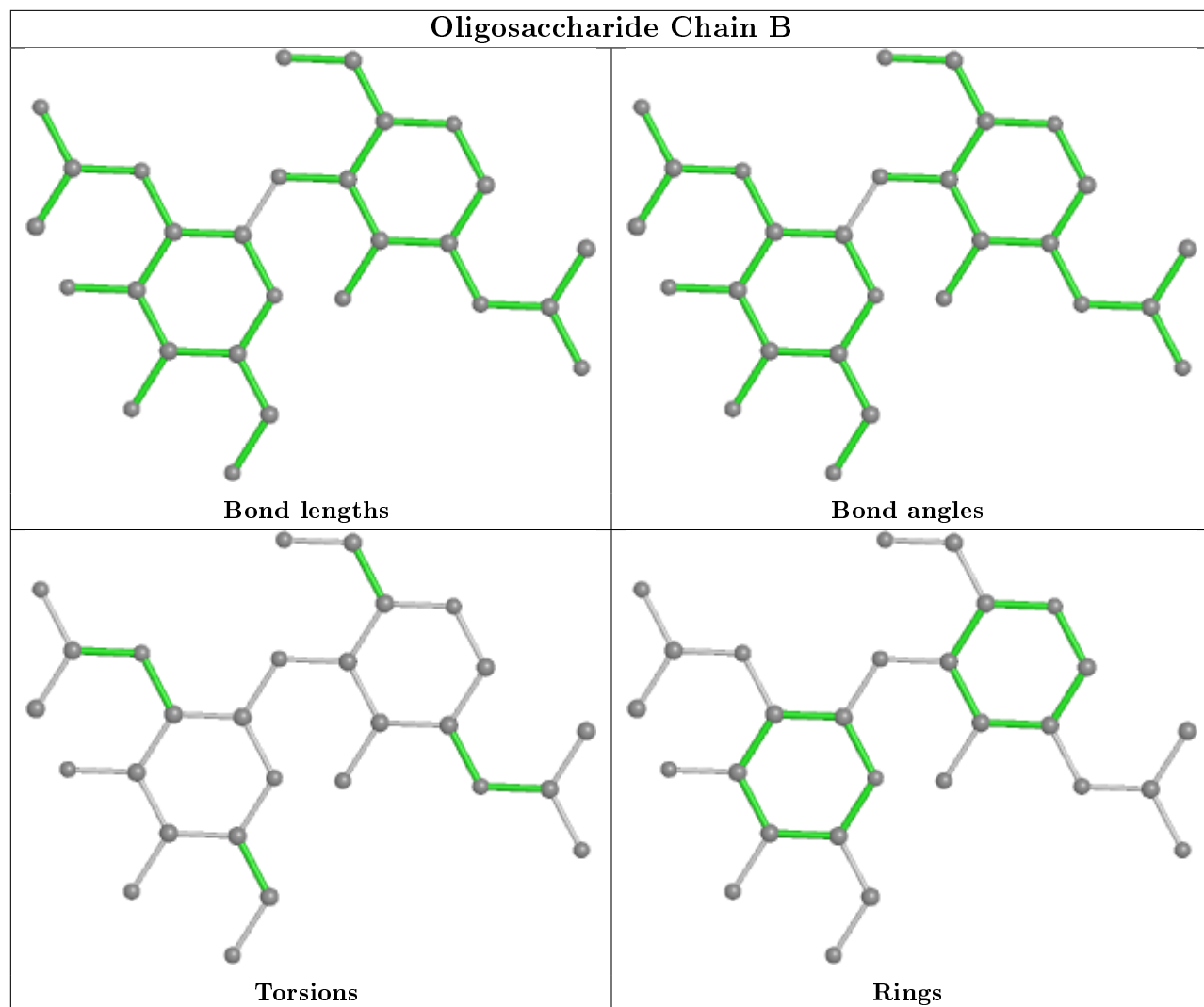
There are no ring outliers.

