



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 12:32 AM EDT

PDB ID : 6PKI  
Title : Zebrafish N-acetylglucosamine-1-phosphodiester alpha-N-acetylglucosaminidase (NAGPA) catalytic domain (C56S C230S) in complex with N-acetyl-alpha-D-glucosamine (alpha-GlcNAc) and mannose 6-phosphate (M6P)  
Authors : Gorelik, A.; Illes, K.; Nagar, B.  
Deposited on : 2019-06-29  
Resolution : 2.29 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

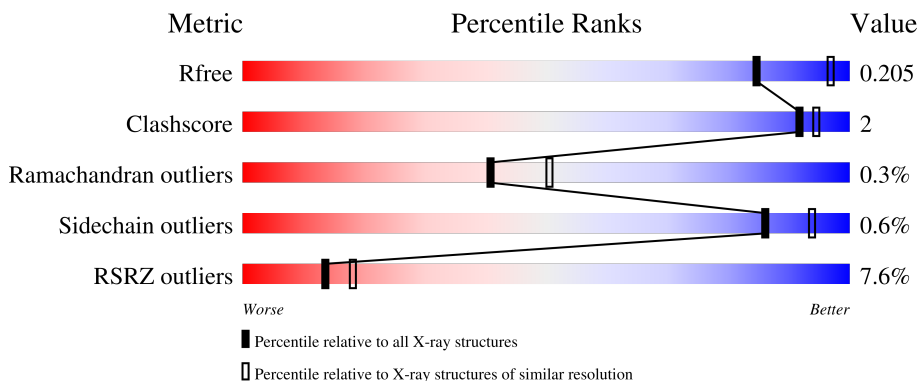
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	309	 4% 95%
1	B	309	 5% 92%
1	C	309	 7% 91% 5%
1	D	309	 14% 93%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	NAG	D	401	-	-	-	X
2	NAG	D	402	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19042 atoms, of which 8964 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 N-acetylglucosamine-1-phosphodiester alpha-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	301	4544	1435	2226	426	449	8	0	0	0
1	B	298	4498	1421	2205	422	442	8	0	0	0
1	C	298	4497	1421	2204	422	442	8	0	0	0
1	D	296	4462	1411	2185	419	439	8	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	expression tag	UNP F1QSF9
A	29	ARG	-	expression tag	UNP F1QSF9
A	30	HIS	-	expression tag	UNP F1QSF9
A	31	HIS	-	expression tag	UNP F1QSF9
A	32	HIS	-	expression tag	UNP F1QSF9
A	33	HIS	-	expression tag	UNP F1QSF9
A	34	HIS	-	expression tag	UNP F1QSF9
A	35	HIS	-	expression tag	UNP F1QSF9
A	36	GLY	-	expression tag	UNP F1QSF9
A	37	SER	-	expression tag	UNP F1QSF9
A	38	GLY	-	expression tag	UNP F1QSF9
A	56	SER	CYS	engineered mutation	UNP F1QSF9
A	230	SER	CYS	engineered mutation	UNP F1QSF9
B	28	ASP	-	expression tag	UNP F1QSF9
B	29	ARG	-	expression tag	UNP F1QSF9
B	30	HIS	-	expression tag	UNP F1QSF9
B	31	HIS	-	expression tag	UNP F1QSF9
B	32	HIS	-	expression tag	UNP F1QSF9
B	33	HIS	-	expression tag	UNP F1QSF9
B	34	HIS	-	expression tag	UNP F1QSF9

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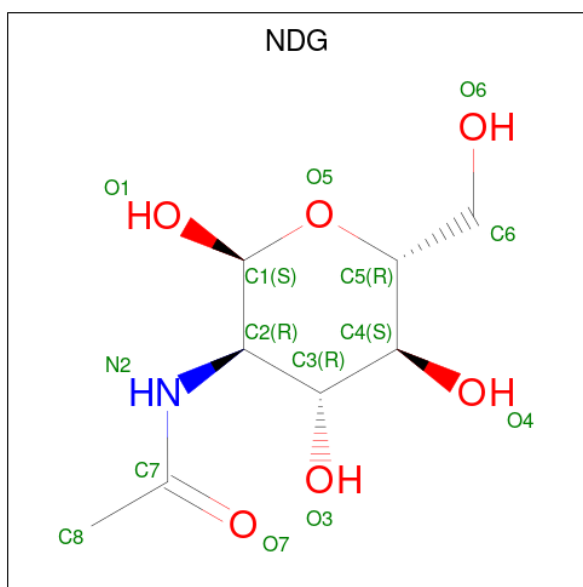
Chain	Residue	Modelled	Actual	Comment	Reference
B	35	HIS	-	expression tag	UNP F1QSF9
B	36	GLY	-	expression tag	UNP F1QSF9
B	37	SER	-	expression tag	UNP F1QSF9
B	38	GLY	-	expression tag	UNP F1QSF9
B	56	SER	CYS	engineered mutation	UNP F1QSF9
B	230	SER	CYS	engineered mutation	UNP F1QSF9
C	28	ASP	-	expression tag	UNP F1QSF9
C	29	ARG	-	expression tag	UNP F1QSF9
C	30	HIS	-	expression tag	UNP F1QSF9
C	31	HIS	-	expression tag	UNP F1QSF9
C	32	HIS	-	expression tag	UNP F1QSF9
C	33	HIS	-	expression tag	UNP F1QSF9
C	34	HIS	-	expression tag	UNP F1QSF9
C	35	HIS	-	expression tag	UNP F1QSF9
C	36	GLY	-	expression tag	UNP F1QSF9
C	37	SER	-	expression tag	UNP F1QSF9
C	38	GLY	-	expression tag	UNP F1QSF9
C	56	SER	CYS	engineered mutation	UNP F1QSF9
C	230	SER	CYS	engineered mutation	UNP F1QSF9
D	28	ASP	-	expression tag	UNP F1QSF9
D	29	ARG	-	expression tag	UNP F1QSF9
D	30	HIS	-	expression tag	UNP F1QSF9
D	31	HIS	-	expression tag	UNP F1QSF9
D	32	HIS	-	expression tag	UNP F1QSF9
D	33	HIS	-	expression tag	UNP F1QSF9
D	34	HIS	-	expression tag	UNP F1QSF9
D	35	HIS	-	expression tag	UNP F1QSF9
D	36	GLY	-	expression tag	UNP F1QSF9
D	37	SER	-	expression tag	UNP F1QSF9
D	38	GLY	-	expression tag	UNP F1QSF9
D	56	SER	CYS	engineered mutation	UNP F1QSF9
D	230	SER	CYS	engineered mutation	UNP F1QSF9

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



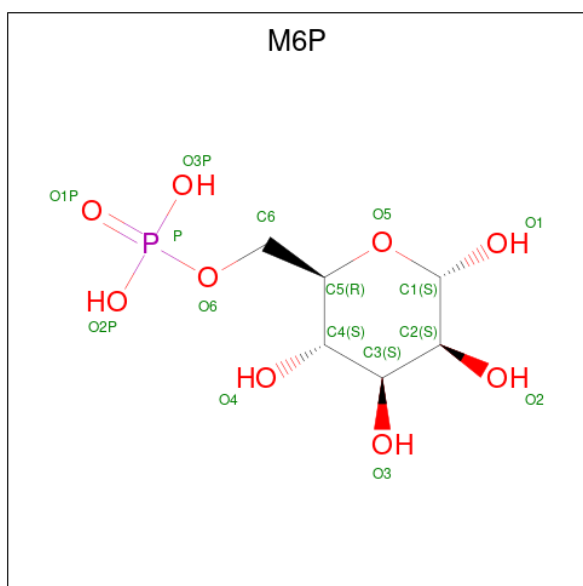
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



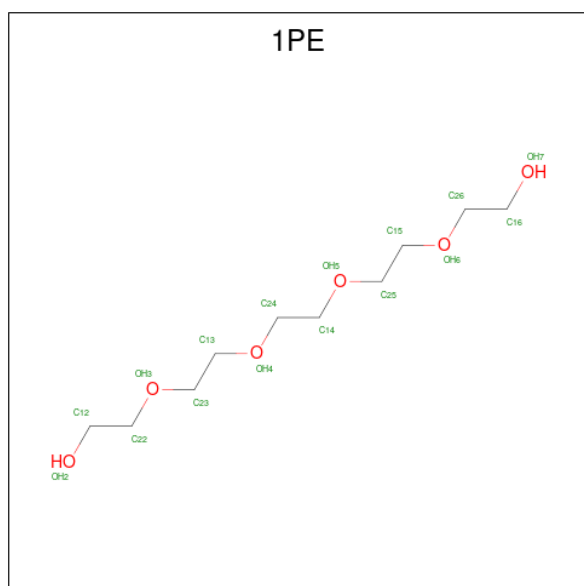
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	C	1	Total	C	N	O	0	0
			15	8	1	6		
3	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is 6-O-phosphono-alpha-D-mannopyranose (three-letter code: M6P) (formula:  $C_6H_{13}O_9P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 16 6 9 1	0	0
4	B	1	Total C O P 16 6 9 1	0	0
4	C	1	Total C O P 16 6 9 1	0	0
4	C	1	Total C H O P 26 6 10 9 1	0	0
4	D	1	Total C O P 16 6 9 1	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 38 10 22 6	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	B	2	Total Cl 2 2	0	0
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is water.

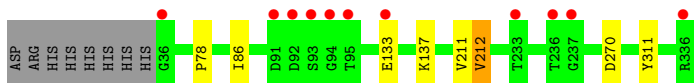


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total 212	O 212	0	0
7	B	196	Total 196	O 196	0	0
7	C	121	Total 121	O 121	0	0
7	D	96	Total 96	O 96	0	0

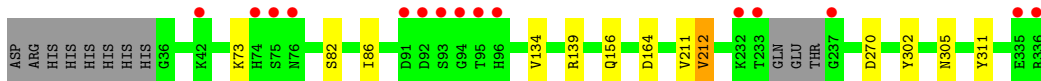
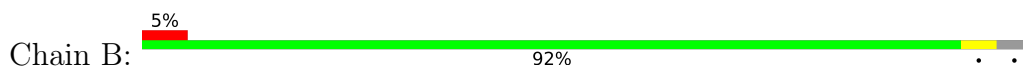
### 3 Residue-property plots [i](#)

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.

