



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 01:00 PM EDT

PDB ID : 8E0V  
Title : DAHP (3-deoxy-D-arabinoheptulosonate-7-phosphate) Synthase complexed with Mn(II), PEP, and Pi in unbound:(bound)2:other Conformations  
Authors : Berti, P.J.; Junop, M.S.; Grainger, R.  
Deposited on : 2022-08-09  
Resolution : 2.30 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)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

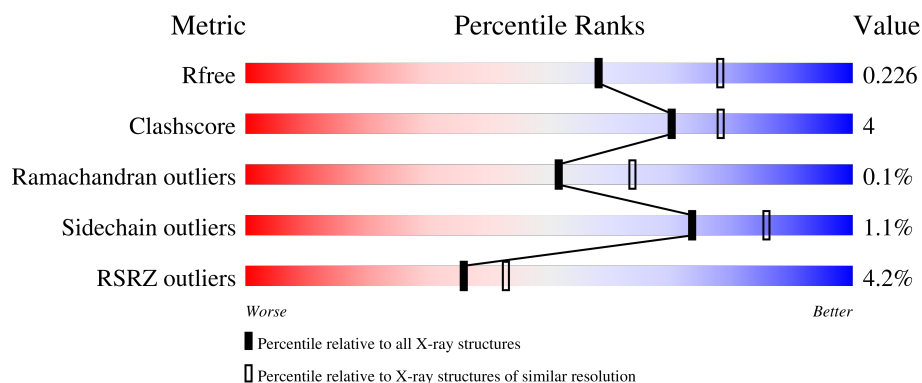
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	351	<div> <div>5%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	B	351	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	351	<div> <div>94%</div> <div>..</div> </div>
1	D	351	<div> <div>9%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11265 atoms, of which 36 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 Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	1	0
			2572	1614	458	486	14			
1	B	340	Total	C	N	O	S	0	0	0
			2547	1601	451	481	14			
1	C	344	Total	C	N	O	S	0	0	0
			2572	1615	455	488	14			
1	D	343	Total	C	N	O	S	0	0	0
			2543	1600	451	478	14			

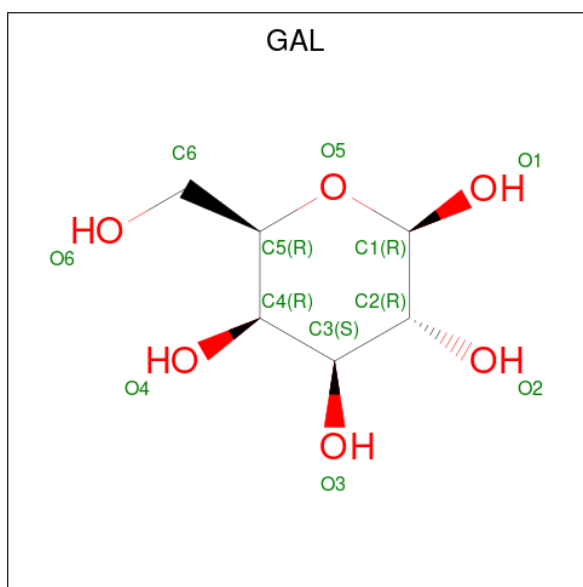
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0AB91
B	0	GLY	-	expression tag	UNP P0AB91
C	0	GLY	-	expression tag	UNP P0AB91
D	0	GLY	-	expression tag	UNP P0AB91

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

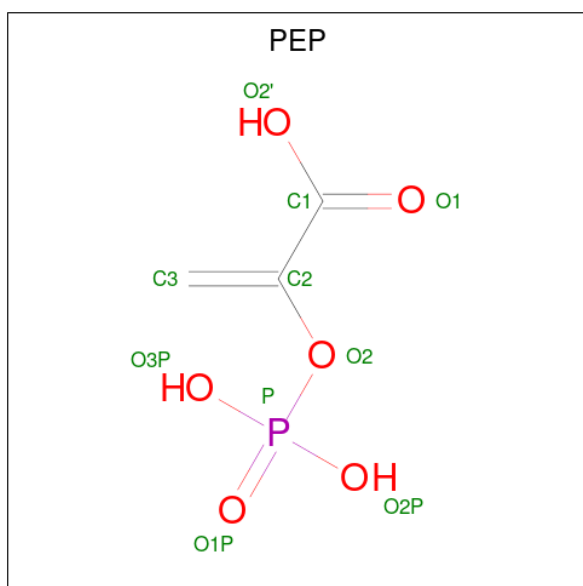
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is beta-D-galactopyranose (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