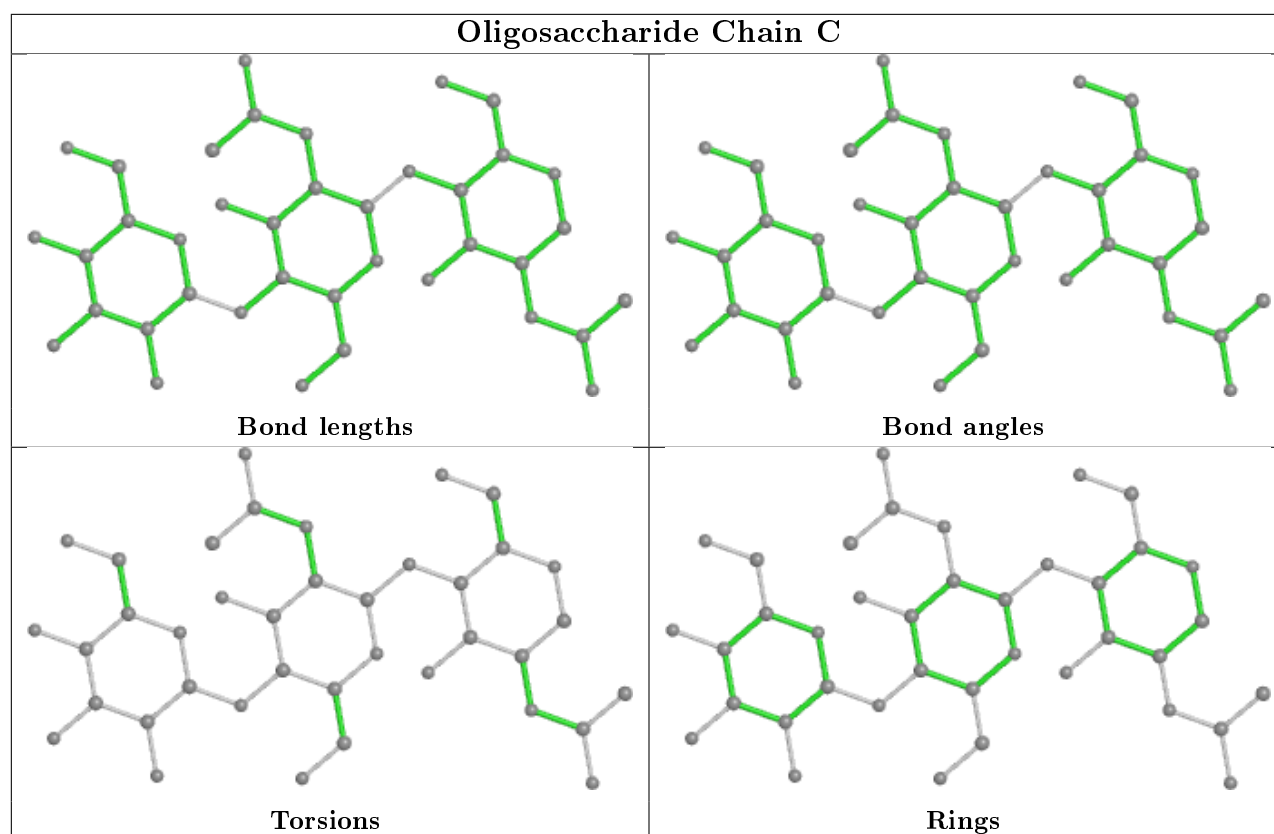
1 monomer is involved in 1 short contact:

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

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







## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 4 are monoatomic - leaving 37 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	$\# Z  > 2$
8	EDO	A	1017	-	3,3,3	0.33	0	2,2,2	0.44	0
8	EDO	A	1040	-	3,3,3	0.48	0	2,2,2	0.32	0
8	EDO	A	1038	-	3,3,3	0.46	0	2,2,2	0.46	0
8	EDO	A	1039	-	3,3,3	0.45	0	2,2,2	0.16	0
8	EDO	A	1014	-	3,3,3	0.29	0	2,2,2	0.24	0
11	PG4	A	1043	-	12,12,12	0.56	0	11,11,11	0.44	0
8	EDO	A	1031	-	3,3,3	0.47	0	2,2,2	0.48	0
8	EDO	A	1016	-	3,3,3	0.34	0	2,2,2	0.72	0
4	NAG	A	1006	1	14,14,15	0.37	0	17,19,21	0.44	0
8	EDO	A	1029	-	3,3,3	0.43	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	EDO	A	1025	-	3,3,3	0.41	0	2,2,2	0.39	0
8	EDO	A	1028	-	3,3,3	0.51	0	2,2,2	0.11	0
8	EDO	A	1024	-	3,3,3	0.42	0	2,2,2	0.35	0
8	EDO	A	1036	-	3,3,3	0.48	0	2,2,2	0.23	0
8	EDO	A	1033	-	3,3,3	0.32	0	2,2,2	0.36	0
8	EDO	A	1027	-	3,3,3	0.39	0	2,2,2	0.36	0
10	P6G	A	1042	-	18,18,18	0.54	0	17,17,17	0.40	0
8	EDO	A	1022	-	3,3,3	0.45	0	2,2,2	0.47	0
8	EDO	A	1030	-	3,3,3	0.46	0	2,2,2	0.12	0
8	EDO	A	1032	-	3,3,3	0.35	0	2,2,2	0.39	0
8	EDO	A	1020	-	3,3,3	0.25	0	2,2,2	0.37	0
4	NAG	A	1007	1	14,14,15	0.60	0	17,19,21	0.56	0
9	MLT	A	1041	-	2,8,8	0.36	0	3,10,10	0.50	0
8	EDO	A	1034	-	3,3,3	0.36	0	2,2,2	0.71	0
7	B3P	A	1010	-	18,18,18	0.59	0	21,23,23	1.21	4 (19%)
8	EDO	A	1012	-	3,3,3	0.50	0	2,2,2	0.24	0
8	EDO	A	1019	-	3,3,3	0.14	0	2,2,2	0.91	0
8	EDO	A	1013	-	3,3,3	0.41	0	2,2,2	0.44	0
6	HJ5	A	1009	5	29,33,33	1.10	3 (10%)	31,44,44	0.94	2 (6%)
8	EDO	A	1021	-	3,3,3	0.31	0	2,2,2	0.55	0
8	EDO	A	1035	-	3,3,3	0.47	0	2,2,2	0.46	0
8	EDO	A	1037	-	3,3,3	0.46	0	2,2,2	0.38	0
8	EDO	A	1015	-	3,3,3	0.41	0	2,2,2	0.38	0
8	EDO	A	1018	-	3,3,3	0.50	0	2,2,2	0.04	0
8	EDO	A	1026	-	3,3,3	0.37	0	2,2,2	0.37	0
8	EDO	A	1023	-	3,3,3	0.47	0	2,2,2	0.15	0
8	EDO	A	1011	-	3,3,3	0.43	0	2,2,2	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	1017	-	-	1/1/1/1	-
8	EDO	A	1040	-	-	0/1/1/1	-
8	EDO	A	1038	-	-	0/1/1/1	-
8	EDO	A	1039	-	-	1/1/1/1	-
8	EDO	A	1014	-	-	0/1/1/1	-
11	PG4	A	1043	-	-	6/10/10/10	-
8	EDO	A	1031	-	-	1/1/1/1	-
8	EDO	A	1016	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
8	EDO	A	1029	-	-	0/1/1/1	-
8	EDO	A	1025	-	-	1/1/1/1	-
8	EDO	A	1028	-	-	1/1/1/1	-
8	EDO	A	1024	-	-	1/1/1/1	-
8	EDO	A	1036	-	-	0/1/1/1	-
8	EDO	A	1033	-	-	1/1/1/1	-
8	EDO	A	1027	-	-	0/1/1/1	-
10	P6G	A	1042	-	-	11/16/16/16	-
8	EDO	A	1022	-	-	0/1/1/1	-
8	EDO	A	1030	-	-	1/1/1/1	-
8	EDO	A	1032	-	-	1/1/1/1	-
8	EDO	A	1020	-	-	0/1/1/1	-
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
9	MLT	A	1041	-	-	0/2/8/8	-
8	EDO	A	1034	-	-	0/1/1/1	-
7	B3P	A	1010	-	-	0/28/28/28	-
8	EDO	A	1012	-	-	0/1/1/1	-
8	EDO	A	1019	-	-	1/1/1/1	-
8	EDO	A	1013	-	-	0/1/1/1	-
6	HJ5	A	1009	5	-	0/28/35/35	0/2/2/2
8	EDO	A	1021	-	-	1/1/1/1	-
8	EDO	A	1035	-	-	1/1/1/1	-
8	EDO	A	1037	-	-	0/1/1/1	-
8	EDO	A	1015	-	-	1/1/1/1	-
8	EDO	A	1018	-	-	1/1/1/1	-
8	EDO	A	1026	-	-	0/1/1/1	-
8	EDO	A	1023	-	-	1/1/1/1	-
8	EDO	A	1011	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1009	HJ5	C17-C21	3.47	1.28	1.18
6	A	1009	HJ5	C32-N34	3.41	1.41	1.32
6	A	1009	HJ5	P11-C14	2.27	1.81	1.79

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1009	HJ5	O22-C20-C15	-2.79	118.49	122.12
7	A	1010	B3P	C7-C4-C5	-2.72	104.29	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1009	HJ5	O33-C32-N34	-2.23	119.12	123.00
7	A	1010	B3P	O4-C5-C4	-2.20	107.19	111.63
7	A	1010	B3P	O6-C7-C4	-2.12	107.34	111.63

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1042	P6G	C5-C6-O7-C8
10	A	1042	P6G	O4-C5-C6-O7
10	A	1042	P6G	O1-C2-C3-O4
4	A	1006	NAG	O5-C5-C6-O6
11	A	1043	PG4	O3-C5-C6-O4