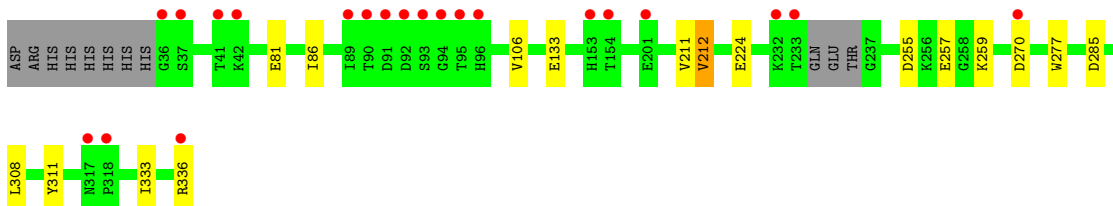
- Molecule 1: N-acetylglucosamine-1-phosphodiester alpha-N-acetylglucosaminidase



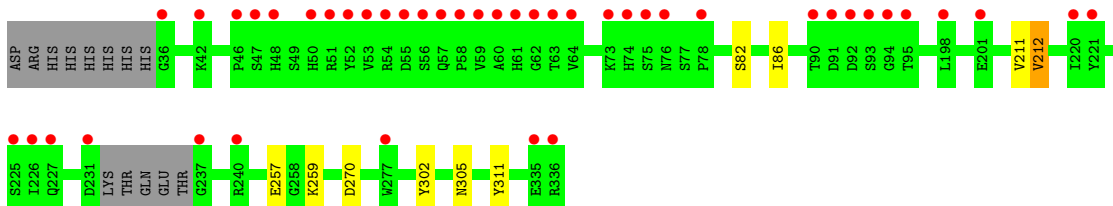
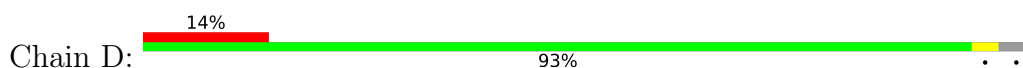
- Molecule 1: N-acetylglucosamine-1-phosphodiester alpha-N-acetylglucosaminidase



- Molecule 1: N-acetylglucosamine-1-phosphodiester alpha-N-acetylglucosaminidase



- Molecule 1: N-acetylglucosamine-1-phosphodiester alpha-N-acetylglucosaminidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.17Å 124.17Å 276.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.66 – 2.29 47.59 – 2.29	Depositor EDS
% Data completeness (in resolution range)	80.1 (22.66-2.29) 74.1 (47.59-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.15_3459: ???)	Depositor
R, $R_{free}$	0.170 , 0.204 0.172 , 0.205	Depositor DCC
$R_{free}$ test set	2000 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: CL, M6P, NAG, NDG, 1PE

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	0.29	0/2369	0.49	0/3211
1	B	0.28	0/2343	0.48	0/3174
1	C	0.27	0/2343	0.47	0/3174
1	D	0.26	0/2327	0.46	0/3153
All	All	0.28	0/9382	0.48	0/12712

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2318	2226	2226	5	0
1	B	2293	2205	2204	8	0
1	C	2293	2204	2204	16	0
1	D	2277	2185	2184	5	0
2	A	28	28	26	0	0
2	B	28	28	26	0	0
2	C	28	28	26	2	0
2	D	28	28	26	1	0
3	A	15	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	12	0	0
3	C	15	0	12	1	0
3	D	15	0	12	0	0
4	A	16	0	10	0	0
4	B	16	0	10	0	0
4	C	32	10	20	2	0
4	D	16	0	10	0	0
5	A	16	22	22	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	212	0	0	0	1
7	B	196	0	0	2	1
7	C	121	0	0	0	0
7	D	96	0	0	1	0
All	All	10078	8964	9042	30	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (30) 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:B:82:SER:HG	1:B:302:TYR:HH	1.18	0.89
1:C:285:ASP:OD1	4:C:405:M6P:O1	1.96	0.83
1:C:257:GLU:OE1	1:C:259:LYS:NZ	2.20	0.75
1:B:134:VAL:HG13	1:C:336:ARG:HD3	1.70	0.74
1:A:133:GLU:OE2	1:A:137:LYS:NZ	2.26	0.67
1:C:277:TRP:HZ3	2:C:401:NAG:H82	1.64	0.62
2:D:401:NAG:O7	7:D:501:HOH:O	2.17	0.57
1:C:211:VAL:O	1:C:212:VAL:HB	2.09	0.52
1:C:86:ILE:HD11	1:D:311:TYR:HB3	1.92	0.51
1:D:211:VAL:O	1:D:212:VAL:HB	2.12	0.50
1:B:211:VAL:O	1:B:212:VAL:HB	2.12	0.50
1:A:211:VAL:O	1:A:212:VAL:HB	2.12	0.49
1:C:257:GLU:O	1:C:257:GLU:HG2	2.13	0.49
1:D:257:GLU:OE1	1:D:259:LYS:NZ	2.47	0.48
1:B:156:GLN:NE2	7:B:507:HOH:O	2.44	0.48
1:D:82:SER:OG	1:D:302:TYR:OH	2.20	0.47
1:B:139:ARG:NH1	1:B:164:ASP:OD1	2.49	0.46
1:C:277:TRP:CZ3	2:C:401:NAG:H82	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:CE	7:B:679:HOH:O	2.64	0.45
1:C:311:TYR:HB3	1:D:86:ILE:HD11	1.99	0.44
1:A:86:ILE:HD11	1:B:311:TYR:HB3	2.00	0.43
1:C:133:GLU:OE2	1:C:308:LEU:HB2	2.18	0.43
1:A:78:PRO:HD2	1:C:81:GLU:OE1	2.18	0.43
3:C:403:NDG:O1	4:C:404:M6P:O3P	2.36	0.42
1:C:224:GLU:OE1	1:C:224:GLU:N	2.42	0.42
1:A:311:TYR:HB3	1:B:86:ILE:HD11	2.02	0.42
1:C:106:VAL:HG22	1:C:333:ILE:HD13	2.01	0.42
1:C:211:VAL:O	1:C:212:VAL:CB	2.68	0.41
1:C:255:ASP:OD2	1:C:259:LYS:HE2	2.21	0.41
1:C:257:GLU:O	1:C:257:GLU:CG	2.69	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:665:HOH:O	7:B:575:HOH:O[4_554]	2.17	0.03

## 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	299/309 (97%)	288 (96%)	10 (3%)	1 (0%)	41	50
1	B	294/309 (95%)	287 (98%)	6 (2%)	1 (0%)	41	50
1	C	294/309 (95%)	287 (98%)	6 (2%)	1 (0%)	41	50
1	D	292/309 (94%)	285 (98%)	6 (2%)	1 (0%)	41	50
All	All	1179/1236 (95%)	1147 (97%)	28 (2%)	4 (0%)	41	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	VAL
1	B	212	VAL
1	C	212	VAL
1	D	212	VAL

### 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	255/263 (97%)	254 (100%)	1 (0%)	91	96
1	B	252/263 (96%)	250 (99%)	2 (1%)	81	91
1	C	252/263 (96%)	251 (100%)	1 (0%)	91	96
1	D	250/263 (95%)	248 (99%)	2 (1%)	81	91
All	All	1009/1052 (96%)	1003 (99%)	6 (1%)	86	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	ASP
1	B	270	ASP
1	B	305	ASN
1	C	270	ASP
1	D	270	ASP
1	D	305	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	227	GLN
1	D	61	HIS
1	D	145	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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
4	M6P	C	404	-	16,16,16	1.19	1 (6%)	24,24,24	1.05	3 (12%)
3	NDG	D	403	-	15,15,15	0.64	0	21,21,21	1.03	1 (4%)
5	1PE	A	405	-	15,15,15	0.52	0	14,14,14	0.28	0
2	NAG	D	401	1	14,14,15	0.19	0	17,19,21	0.36	0
4	M6P	A	404	-	16,16,16	1.14	1 (6%)	24,24,24	0.93	1 (4%)
4	M6P	C	405	-	16,16,16	1.25	1 (6%)	24,24,24	0.88	1 (4%)
3	NDG	A	403	-	15,15,15	0.74	1 (6%)	21,21,21	1.21	1 (4%)
3	NDG	B	403	-	15,15,15	0.64	0	21,21,21	1.09	1 (4%)
3	NDG	C	403	-	15,15,15	0.69	0	21,21,21	1.11	2 (9%)
2	NAG	B	402	1	14,14,15	1.16	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	D	402	1	14,14,15	0.46	0	17,19,21	0.48	0
2	NAG	C	402	1	14,14,15	0.16	0	17,19,21	0.61	0
2	NAG	A	401	1	14,14,15	0.68	1 (7%)	17,19,21	0.54	0
2	NAG	A	402	1	14,14,15	0.26	0	17,19,21	0.59	0
2	NAG	B	401	1	14,14,15	0.45	0	17,19,21	0.87	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	401	1	14,14,15	0.42	0	17,19,21	0.63	1 (5%)
4	M6P	B	404	-	16,16,16	1.20	1 (6%)	24,24,24	1.09	2 (8%)
4	M6P	D	404	-	16,16,16	1.18	1 (6%)	24,24,24	0.81	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
4	M6P	C	404	-	-	3/6/26/26	0/1/1/1
3	NDG	D	403	-	-	2/6/26/26	0/1/1/1
5	1PE	A	405	-	-	7/13/13/13	-
2	NAG	D	401	1	-	1/6/23/26	0/1/1/1
4	M6P	A	404	-	-	2/6/26/26	0/1/1/1
4	M6P	C	405	-	-	4/6/26/26	0/1/1/1
3	NDG	A	403	-	-	0/6/26/26	0/1/1/1
3	NDG	B	403	-	-	2/6/26/26	0/1/1/1
3	NDG	C	403	-	-	2/6/26/26	0/1/1/1
2	NAG	B	402	1	-	0/6/23/26	0/1/1/1
2	NAG	D	402	1	-	1/6/23/26	0/1/1/1
2	NAG	C	402	1	-	2/6/23/26	0/1/1/1
2	NAG	A	401	1	-	2/6/23/26	0/1/1/1
2	NAG	A	402	1	-	2/6/23/26	0/1/1/1
2	NAG	B	401	1	-	2/6/23/26	0/1/1/1
2	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	M6P	B	404	-	-	2/6/26/26	0/1/1/1
4	M6P	D	404	-	-	5/6/26/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	NAG	O5-C1	-4.13	1.37	1.43
4	C	405	M6P	O5-C1	3.56	1.51	1.42
4	B	404	M6P	O5-C1	3.42	1.51	1.42
4	D	404	M6P	O5-C1	3.35	1.51	1.42
4	A	404	M6P	O5-C1	3.21	1.50	1.42
4	C	404	M6P	O5-C1	3.18	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAG	C1-C2	2.36	1.55	1.52
3	A	403	NDG	C1-C2	2.14	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NDG	C1-C2-N2	4.02	115.38	110.73
3	B	403	NDG	C1-C2-N2	3.69	115.01	110.73
2	B	401	NAG	C1-O5-C5	3.25	116.60	112.19
3	C	403	NDG	C1-C2-N2	3.20	114.43	110.73
3	D	403	NDG	C1-C2-N2	3.16	114.39	110.73
4	C	404	M6P	O5-C5-C4	3.03	115.20	109.69
2	B	402	NAG	C3-C4-C5	2.97	115.54	110.24
4	C	405	M6P	O5-C1-C2	2.44	114.65	110.28
4	A	404	M6P	C1-O5-C5	-2.43	109.08	113.66
4	B	404	M6P	C1-C2-C3	2.40	115.29	110.31
4	B	404	M6P	O6-P-O1P	2.30	112.94	106.47
4	C	404	M6P	C3-C4-C5	2.27	114.29	110.24
3	C	403	NDG	C1-O5-C5	2.23	117.87	113.66
2	C	401	NAG	C1-O5-C5	2.15	115.10	112.19
4	C	404	M6P	C6-C5-C4	-2.03	107.85	112.09

