



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 01:03 am BST

PDB ID : 9EP0 / pdb\_00009ep0  
Title : Dolichyl phosphate mannose synthase in complex with donor (GDP-Man) and traces of acceptor (Dol55P) and product (Dol55P-Man)  
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Deposited on : 2024-03-16  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

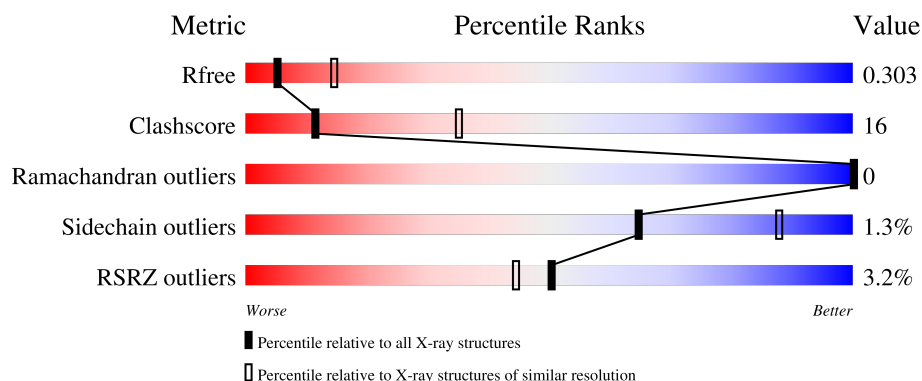
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.90 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	374	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2859 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.

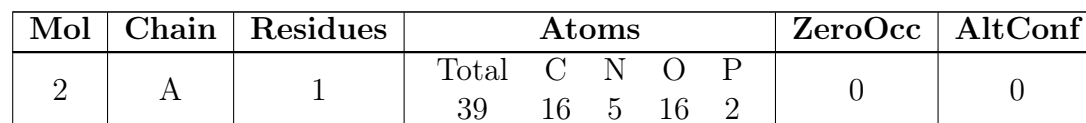
- Molecule 1 is a protein called Dolichol monophosphate mannose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2771	1826	464	476	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q8U4M3
A	-20	HIS	-	expression tag	UNP Q8U4M3
A	-19	HIS	-	expression tag	UNP Q8U4M3
A	-18	HIS	-	expression tag	UNP Q8U4M3
A	-17	HIS	-	expression tag	UNP Q8U4M3
A	-16	HIS	-	expression tag	UNP Q8U4M3
A	-15	HIS	-	expression tag	UNP Q8U4M3
A	-14	SER	-	expression tag	UNP Q8U4M3
A	-13	SER	-	expression tag	UNP Q8U4M3
A	-12	GLY	-	expression tag	UNP Q8U4M3
A	-11	VAL	-	expression tag	UNP Q8U4M3
A	-10	ASP	-	expression tag	UNP Q8U4M3
A	-9	LEU	-	expression tag	UNP Q8U4M3
A	-8	GLY	-	expression tag	UNP Q8U4M3
A	-7	THR	-	expression tag	UNP Q8U4M3
A	-6	GLU	-	expression tag	UNP Q8U4M3
A	-5	ASN	-	expression tag	UNP Q8U4M3
A	-4	LEU	-	expression tag	UNP Q8U4M3
A	-3	TYR	-	expression tag	UNP Q8U4M3
A	-2	PHE	-	expression tag	UNP Q8U4M3
A	-1	GLN	-	expression tag	UNP Q8U4M3
A	0	SER	-	expression tag	UNP Q8U4M3

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (CCD ID: GDD) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>5</sub>O<sub>16</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

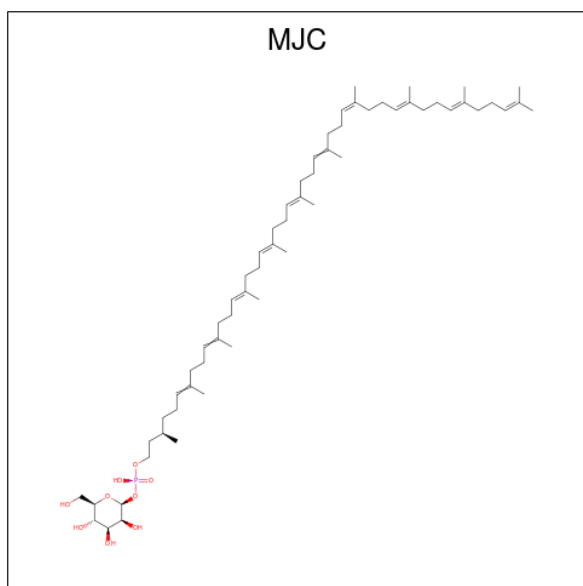


- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |

- EFS
- 
- Chemical structure diagram showing a phosphate group (EFS) with a central phosphorus atom (P) bonded to four oxygen atoms (O). The phosphorus atom is labeled 'P' in green. The oxygen atoms are labeled O1, O2, O3, and O4 in green. O1 and O2 are single-bonded to the phosphorus, while O3 and O4 are double-bonded. O1 is bonded to a hydrogen atom (H) in red. O2 is bonded to a carbon atom (C11) in green, which is further bonded to a carbon atom (C12) in green. The bonds are colored: single bonds are purple, double bonds are red, and the C11-C12 bond is black.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			7	2	4	1		

- Molecule 5 is dolichyl phosphate mannose (CCD ID: MJC) (formula:  $C_{61}H_{103}O_9P$ ) (labeled as "Ligand of Interest" by depositor).