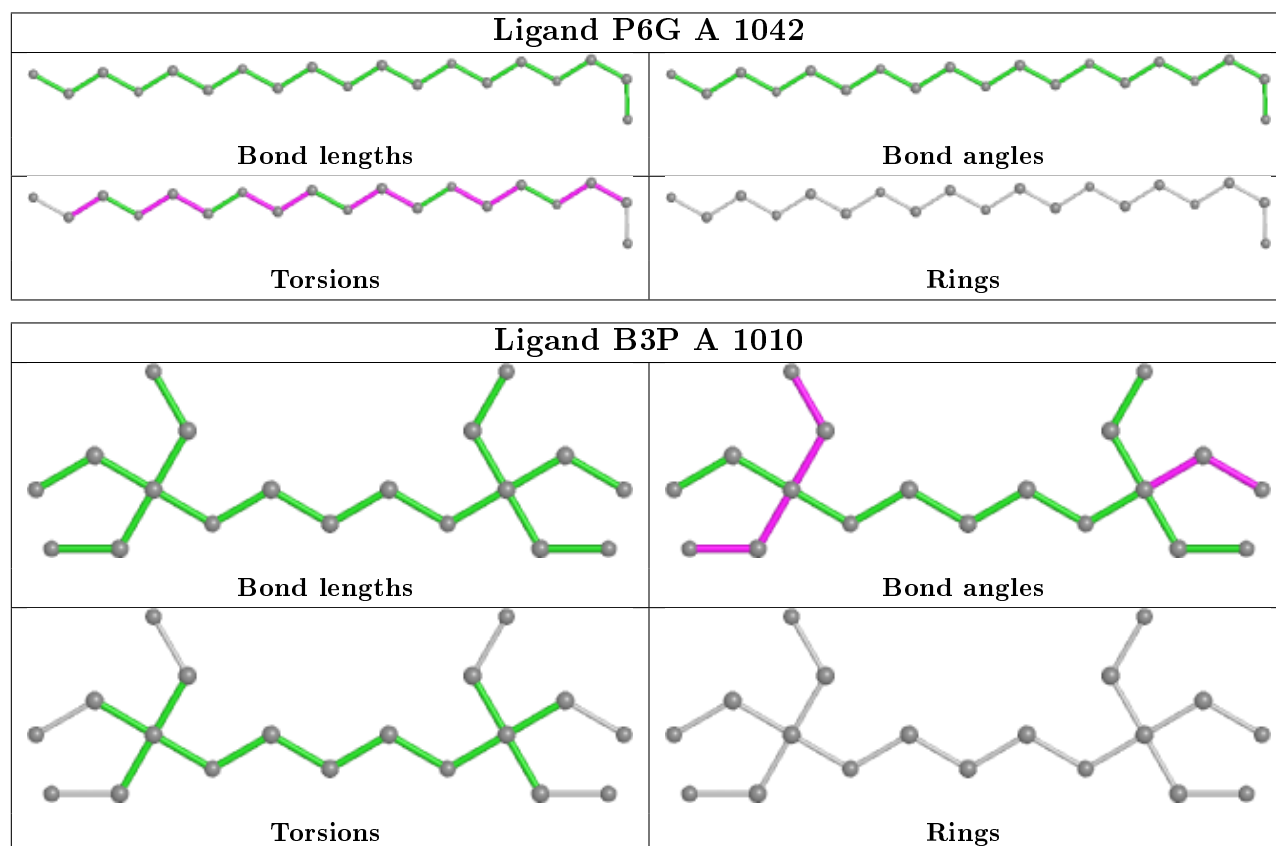
There are no ring outliers.