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	M6P	C4-C5-C6-O6
4	B	404	M6P	C4-C5-C6-O6
4	B	404	M6P	O5-C5-C6-O6
4	C	404	M6P	C4-C5-C6-O6
4	C	404	M6P	O5-C5-C6-O6
4	C	405	M6P	C4-C5-C6-O6
4	C	405	M6P	O5-C5-C6-O6
4	C	405	M6P	C6-O6-P-O2P
4	C	405	M6P	C6-O6-P-O3P
4	D	404	M6P	C4-C5-C6-O6
4	D	404	M6P	O5-C5-C6-O6
4	D	404	M6P	C6-O6-P-O2P
4	D	404	M6P	C6-O6-P-O3P
2	B	401	NAG	O5-C5-C6-O6
2	A	401	NAG	O5-C5-C6-O6
2	A	402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	401	NAG	C4-C5-C6-O6
3	C	403	NDG	C4-C5-C6-O6
2	C	402	NAG	O5-C5-C6-O6
5	A	405	1PE	OH4-C13-C23-OH3
2	C	401	NAG	O5-C5-C6-O6
2	A	402	NAG	C4-C5-C6-O6
2	B	401	NAG	C4-C5-C6-O6
2	C	402	NAG	C4-C5-C6-O6
2	C	401	NAG	C4-C5-C6-O6
3	C	403	NDG	O5-C5-C6-O6
5	A	405	1PE	OH6-C15-C25-OH5
2	D	401	NAG	O5-C5-C6-O6
3	B	403	NDG	C4-C5-C6-O6
4	D	404	M6P	C6-O6-P-O1P
3	D	403	NDG	C4-C5-C6-O6
5	A	405	1PE	OH7-C16-C26-OH6
4	C	404	M6P	C5-C6-O6-P
5	A	405	1PE	C16-C26-OH6-C15
3	B	403	NDG	O5-C5-C6-O6
3	D	403	NDG	O5-C5-C6-O6
5	A	405	1PE	C23-C13-OH4-C24
5	A	405	1PE	C24-C14-OH5-C25
4	A	404	M6P	O5-C5-C6-O6
2	D	402	NAG	C4-C5-C6-O6
5	A	405	1PE	OH2-C12-C22-OH3

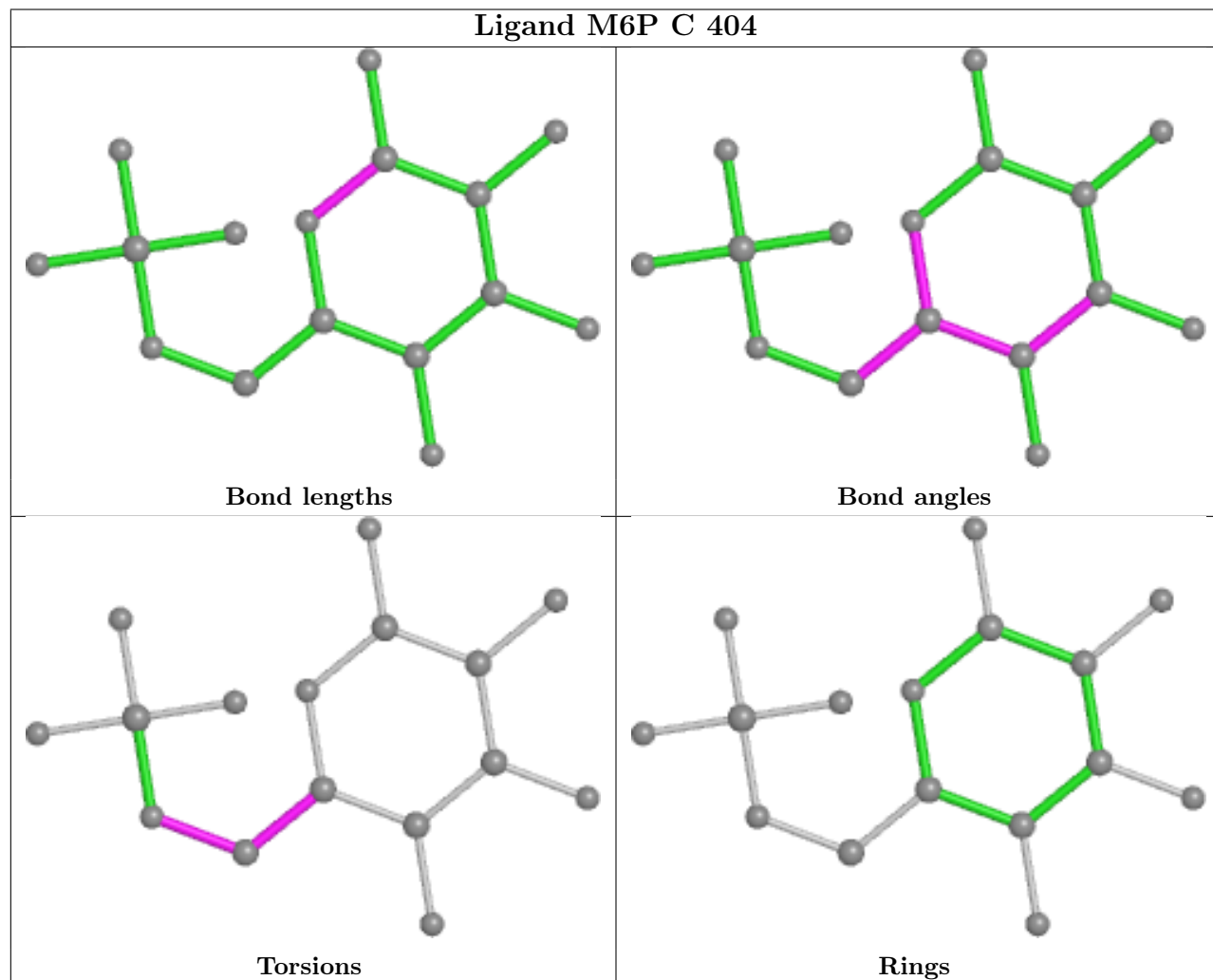
There are no ring outliers.

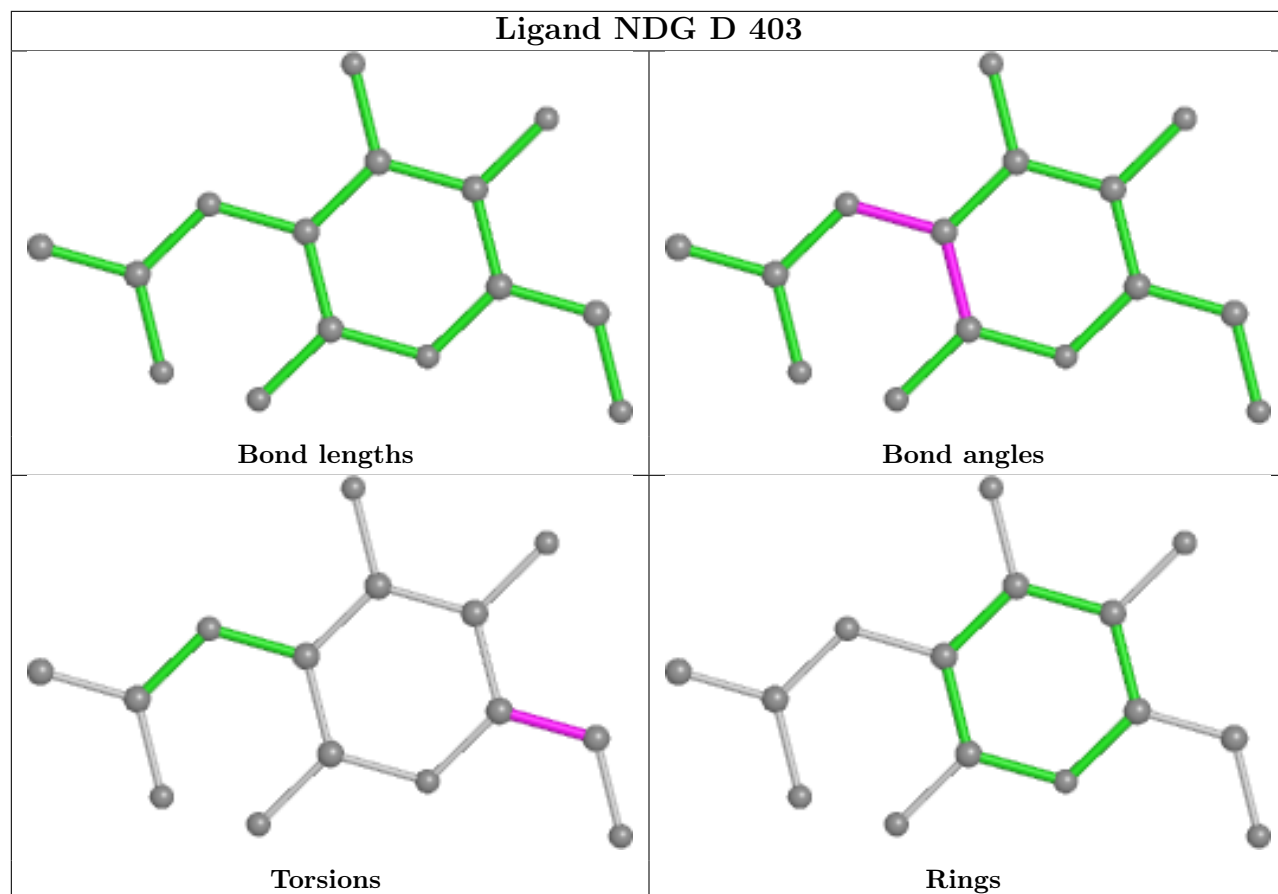
5 monomers are involved in 5 short contacts:

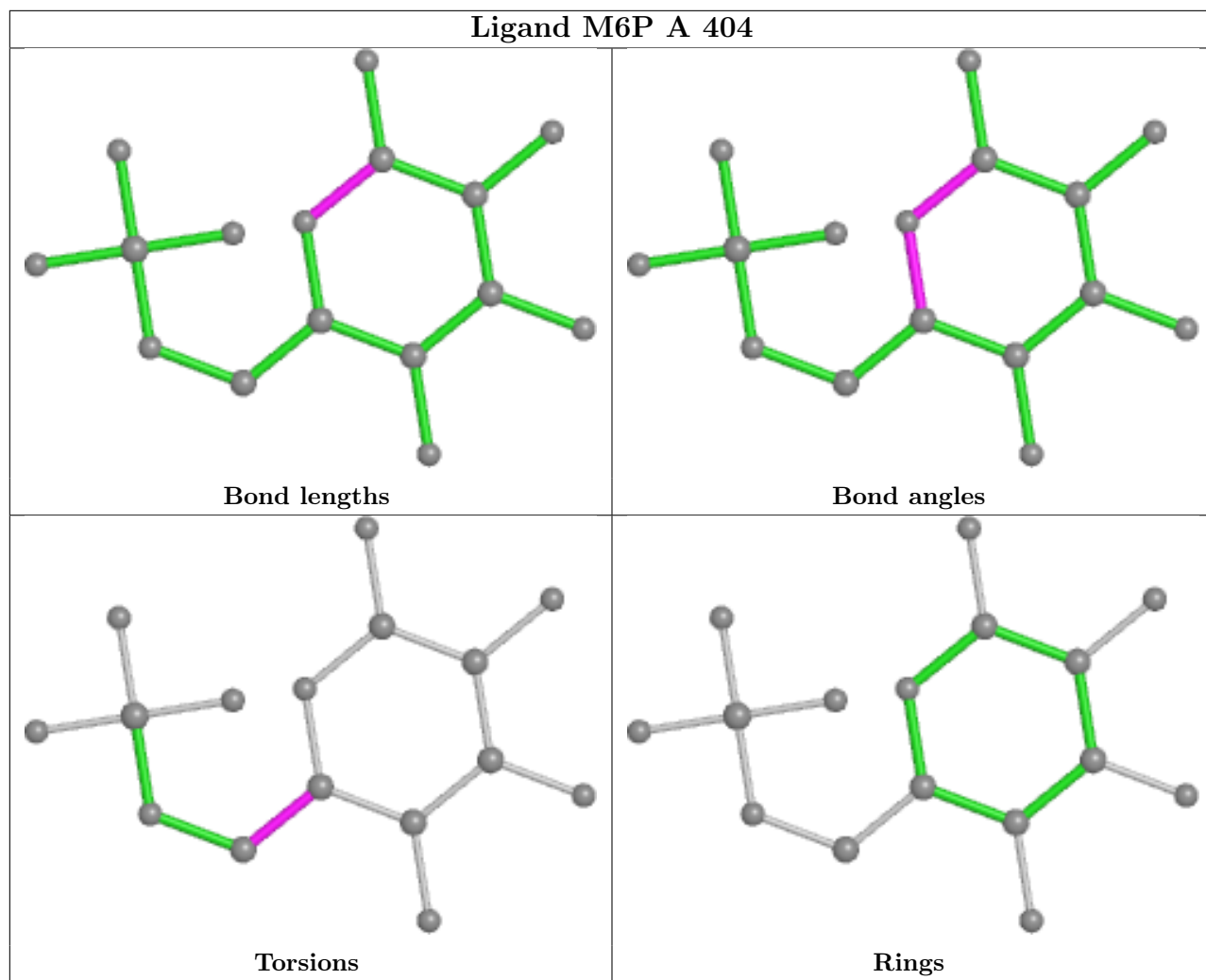
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	M6P	1	0
2	D	401	NAG	1	0
4	C	405	M6P	1	0
3	C	403	NDG	1	0
2	C	401	NAG	2	0

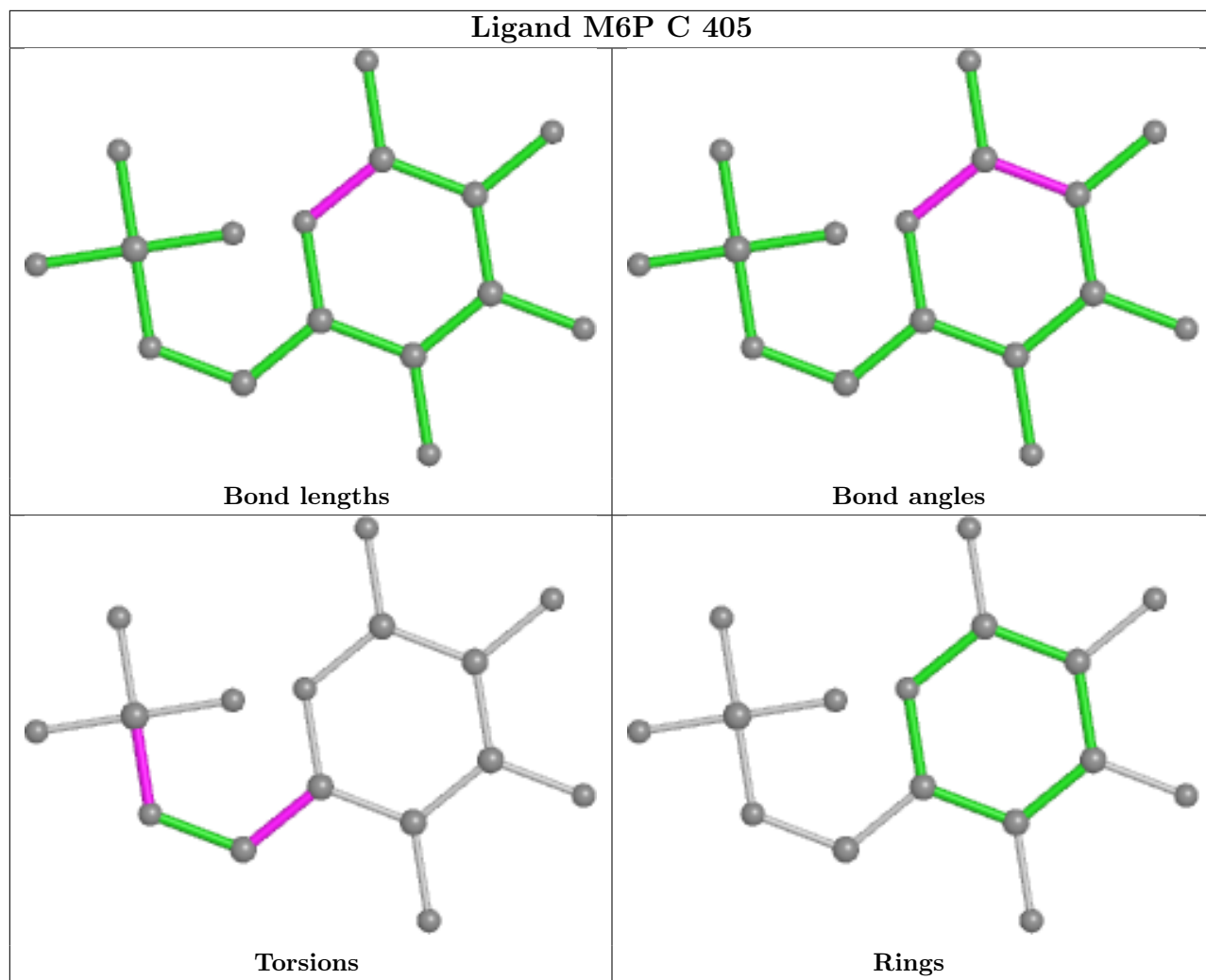
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