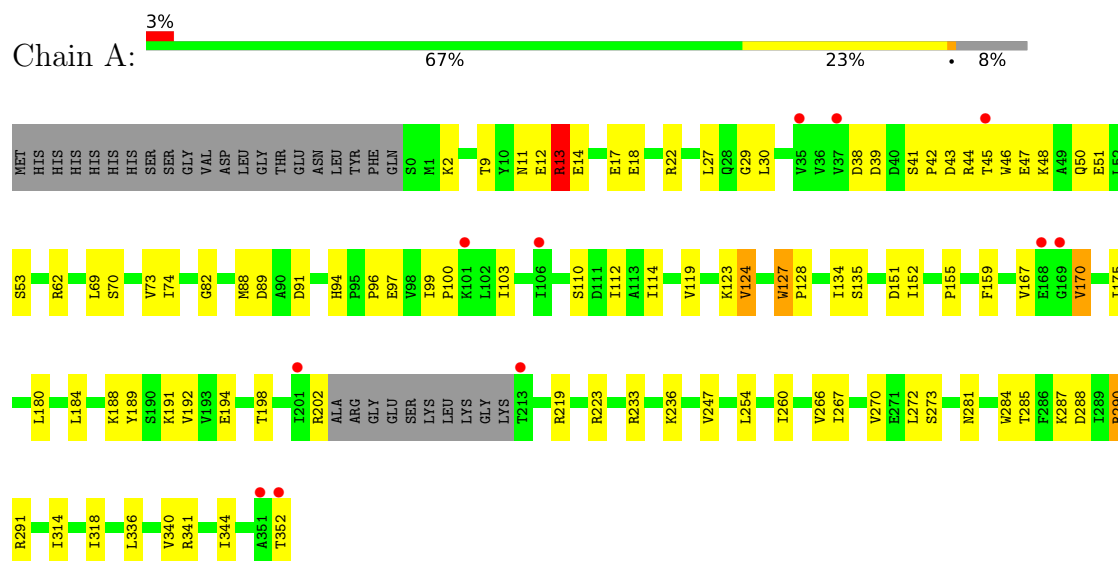


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			41	31	9	1		

### 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: Dolichol monophosphate mannose synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.80Å 145.25Å 99.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.90 43.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.90-2.90) 99.6 (43.90-2.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.237 , 0.301 0.249 , 0.303	Depositor DCC
$R_{free}$ test set	1443 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.0	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EFS, MJC, GDD, MG

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	0.44	0/2835	0.67	2/3834 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	13	ARG	CB-CG-CD	6.12	125.37	111.30
1	A	42	PRO	N-CA-C	-5.22	107.60	114.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	290	ARG	Sidechain

### 5.2 Too-close contacts

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



the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2771	0	2881	90	2
2	A	39	0	23	3	0
3	A	1	0	0	0	0
4	A	7	0	5	0	0
5	A	41	0	0	1	0
All	All	2859	0	2909	91	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 16.