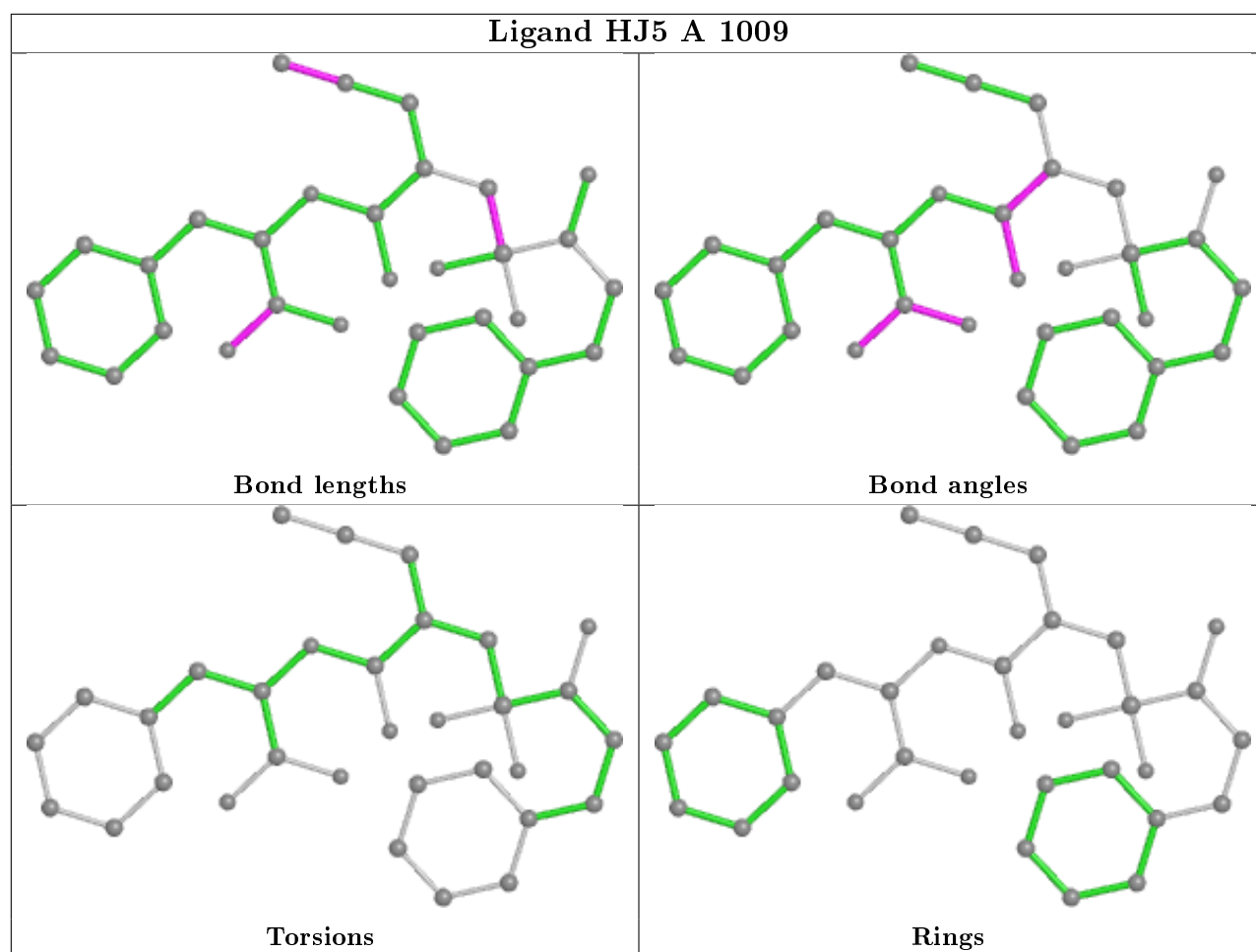
17 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1039	EDO	1	0
11	A	1043	PG4	11	0
8	A	1016	EDO	3	0
4	A	1006	NAG	1	0
8	A	1029	EDO	1	0
8	A	1025	EDO	1	0
8	A	1033	EDO	2	0
8	A	1027	EDO	2	0
10	A	1042	P6G	7	0
8	A	1032	EDO	2	0
8	A	1020	EDO	2	0
9	A	1041	MLT	1	0
8	A	1019	EDO	2	0
8	A	1013	EDO	3	0
8	A	1021	EDO	1	0
8	A	1018	EDO	1	0
8	A	1023	EDO	2	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	855/912 (93%)	0.39	40 (4%) 31 28	14, 22, 45, 82	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	PRO	7.5
1	A	45	THR	6.9
1	A	552	GLY	6.4
1	A	115	LEU	6.0
1	A	46	PRO	5.8

### 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.

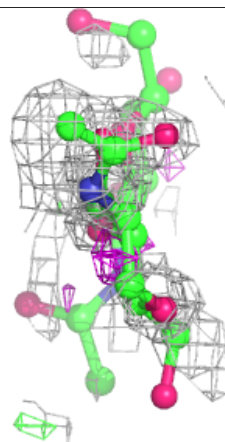
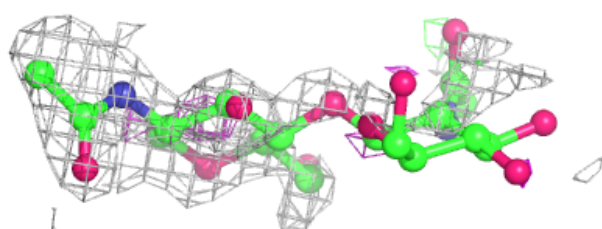
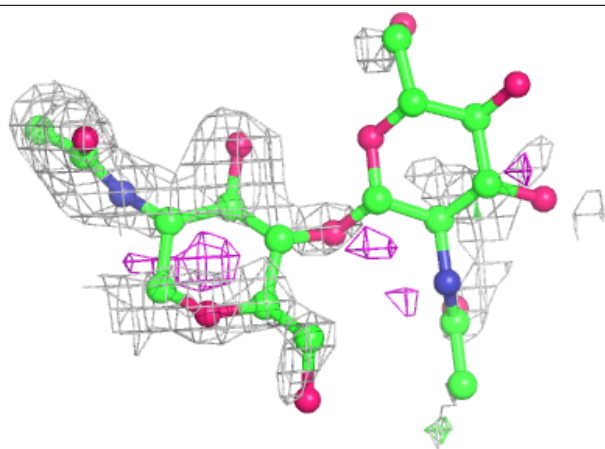
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.33	0.76	58,68,72,78	0
3	BMA	C	3	11/12	0.40	0.55	60,63,66,67	0
2	NAG	B	1	14/15	0.43	0.36	44,54,64,70	0
3	NAG	C	2	14/15	0.55	0.41	51,57,62,67	0
3	NAG	C	1	14/15	0.84	0.21	22,35,44,49	0

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.