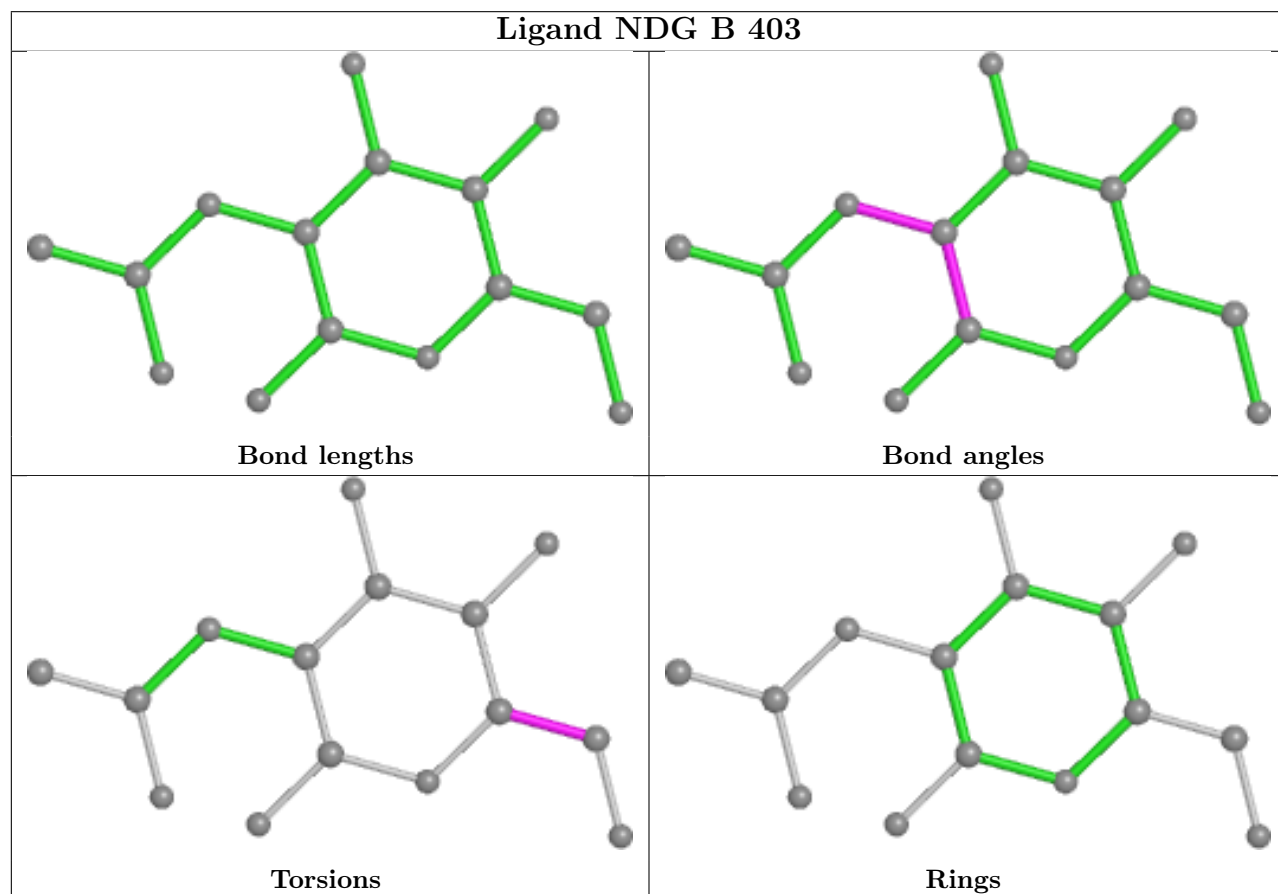
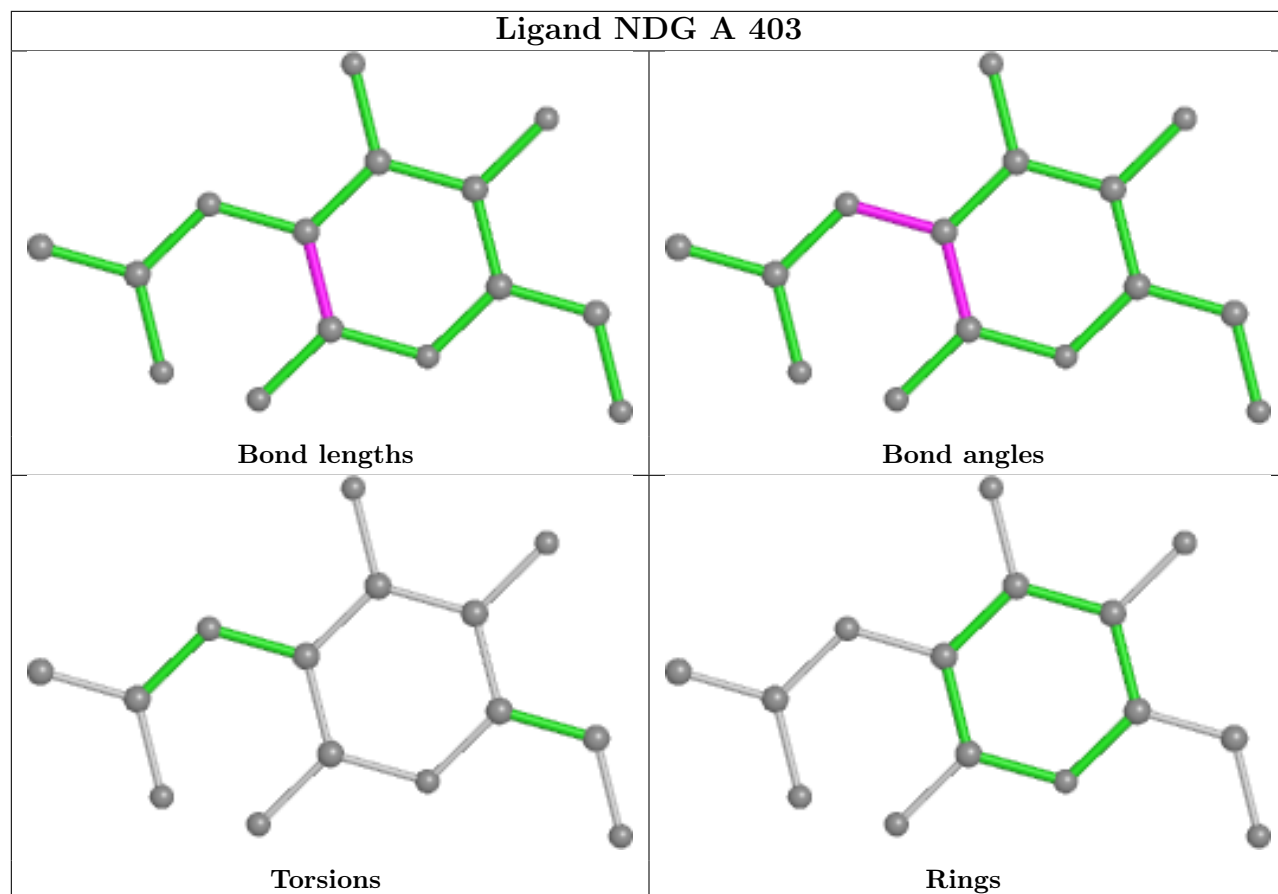
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