All (91) 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:46:TRP:CZ2	1:A:62:ARG:NH2	2.20	1.09
1:A:46:TRP:CE2	1:A:62:ARG:NH2	2.40	0.87
1:A:46:TRP:CG	1:A:62:ARG:HE	1.93	0.85
1:A:13:ARG:HD3	1:A:14:GLU:HG3	1.69	0.74
1:A:89:ASP:H	1:A:94:HIS:HD2	1.38	0.72
1:A:340:VAL:O	1:A:344:ILE:HG13	1.91	0.68
1:A:352:THR:HG23	1:A:352:THR:O	1.95	0.67
1:A:123:LYS:HB2	1:A:198:THR:HG23	1.77	0.66
1:A:91:ASP:HB2	1:A:202:ARG:HD2	1.78	0.66
1:A:46:TRP:CD1	1:A:62:ARG:NE	2.65	0.65
1:A:236:LYS:HG2	1:A:284:TRP:CZ2	2.33	0.63
1:A:11:ASN:HA	1:A:43:ASP:HB2	1.81	0.63
1:A:46:TRP:CG	1:A:62:ARG:NE	2.67	0.62
1:A:46:TRP:CD1	1:A:62:ARG:HE	2.18	0.61
1:A:46:TRP:CE2	1:A:62:ARG:NE	2.68	0.60
1:A:50:GLN:CD	1:A:50:GLN:H	2.08	0.60
1:A:17:GLU:OE2	1:A:48:LYS:NZ	2.26	0.59
1:A:45:THR:HA	1:A:46:TRP:C	2.28	0.59
1:A:266:VAL:O	1:A:270:VAL:HG12	2.02	0.59
1:A:96:PRO:HA	1:A:99:ILE:HG13	1.85	0.58
1:A:39:ASP:OD2	2:A:400:GDD:N2	2.34	0.58
1:A:2:LYS:HB3	1:A:82:GLY:HA2	1.85	0.57
1:A:290:ARG:HG3	1:A:290:ARG:HH11	1.70	0.57
1:A:44:ARG:HG3	1:A:45:THR:N	2.19	0.57
1:A:39:ASP:CG	2:A:400:GDD:H2N1	2.14	0.56
1:A:89:ASP:H	1:A:94:HIS:CD2	2.22	0.55
1:A:46:TRP:CE2	1:A:62:ARG:CZ	2.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:OE2	1:A:202:ARG:NH2	2.40	0.55
1:A:151:ASP:OD1	1:A:151:ASP:N	2.40	0.54
1:A:114:ILE:HD13	1:A:180:LEU:HD21	1.90	0.53
1:A:44:ARG:HB2	1:A:47:GLU:OE2	2.08	0.53
1:A:94:HIS:CE1	1:A:159:PHE:HB2	2.44	0.53
1:A:290:ARG:O	1:A:291:ARG:HG2	2.09	0.53
1:A:12:GLU:O	1:A:45:THR:HG21	2.09	0.52
1:A:233:ARG:NH2	1:A:288:ASP:OD1	2.42	0.51
1:A:46:TRP:C	1:A:50:GLN:HE22	2.19	0.51
1:A:175:ILE:HG22	1:A:175:ILE:O	2.10	0.51
1:A:336:LEU:O	1:A:340:VAL:HG13	2.10	0.51
1:A:89:ASP:N	1:A:94:HIS:HD2	2.07	0.51
1:A:219:ARG:HE	1:A:223:ARG:HH12	1.59	0.51
1:A:260:ILE:HD12	1:A:260:ILE:H	1.75	0.51
1:A:124:VAL:HG21	1:A:127:TRP:CE3	2.47	0.50
1:A:266:VAL:HG23	1:A:267:ILE:HD13	1.93	0.50
1:A:22:ARG:HD2	1:A:97:GLU:OE1	2.11	0.50
1:A:45:THR:HG22	1:A:48:LYS:HB3	1.94	0.50
1:A:134:ILE:HD12	1:A:135:SER:N	2.27	0.50
1:A:70:SER:O	1:A:74:ILE:HG12	2.12	0.49
1:A:236:LYS:HB3	1:A:285:THR:HG22	1.95	0.49
1:A:127:TRP:CD1	1:A:128:PRO:HD2	2.48	0.48
1:A:27:LEU:HD22	1:A:30:LEU:HD12	1.94	0.48
1:A:46:TRP:HB2	1:A:50:GLN:NE2	2.29	0.48
1:A:314:ILE:O	1:A:318:ILE:HG13	2.14	0.47
1:A:110:SER:OG	1:A:191:LYS:HD3	2.14	0.47
1:A:9:THR:OG1	1:A:38:ASP:OD2	2.30	0.47
1:A:44:ARG:HG3	1:A:45:THR:H	1.79	0.47
1:A:152:ILE:O	1:A:155:PRO:HD3	2.16	0.46
1:A:219:ARG:HE	1:A:223:ARG:NH1	2.13	0.46
1:A:50:GLN:O	1:A:53:SER:HB3	2.16	0.46
1:A:236:LYS:HG2	1:A:284:TRP:CH2	2.51	0.46
1:A:44:ARG:CG	1:A:45:THR:N	2.79	0.45
1:A:123:LYS:HD2	1:A:198:THR:OG1	2.17	0.45
1:A:184:LEU:O	1:A:189:TYR:OH	2.33	0.45
1:A:281:ASN:HA	1:A:285:THR:OG1	2.16	0.44
1:A:74:ILE:HG12	1:A:74:ILE:H	1.66	0.44
1:A:110:SER:HA	1:A:191:LYS:HB3	1.98	0.44
1:A:41:SER:OG	1:A:45:THR:O	2.35	0.44
1:A:18:GLU:O	1:A:22:ARG:HG3	2.18	0.44
1:A:46:TRP:NE1	1:A:62:ARG:NE	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:PRO:O	1:A:103:ILE:HG13	2.17	0.43
1:A:236:LYS:CB	1:A:285:THR:HG22	2.49	0.43
1:A:341:ARG:NH2	5:A:403:MJC:OP2	2.52	0.43
1:A:170:VAL:HG12	1:A:188:LYS:HE3	2.00	0.43
1:A:44:ARG:CG	1:A:45:THR:H	2.32	0.43
1:A:284:TRP:O	1:A:287:LYS:HG2	2.19	0.42
1:A:18:GLU:H	1:A:18:GLU:CD	2.26	0.42
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.83	0.42
1:A:167:VAL:O	1:A:170:VAL:HG22	2.20	0.42
1:A:13:ARG:HE	1:A:44:ARG:HH11	1.67	0.42
1:A:46:TRP:HB2	1:A:50:GLN:HE22	1.84	0.42
1:A:124:VAL:HG21	1:A:127:TRP:HE3	1.83	0.42
1:A:112:ILE:HB	1:A:192:VAL:HG22	2.02	0.41
1:A:43:ASP:O	1:A:44:ARG:C	2.62	0.41
1:A:69:LEU:O	1:A:73:VAL:HG23	2.20	0.41
1:A:13:ARG:HG2	1:A:44:ARG:HD3	2.02	0.41
1:A:11:ASN:HA	1:A:43:ASP:CB	2.49	0.41
1:A:175:ILE:O	1:A:175:ILE:CG2	2.68	0.41
1:A:119:VAL:HG21	1:A:194:GLU:CB	2.51	0.41
1:A:13:ARG:CG	1:A:44:ARG:HD3	2.51	0.41
2:A:400:GDD:H8	2:A:400:GDD:O5'	2.21	0.41
1:A:88:MET:HE3	1:A:88:MET:HB2	1.96	0.41
1:A:247:VAL:CG1	1:A:273:SER:HA	2.50	0.41