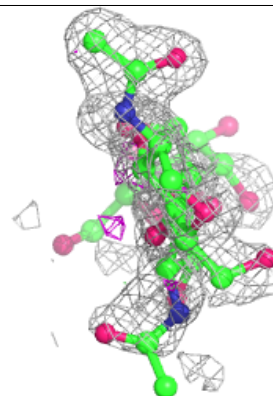
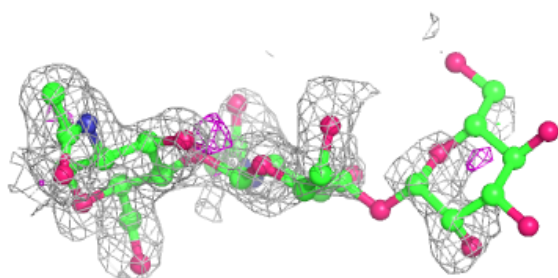
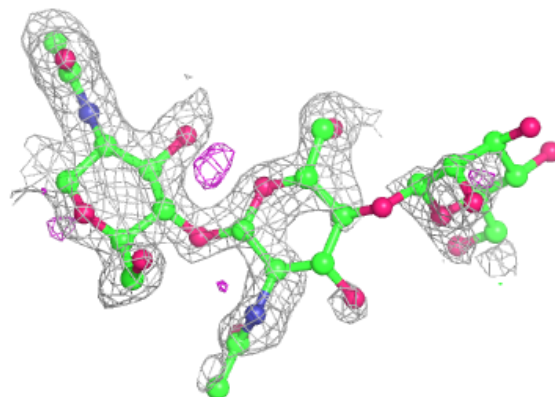


**Electron density around Chain B:**

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

**Electron density around Chain C:**

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



## 6.4 Ligands ⓘ

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.