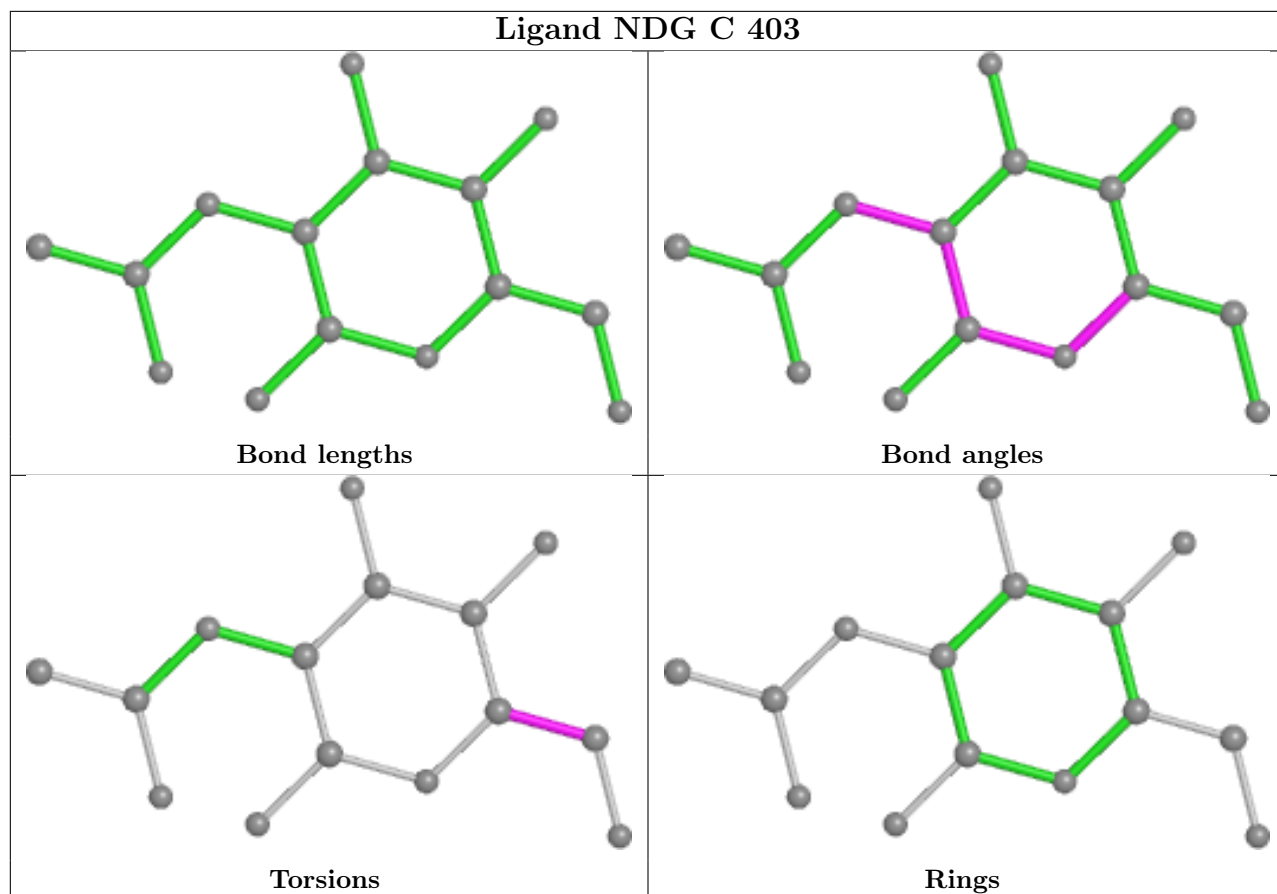


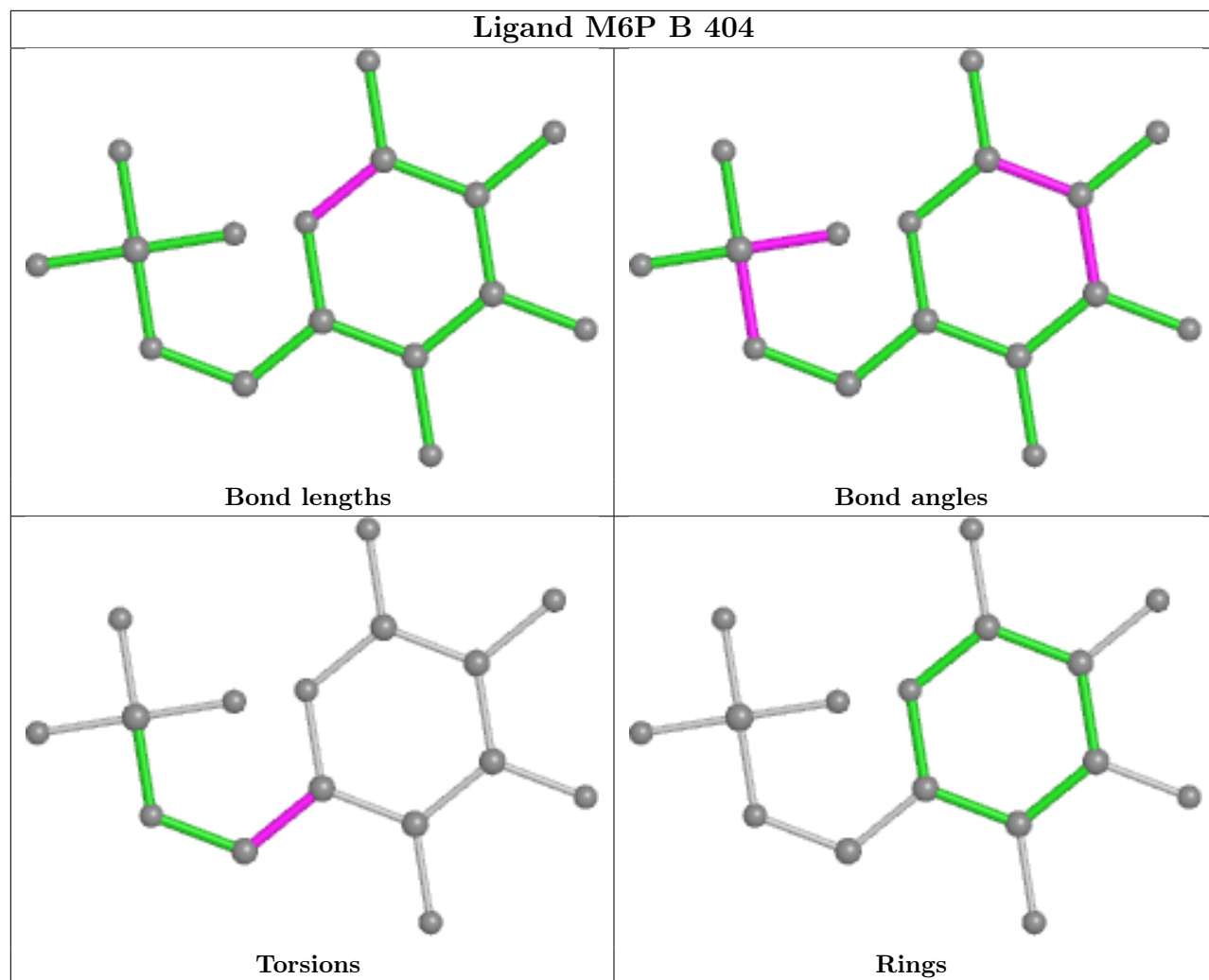


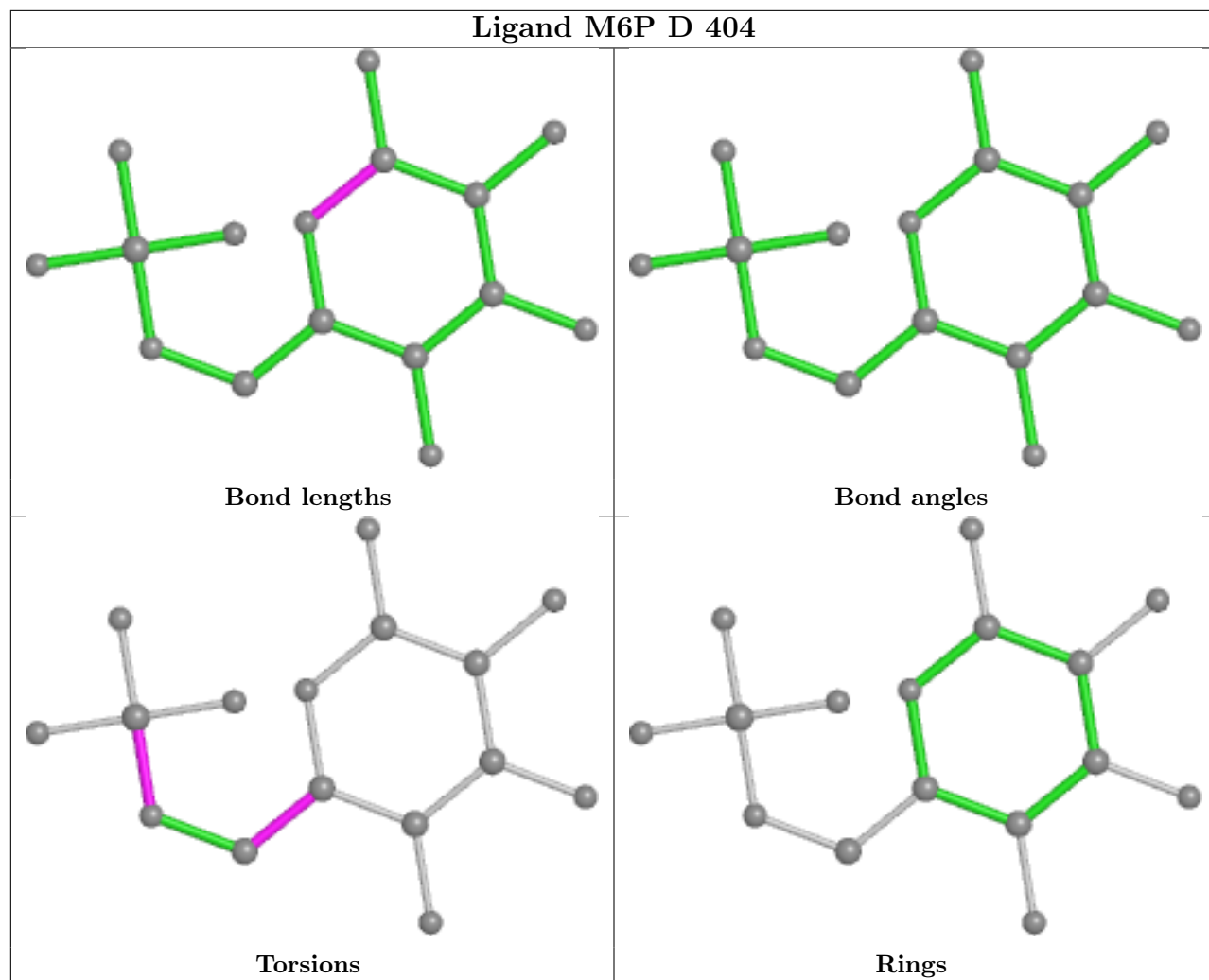












## 5.7 Other polymers [i](#)

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	301/309 (97%)	-0.06	11 (3%) 41 48	16, 31, 79, 126	0
1	B	298/309 (96%)	-0.03	15 (5%) 28 35	20, 34, 85, 131	0
1	C	298/309 (96%)	0.19	21 (7%) 16 21	29, 48, 95, 123	0
1	D	296/309 (95%)	0.74	44 (14%) 2 3	33, 65, 113, 144	0
All	All	1193/1236 (96%)	0.21	91 (7%) 13 18	16, 43, 98, 144	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	SER	7.6
1	D	58	PRO	7.4
1	D	60	ALA	6.5
1	D	63	THR	6.0
1	D	61	HIS	5.8
1	D	59	VAL	5.5
1	C	92	ASP	5.5
1	B	76	ASN	5.4
1	D	62	GLY	5.4
1	D	52	TYR	5.3
1	D	53	VAL	5.2
1	C	95	THR	5.0
1	C	91	ASP	4.9
1	D	92	ASP	4.8
1	D	76	ASN	4.7
1	D	75	SER	4.6
1	D	47	SER	4.6
1	C	94	GLY	4.3
1	D	237	GLY	4.3
1	D	240	ARG	4.3
1	D	56	SER	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	237	GLY	4.1
1	C	318	PRO	4.0
1	C	317	ASN	4.0
1	B	92	ASP	3.9
1	D	36	GLY	3.9
1	D	201	GLU	3.9
1	A	236	THR	3.8
1	B	94	GLY	3.8
1	B	93	SER	3.8
1	D	336	ARG	3.8
1	B	75	SER	3.7
1	C	153	HIS	3.7
1	C	336	ARG	3.7
1	D	42	LYS	3.7
1	A	336	ARG	3.6
1	A	233	THR	3.5
1	D	220	ILE	3.5
1	B	232	LYS	3.5
1	C	233	THR	3.5
1	D	55	ASP	3.4
1	D	51	ARG	3.4
1	C	36	GLY	3.4
1	D	94	GLY	3.3
1	D	335	GLU	3.3
1	D	64	VAL	3.2
1	D	46	PRO	3.2
1	D	277	TRP	3.1
1	C	232	LYS	3.1
1	D	227	GLN	3.0
1	D	48	HIS	3.0
1	B	335	GLU	3.0
1	B	95	THR	3.0
1	B	96	HIS	3.0
1	B	336	ARG	2.9
1	C	42	LYS	2.8
1	D	221	TYR	2.8
1	A	95	THR	2.7
1	C	41	THR	2.7
1	A	94	GLY	2.7
1	B	233	THR	2.7
1	A	36	GLY	2.7
1	B	91	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	237	GLY	2.6
1	A	133	GLU	2.6
1	D	90	THR	2.6
1	C	270	ASP	2.6
1	D	231	ASP	2.5
1	A	93	SER	2.5
1	D	226	ILE	2.5
1	D	93	SER	2.4
1	C	96	HIS	2.4
1	D	95	THR	2.4
1	C	89	ILE	2.4
1	A	92	ASP	2.3
1	D	78	PRO	2.3
1	C	90	THR	2.3
1	C	201	GLU	2.3
1	A	91	ASP	2.3
1	D	57	GLN	2.3
1	D	198	LEU	2.2
1	B	74	HIS	2.2
1	C	37	SER	2.2
1	D	225	SER	2.2
1	D	50	HIS	2.1
1	D	54	ARG	2.1
1	D	73	LYS	2.1
1	D	91	ASP	2.1
1	B	42	LYS	2.0
1	D	74	HIS	2.0
1	C	154	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 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,