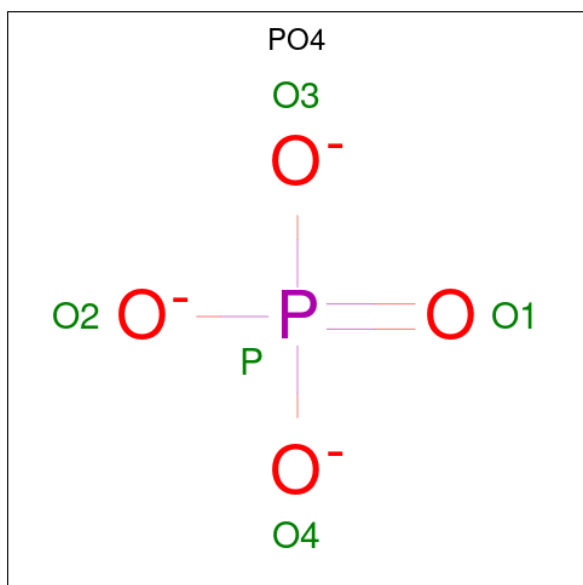
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			24	6	12	6		
3	A	1	Total	C	H	O	0	0
			24	6	12	6		
3	C	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

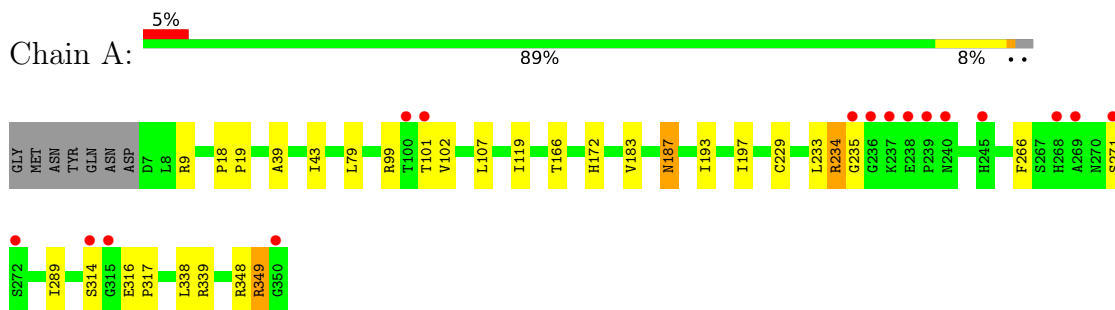
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	231	Total	O	0	0
			231	231		
6	B	165	Total	O	0	0
			165	165		
6	C	329	Total	O	0	0
			329	329		
6	D	200	Total	O	0	0
			200	200		

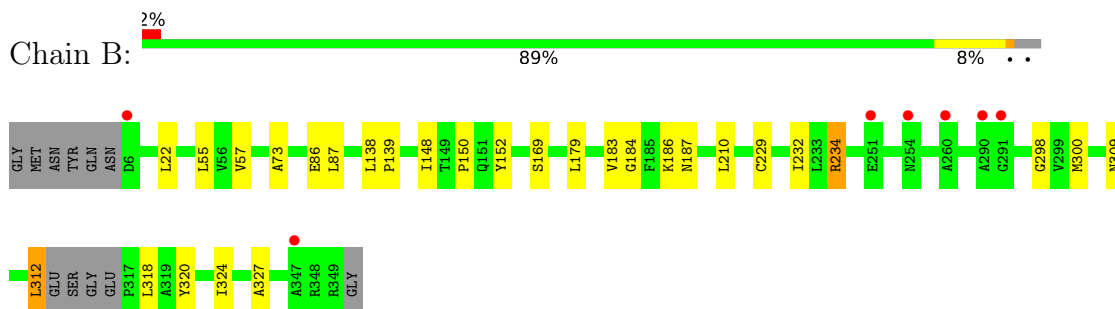
### 3 Residue-property plots [i](#)

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.