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)
1:A:29:GLY:CA	1:A:290:ARG:NH1[8_455]	1.80	0.40
1:A:51:GLU:OE2	1:A:191:LYS:NZ[8_455]	2.19	0.01

## 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	339/374 (91%)	325 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	301/327 (92%)	297 (99%)	4 (1%)	65	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	127	TRP
1	A	170	VAL
1	A	254	LEU

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	94	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](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	EFS	A	402	-	6,6,6	0.58	0	8,8,8	1.05	1 (12%)
5	MJC	A	403	-	40,41,71	3.25	11 (27%)	52,54,90	2.56	15 (28%)
2	GDD	A	400	3	35,42,42	3.33	13 (37%)	46,65,65	1.81	13 (28%)

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	EFS	A	402	-	-	1/4/4/4	-
5	MJC	A	403	-	-	19/38/58/94	0/1/1/1
2	GDD	A	400	3	-	3/19/59/59	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GDD	O4'-C1'	12.61	1.58	1.41
5	A	403	MJC	C12-C13	11.63	1.60	1.33
5	A	403	MJC	C17-C18	9.63	1.56	1.33
5	A	403	MJC	C7-C8	9.07	1.54	1.33
5	A	403	MJC	C22-C23	7.40	1.53	1.32
2	A	400	GDD	O4'-C4'	-7.30	1.28	1.45
2	A	400	GDD	C3'-C2'	-6.90	1.34	1.53
2	A	400	GDD	C2-N3	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	GDD	C3'-C4'	4.11	1.63	1.53
2	A	400	GDD	C2-N2	3.38	1.42	1.34
2	A	400	GDD	C4-N3	3.21	1.45	1.37
2	A	400	GDD	C2-N1	2.79	1.44	1.37
2	A	400	GDD	O2'-C2'	2.76	1.49	1.43
5	A	403	MJC	C21-C22	2.71	1.59	1.50
5	A	403	MJC	C14-C13	2.54	1.57	1.50
5	A	403	MJC	C24-C23	2.50	1.57	1.50
2	A	400	GDD	C31-C21	-2.47	1.46	1.52
5	A	403	MJC	C16-C17	2.43	1.58	1.50
2	A	400	GDD	C2'-C1'	-2.40	1.50	1.53
2	A	400	GDD	C5-C6	2.39	1.52	1.47
5	A	403	MJC	C20-C18	2.20	1.55	1.51
2	A	400	GDD	C5-C4	-2.14	1.37	1.43
5	A	403	MJC	C15-C13	2.04	1.55	1.51
5	A	403	MJC	C11-C12	2.04	1.57	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	MJC	C9-C8-C7	-6.45	107.13	123.68
5	A	403	MJC	C16-C17-C18	-6.15	112.86	127.66
5	A	403	MJC	C15-C13-C12	-5.33	110.33	121.12
5	A	403	MJC	C14-C13-C12	-4.98	110.91	123.68
5	A	403	MJC	C19-C18-C17	-4.64	111.78	123.68
5	A	403	MJC	C19-C18-C20	-4.60	107.54	115.27
5	A	403	MJC	C9-C8-C10	-4.51	107.68	115.27
5	A	403	MJC	C14-C13-C15	-4.50	107.69	115.27
5	A	403	MJC	C11-C12-C13	-4.46	116.91	127.66
2	A	400	GDD	O51-C11-O1B	-4.40	105.61	111.36
5	A	403	MJC	C6-C7-C8	-4.21	117.53	127.66
5	A	403	MJC	C10-C8-C7	-3.98	113.06	121.12
5	A	403	MJC	C21-C22-C23	-3.94	114.28	127.75
2	A	400	GDD	C5-C6-N1	3.87	120.78	113.95
2	A	400	GDD	O3A-PB-O1B	3.40	109.34	102.48
2	A	400	GDD	C2-N1-C6	-3.29	119.04	125.10
2	A	400	GDD	O31-C31-C21	-3.26	102.82	110.35
2	A	400	GDD	O4'-C1'-C2'	-3.08	102.42	106.93
5	A	403	MJC	C24-C23-C22	-3.08	113.75	122.65
2	A	400	GDD	O21-C21-C31	-3.06	103.27	110.35
5	A	403	MJC	C20-C18-C17	-2.82	115.41	121.12
5	A	403	MJC	C25-C23-C22	-2.74	114.72	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GDD	C31-C41-C51	2.73	115.10	110.24
2	A	400	GDD	C8-N7-C5	2.63	108.01	102.99
2	A	400	GDD	C11-O51-C51	-2.49	108.79	113.69
4	A	402	EFS	O1-P-O2	2.43	113.21	106.73
2	A	400	GDD	O6-C6-C5	-2.39	119.71	124.37
2	A	400	GDD	O51-C51-C41	2.10	113.50	109.69
2	A	400	GDD	N2-C2-N1	2.09	121.17	116.71