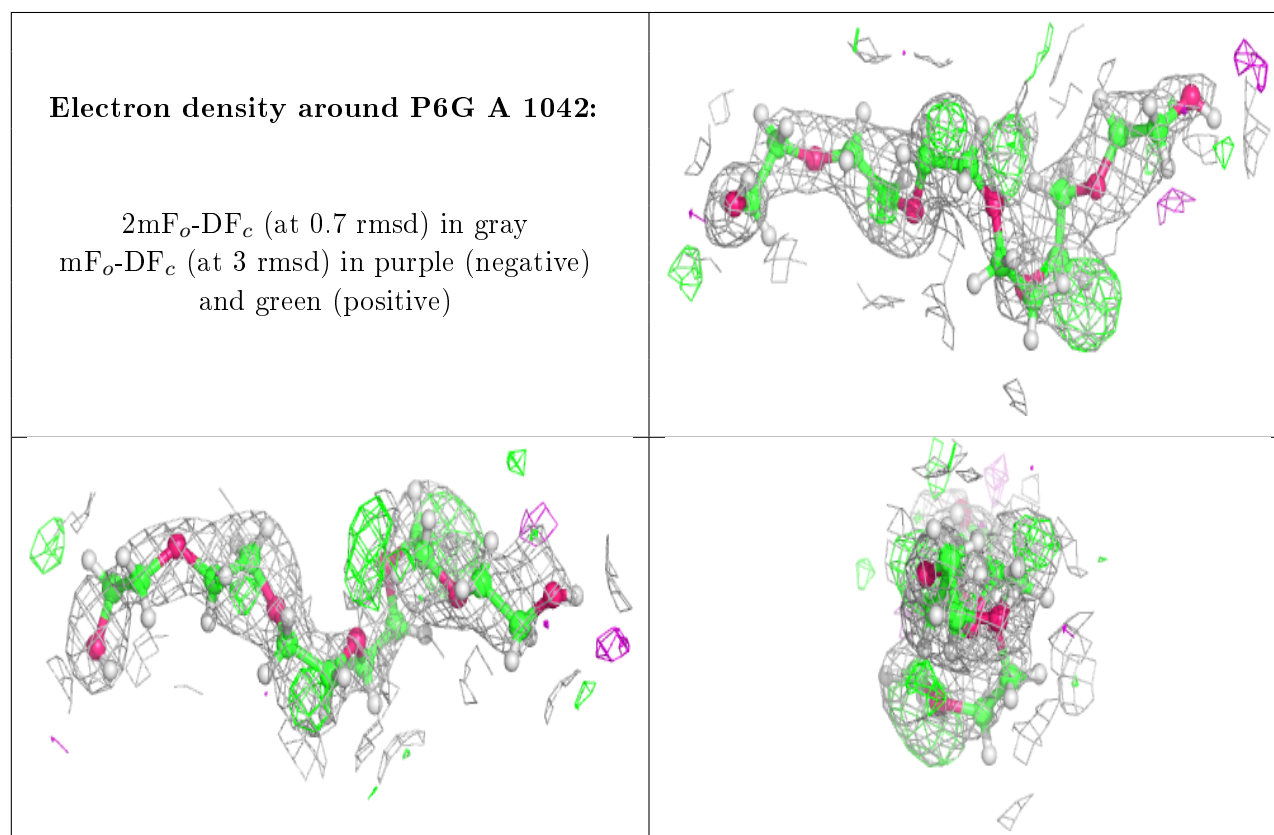
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	1007	14/15	0.46	0.29	40,52,58,64	0
4	NAG	A	1006	14/15	0.51	0.48	56,65,72,73	0
8	EDO	A	1035	4/4	0.67	0.34	37,46,55,55	10
8	EDO	A	1029	4/4	0.71	0.25	41,49,53,53	0
10	P6G	A	1042	19/19	0.74	0.20	16,39,45,49	45
11	PG4	A	1043	13/13	0.76	0.24	15,26,37,44	31
8	EDO	A	1026	4/4	0.78	0.27	34,43,54,56	10
8	EDO	A	1032	4/4	0.79	0.19	37,45,54,54	0
8	EDO	A	1031	4/4	0.79	0.17	51,61,68,68	0
8	EDO	A	1033	4/4	0.80	0.13	41,51,53,64	0
8	EDO	A	1038	4/4	0.82	0.14	33,39,40,48	0
8	EDO	A	1034	4/4	0.82	0.18	26,31,36,43	10
8	EDO	A	1037	4/4	0.83	0.17	40,48,50,50	10
8	EDO	A	1040	4/4	0.84	0.12	42,51,62,71	0
9	MLT	A	1041	9/9	0.84	0.20	32,51,61,69	0
8	EDO	A	1025	4/4	0.85	0.23	28,46,54,55	0
8	EDO	A	1012	4/4	0.86	0.12	21,30,43,43	0
8	EDO	A	1039	4/4	0.86	0.09	50,60,61,66	0
7	B3P	A	1010	19/19	0.87	0.12	22,33,41,42	0
8	EDO	A	1036	4/4	0.88	0.14	41,53,61,64	0
8	EDO	A	1030	4/4	0.89	0.12	40,48,52,59	0
8	EDO	A	1021	4/4	0.90	0.19	34,45,51,55	0
8	EDO	A	1014	4/4	0.91	0.19	11,20,27,27	10
8	EDO	A	1019	4/4	0.91	0.13	26,31,41,41	0
8	EDO	A	1017	4/4	0.91	0.15	30,36,42,42	0
8	EDO	A	1022	4/4	0.91	0.09	26,33,34,40	0
8	EDO	A	1028	4/4	0.91	0.24	23,47,63,69	0
8	EDO	A	1018	4/4	0.91	0.20	23,49,62,62	0
8	EDO	A	1024	4/4	0.91	0.13	31,38,39,39	0
8	EDO	A	1016	4/4	0.92	0.24	25,33,40,40	0
8	EDO	A	1027	4/4	0.92	0.15	36,51,62,65	0
8	EDO	A	1013	4/4	0.93	0.18	19,26,38,38	0
8	EDO	A	1020	4/4	0.93	0.23	18,23,29,29	10
8	EDO	A	1023	4/4	0.93	0.15	28,38,51,53	0
8	EDO	A	1015	4/4	0.94	0.12	20,48,52,61	0
6	HJ5	A	1009	32/32	0.94	0.11	15,20,33,45	0
8	EDO	A	1011	4/4	0.95	0.08	21,25,27,31	0