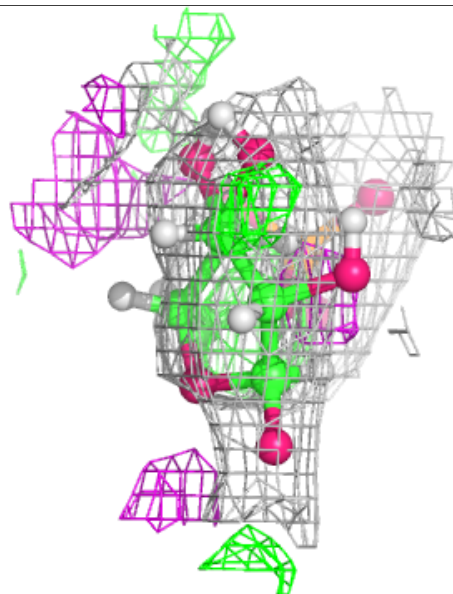
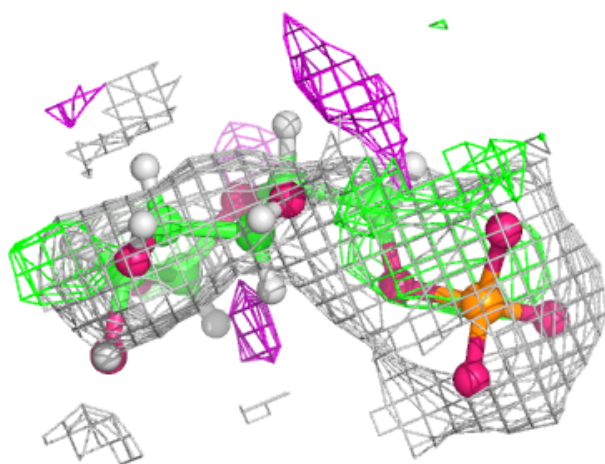
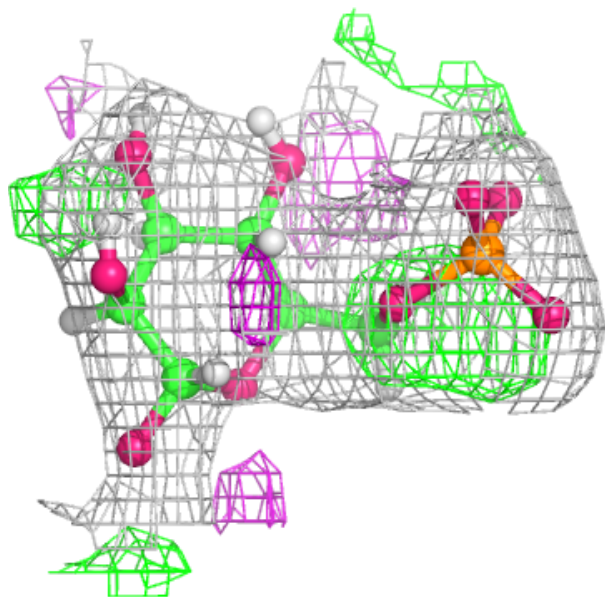
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	401	14/15	0.62	0.45	95,112,131,135	0
2	NAG	C	402	14/15	0.64	0.31	85,97,115,117	0
2	NAG	D	402	14/15	0.66	0.50	96,109,128,130	0
2	NAG	C	401	14/15	0.72	0.32	79,90,107,108	0
6	CL	B	406	1/1	0.83	0.18	81,81,81,81	0
2	NAG	B	402	14/15	0.84	0.30	82,98,117,118	0
2	NAG	A	402	14/15	0.84	0.16	58,71,84,87	0
2	NAG	B	401	14/15	0.84	0.24	71,84,99,101	0
4	M6P	C	405	16/16	0.85	0.24	97,129,155,168	0
6	CL	B	405	1/1	0.86	0.10	75,75,75,75	0
2	NAG	A	401	14/15	0.87	0.18	60,81,104,106	0
5	1PE	A	405	16/16	0.91	0.17	63,78,90,92	0
6	CL	A	406	1/1	0.91	0.21	70,70,70,70	0
3	NDG	D	403	15/15	0.94	0.12	43,46,55,56	0
4	M6P	C	404	16/16	0.95	0.24	51,129,137,138	0
3	NDG	C	403	15/15	0.96	0.14	40,49,54,54	0
4	M6P	D	404	16/16	0.96	0.18	48,114,132,133	0
6	CL	C	406	1/1	0.96	0.13	86,86,86,86	0
4	M6P	A	404	16/16	0.97	0.25	28,108,129,131	0
4	M6P	B	404	16/16	0.98	0.20	30,96,114,119	0
3	NDG	B	403	15/15	0.98	0.11	23,29,34,36	0
3	NDG	A	403	15/15	0.98	0.10	23,29,35,39	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 M6P C 405:**

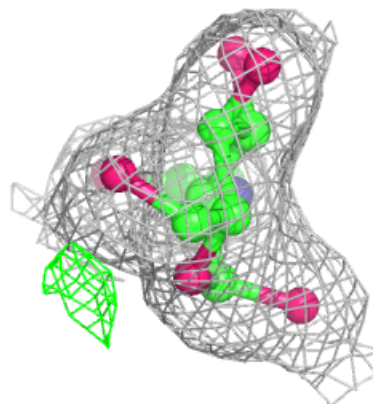
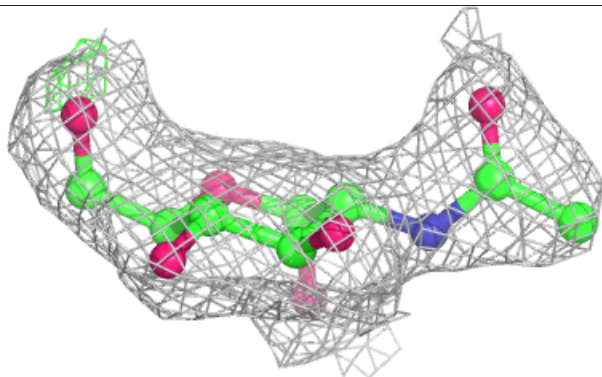
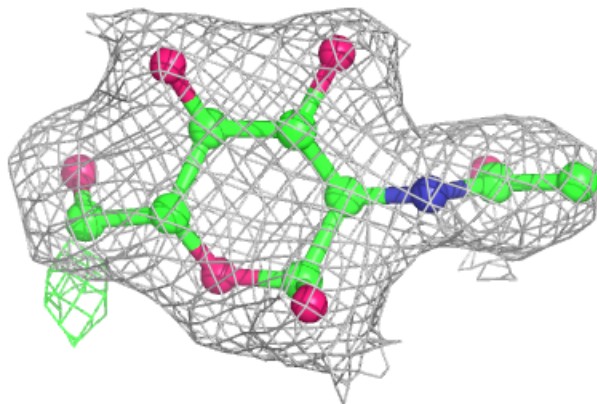
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



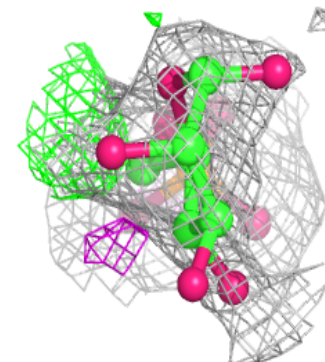
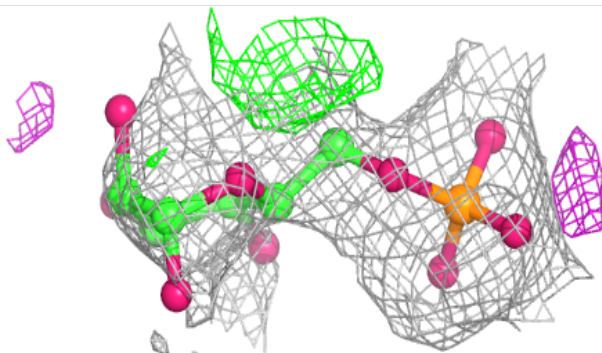
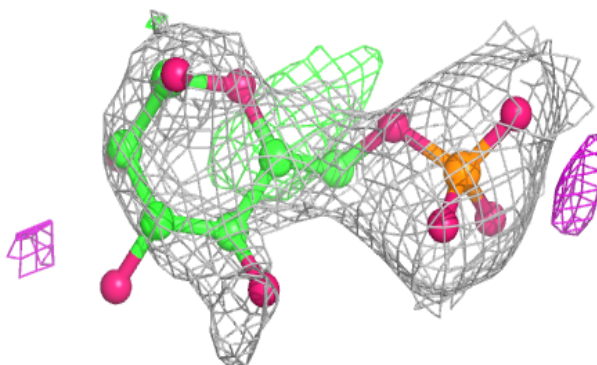


**Electron density around NDG D 403:**

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

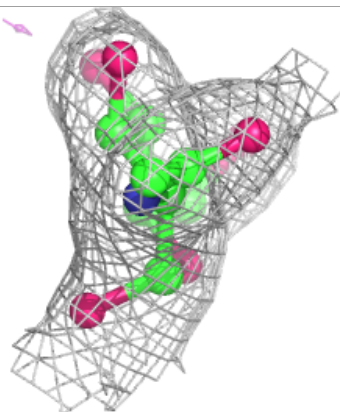
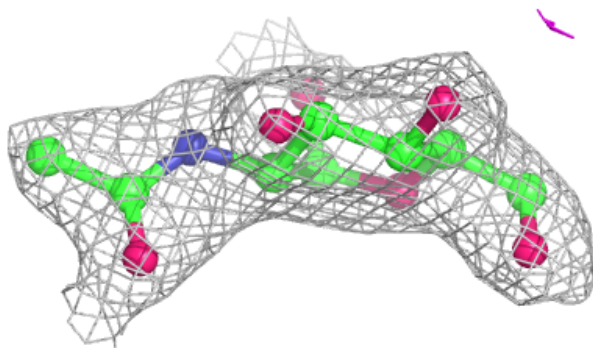
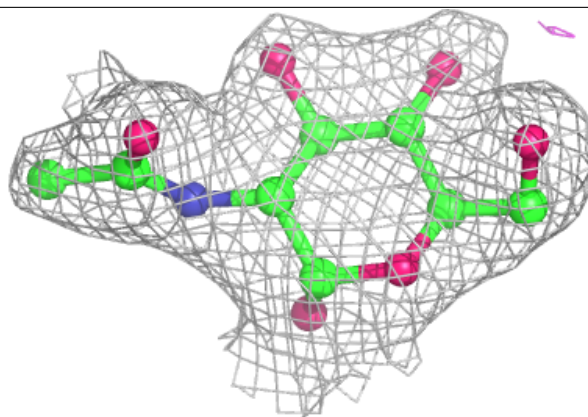
**Electron density around M6P C 404:**