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	MJC	C6-C7-C8-C9
5	A	403	MJC	C11-C10-C8-C7
5	A	403	MJC	C11-C12-C13-C14
5	A	403	MJC	C11-C12-C13-C15
5	A	403	MJC	C13-C15-C16-C17
5	A	403	MJC	C18-C20-C21-C22
5	A	403	MJC	C12-C13-C15-C16
5	A	403	MJC	C21-C22-C23-C24
5	A	403	MJC	C21-C22-C23-C25
5	A	403	MJC	C6-C7-C8-C10
5	A	403	MJC	C16-C17-C18-C20
5	A	403	MJC	C4-C3-C5-C6
5	A	403	MJC	O5'-C5'-C6'-O6'
2	A	400	GDD	C11-O1B-PB-O3A
5	A	403	MJC	C3-C5-C6-C7
5	A	403	MJC	OP-C1-C2-C3
4	A	402	EFS	C11-O2-P-O3
2	A	400	GDD	PA-O3A-PB-O2B
5	A	403	MJC	C11-C10-C8-C9
5	A	403	MJC	C19-C18-C20-C21
5	A	403	MJC	C2-C3-C5-C6
2	A	400	GDD	PA-O3A-PB-O3B
5	A	403	MJC	C4'-C5'-C6'-O6'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

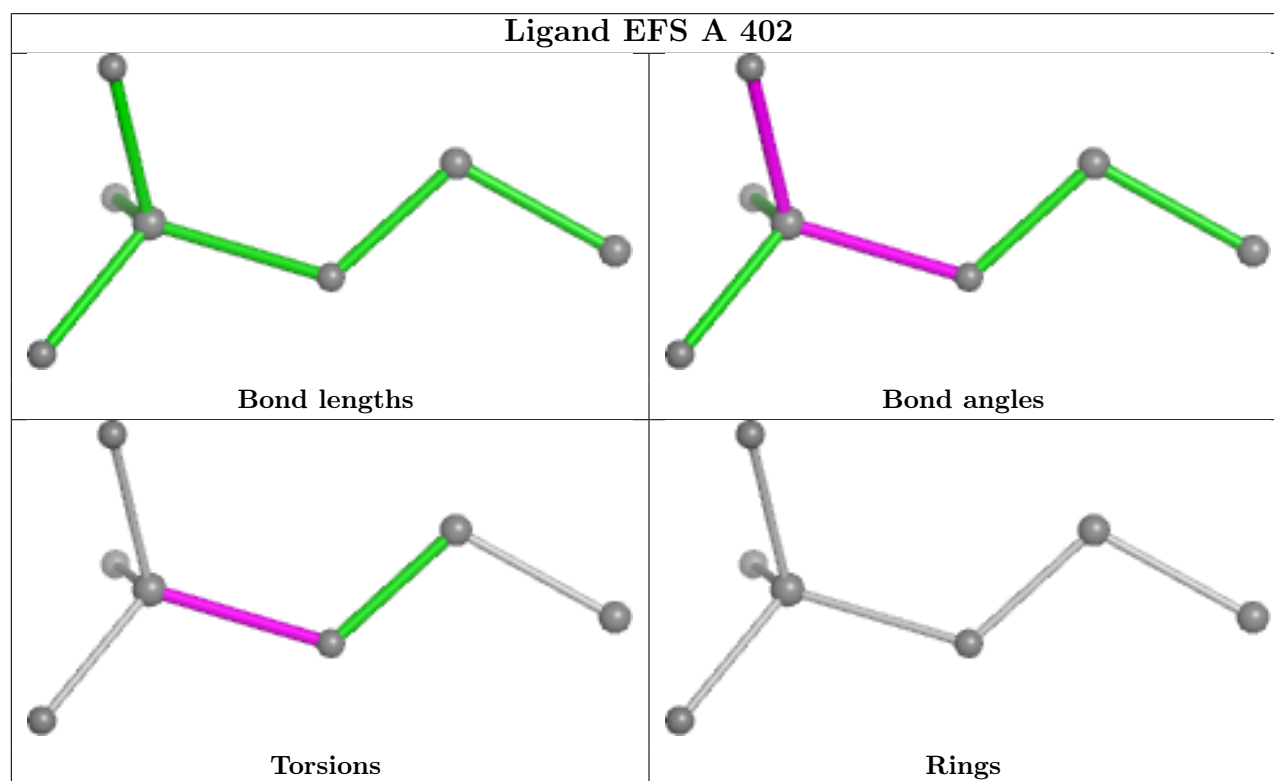
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	MJC	1	0