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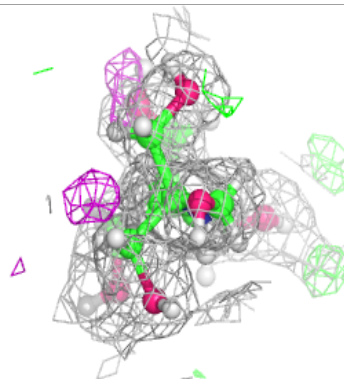
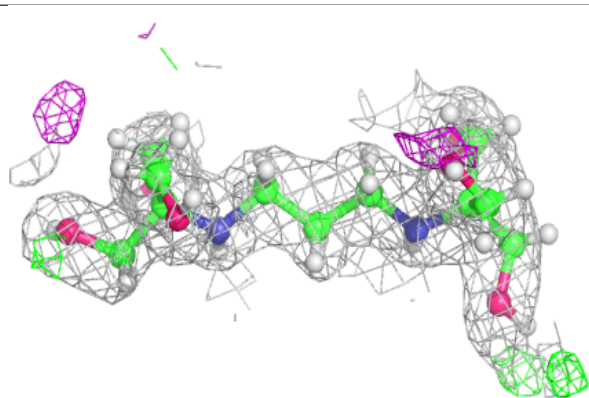
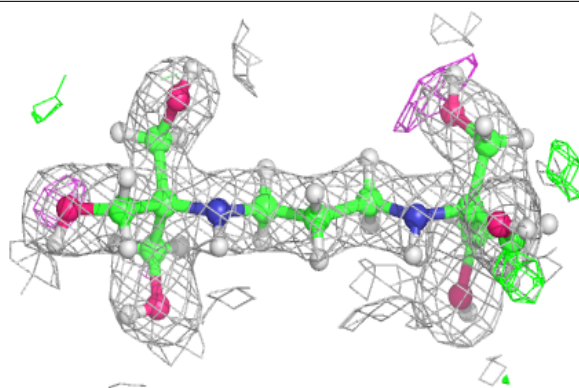
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	NA	A	1045	1/1	0.98	0.27	35,35,35,35	0
12	NA	A	1046	1/1	0.98	0.17	35,35,35,35	0
12	NA	A	1044	1/1	0.99	0.39	35,35,35,35	0
5	ZN	A	1008	1/1	1.00	0.11	18,18,18,18	0

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.



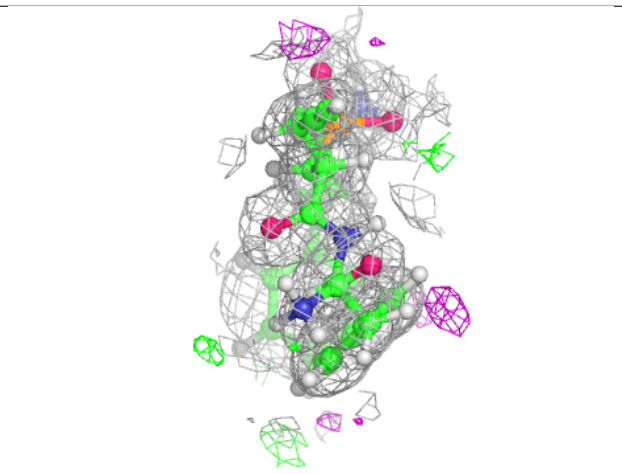
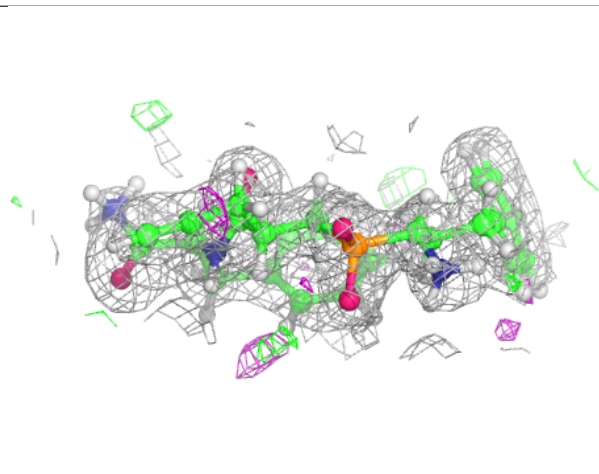
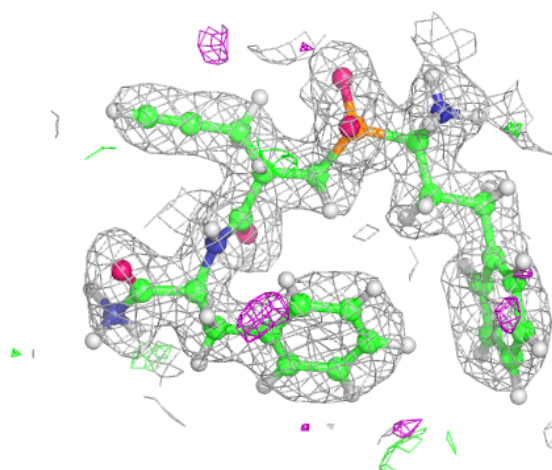
**Electron density around B3P A 1010:**

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



**Electron density around HJ5 A 1009:**

$2mF_o-DF_c$  (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.