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

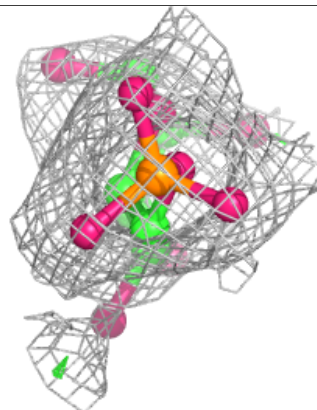
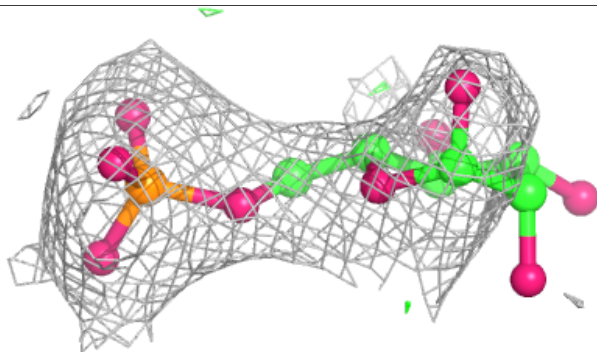
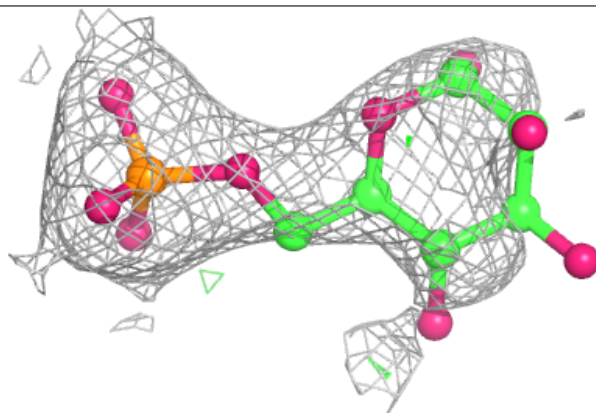


**Electron density around NDG C 403:**

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

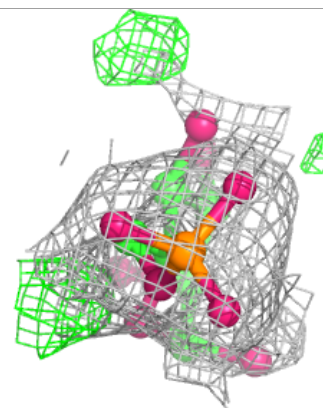
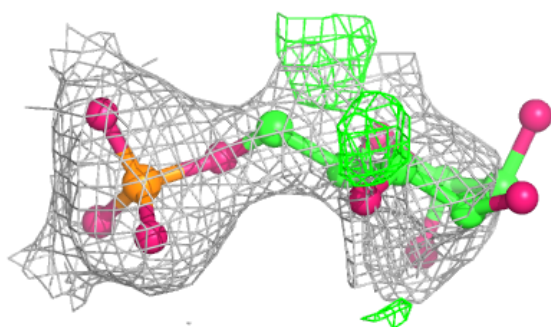
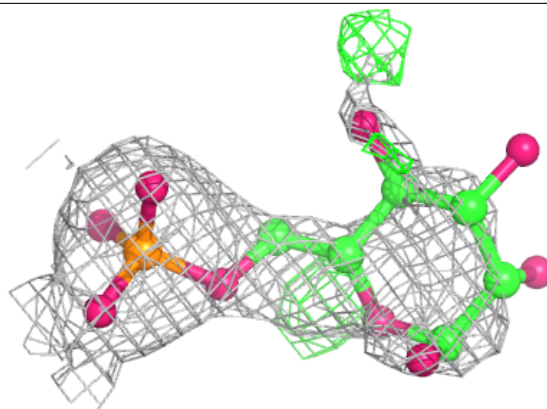
**Electron density around M6P D 404:**

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

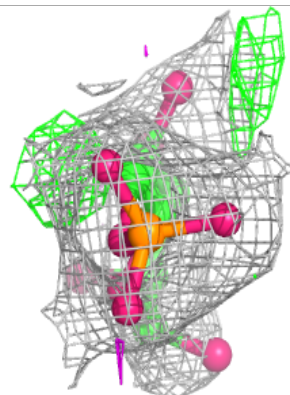
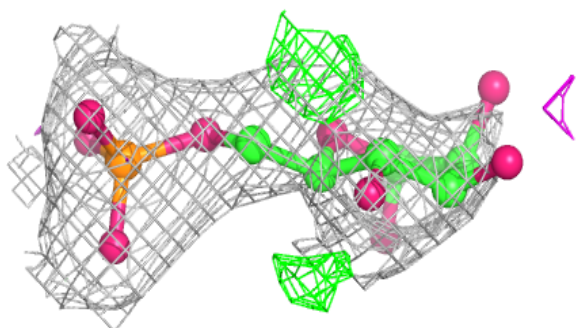
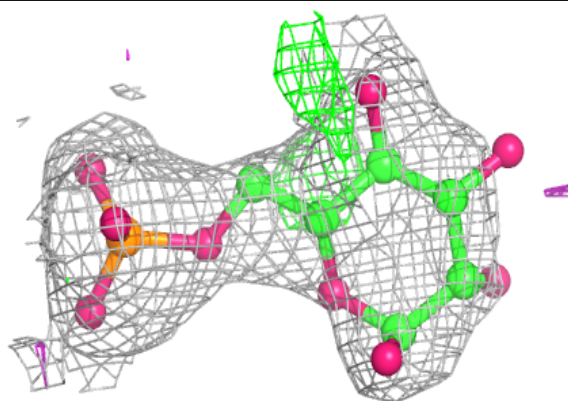


**Electron density around M6P A 404:**

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

**Electron density around M6P B 404:**

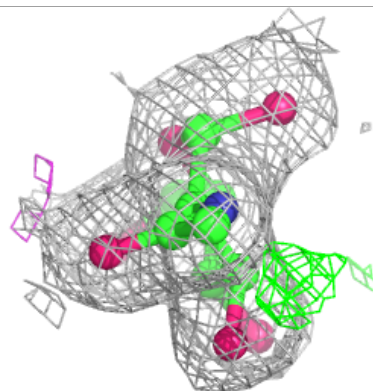
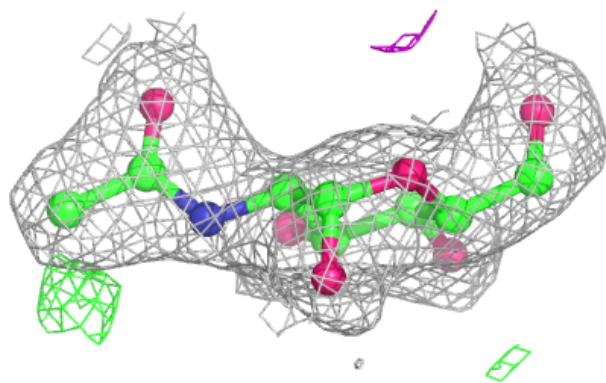
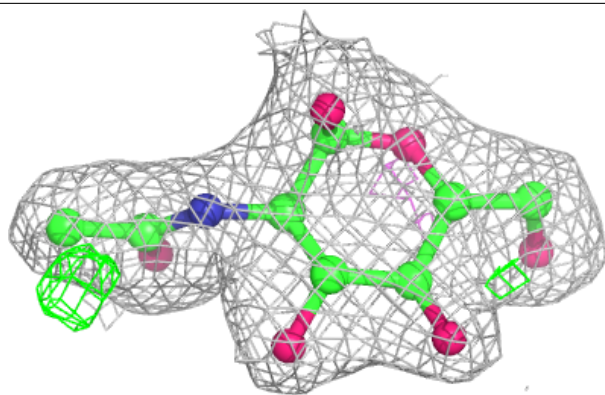
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



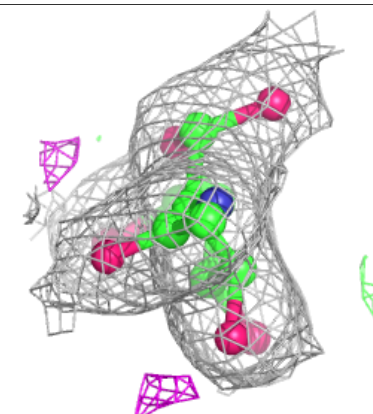
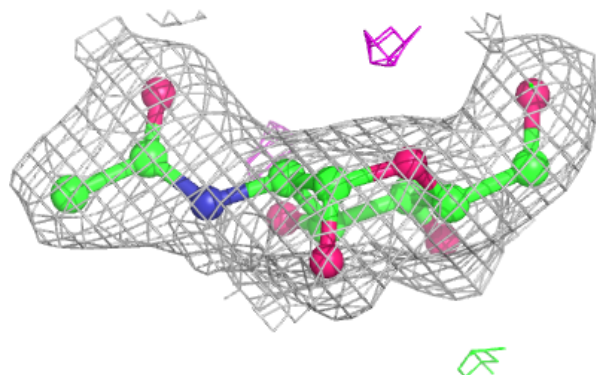
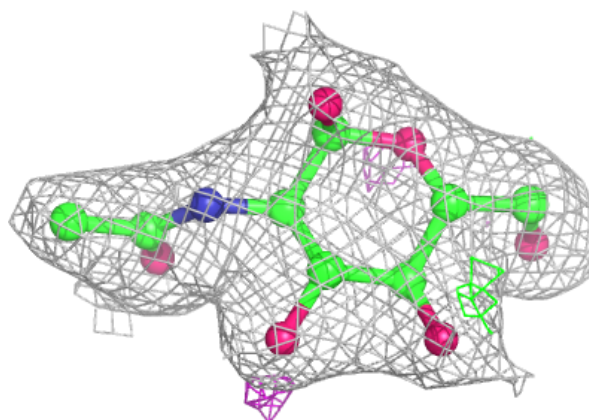


**Electron density around NDG B 403:**

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

**Electron density around NDG A 403:**

$2mF_o-DF_c$  (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.