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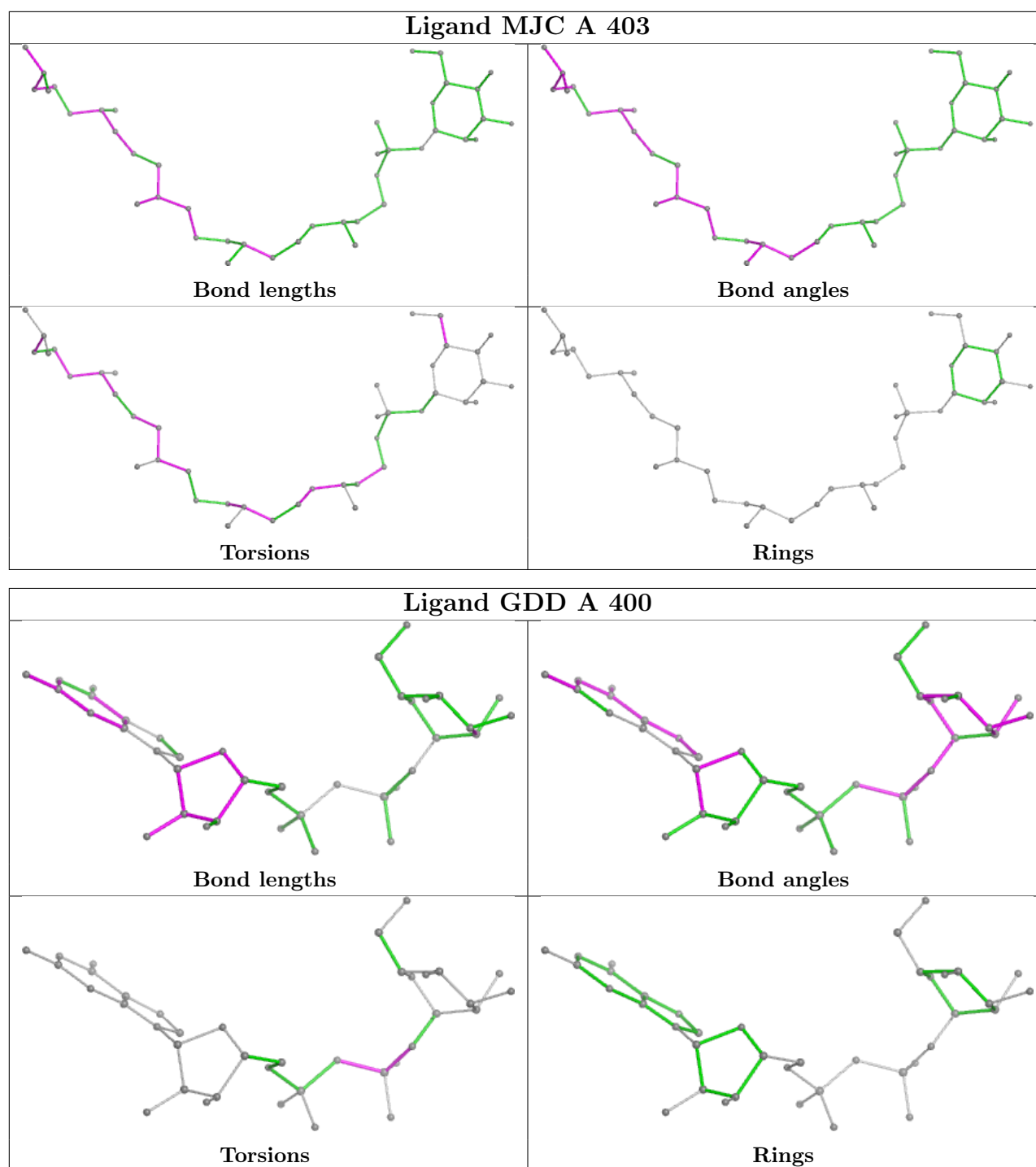
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	GDD	3	0

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	343/374 (91%)	0.30	11 (3%)	50 44	58, 83, 115, 131	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	THR	3.9
1	A	169	GLY	3.7
1	A	45	THR	2.9
1	A	35	VAL	2.5
1	A	351	ALA	2.5
1	A	352	THR	2.3
1	A	101	LYS	2.3
1	A	201	ILE	2.2
1	A	168	GLU	2.2
1	A	37	VAL	2.2
1	A	106	ILE	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 oligosaccharides 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,

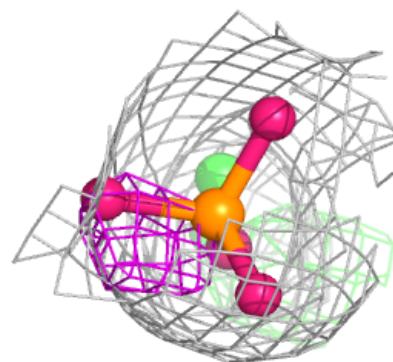
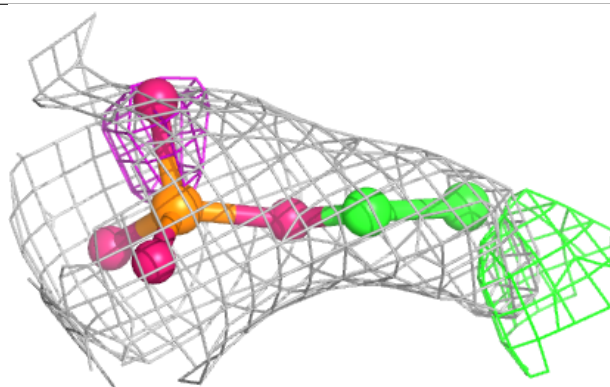
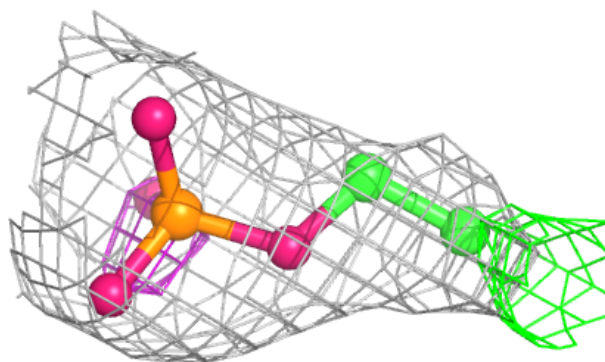
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EFS	A	402	7/7	0.81	0.20	83,91,99,103	0
2	GDD	A	400	39/39	0.89	0.09	83,89,100,106	0
5	MJC	A	403	41/71	0.91	0.18	74,84,97,104	0
3	MG	A	401	1/1	0.93	0.10	83,83,83,83	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.

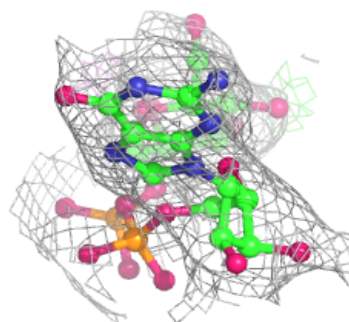
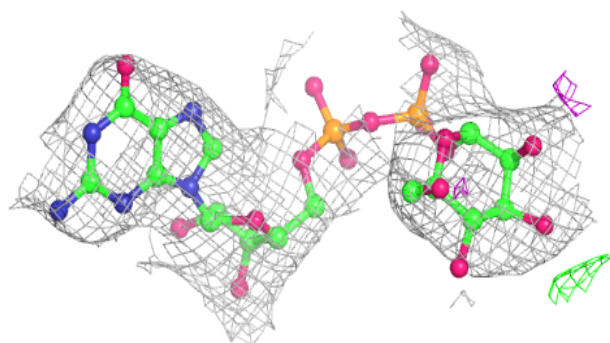
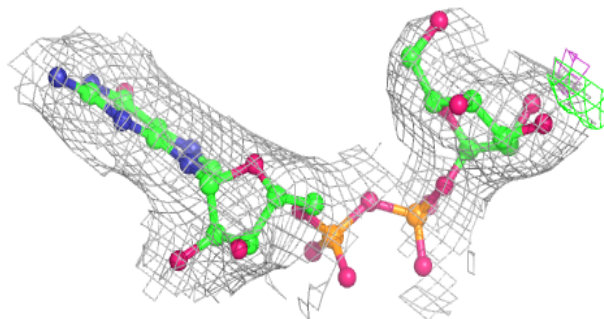
**Electron density around EFS A 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

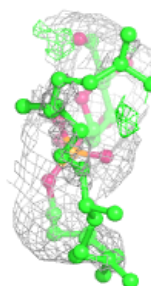
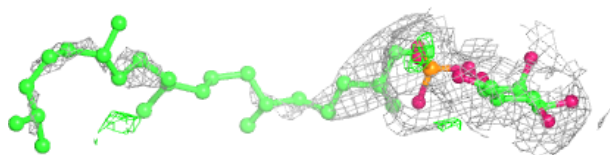
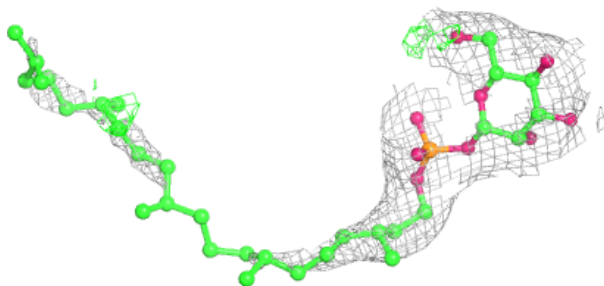


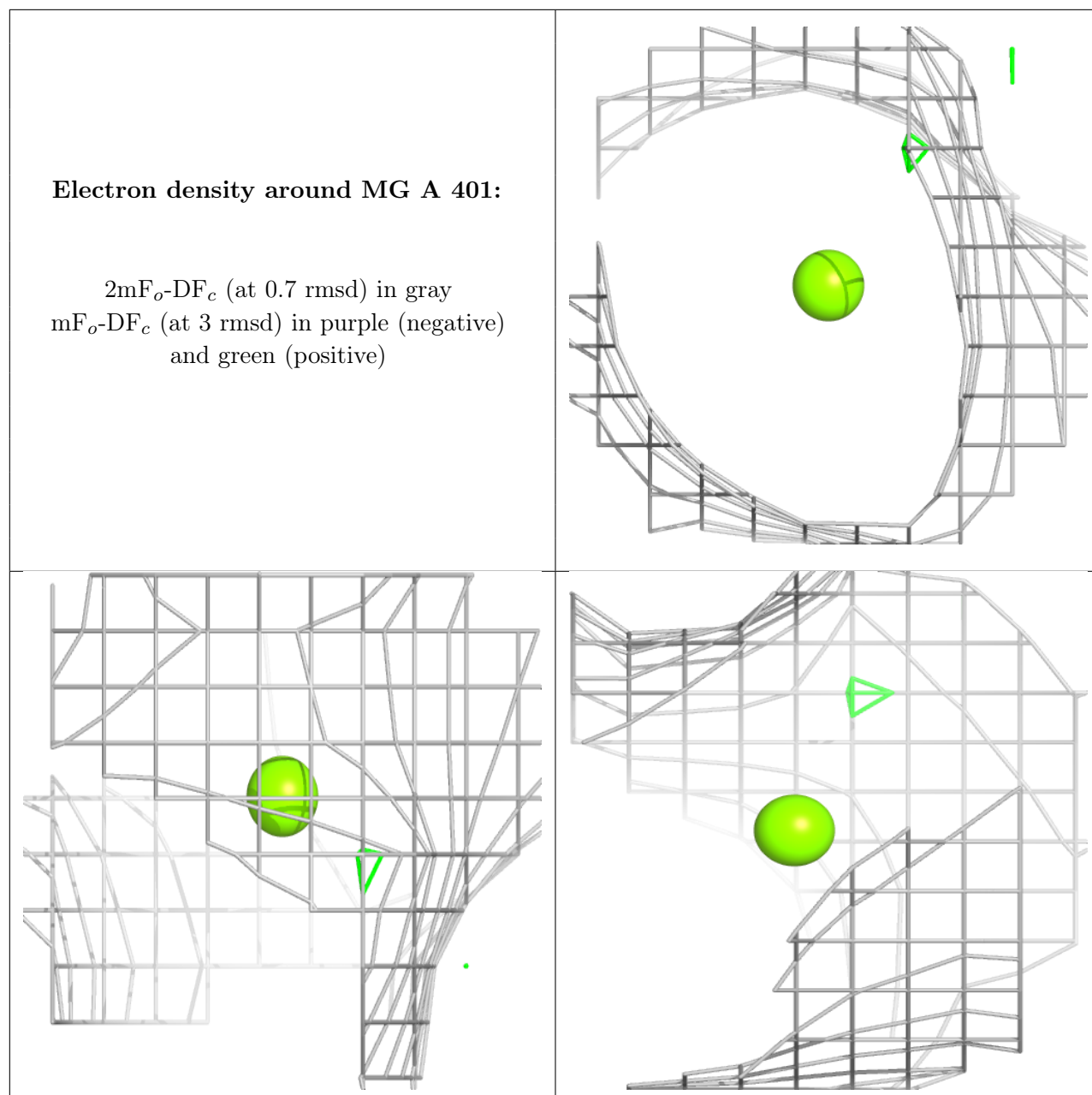
**Electron density around GDD A 400:**

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

**Electron density around MJC 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 ⓘ

There are no such residues in this entry.