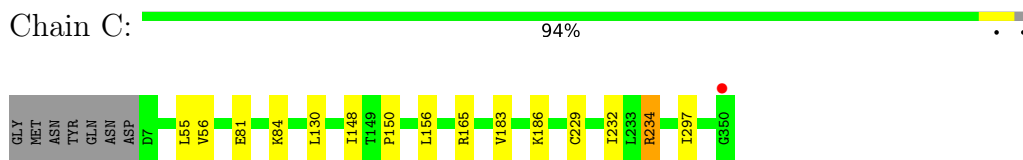
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive



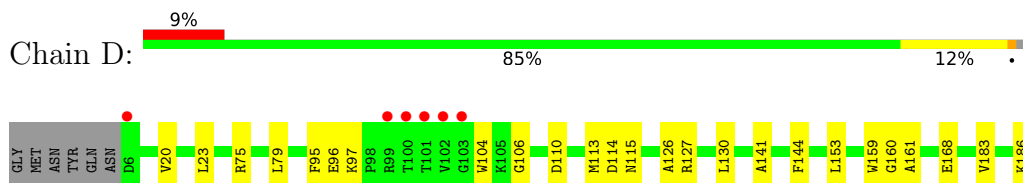
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive

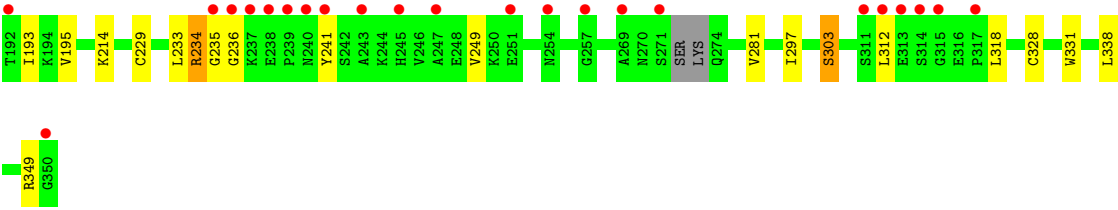


- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.19Å 52.91Å 150.48Å 90.00° 115.71° 90.00°	Depositor
Resolution (Å)	49.65 – 2.30 49.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.65-2.30) 99.7 (49.65-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.194 , 0.228 0.193 , 0.226	Depositor DCC
$R_{free}$ test set	1991 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: GAL, PEP, MN, PO4

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	0.60	0/2620	0.71	0/3554
1	B	0.55	0/2591	0.71	0/3514
1	C	0.63	0/2617	0.71	0/3549
1	D	0.57	0/2587	0.75	0/3510
All	All	0.59	0/10415	0.72	0/14127

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	2572	0	2540	20	0
1	B	2547	0	2516	19	0
1	C	2572	0	2535	9	0
1	D	2543	0	2490	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	12	12	0	0
4	B	10	0	2	0	0
4	C	10	0	2	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	231	0	0	1	0
6	B	165	0	0	0	0
6	C	329	0	0	0	0
6	D	200	0	0	2	0
All	All	11229	36	10121	73	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 4.

All (73) 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:D:20:VAL:HG12	1:D:214:LYS:HE2	1.80	0.64
1:B:312:LEU:HD23	1:B:324:ILE:HD12	1.80	0.63
1:B:312:LEU:HD22	1:B:318:LEU:HD11	1.85	0.57
1:C:186:LYS:HB3	1:C:234:ARG:HG2	1.85	0.57
1:A:193:ILE:HD12	1:A:197:ILE:HD11	1.86	0.56
1:B:57:VAL:O	1:B:300:MET:HA	2.05	0.56
1:D:234:ARG:HD2	1:D:235:GLY:O	2.06	0.56
1:A:9:ARG:HD2	1:B:179:LEU:O	2.07	0.54
1:C:130:LEU:HD13	1:C:156:LEU:HB2	1.89	0.54
1:A:107:LEU:C	1:A:107:LEU:HD23	2.28	0.54
1:D:96:GLU:HG2	1:D:97:LYS:N	2.24	0.53
1:A:187:ASN:OD1	1:A:233:LEU:HA	2.09	0.53
1:D:193:ILE:HG21	1:D:249:VAL:HG22	1.90	0.53
1:B:312:LEU:CD2	1:B:318:LEU:HD11	2.40	0.52
1:D:110:ASP:OD2	1:D:113:MET:HA	2.10	0.51
1:D:95:PHE:CZ	1:D:126:ALA:HB1	2.46	0.50
1:C:148:ILE:C	1:C:150:PRO:HD2	2.32	0.50
1:A:183:VAL:O	1:A:229:CYS:HA	2.12	0.49
1:B:86:GLU:C	1:B:87:LEU:HD23	2.33	0.49
1:D:186:LYS:HD2	6:D:616:HOH:O	2.12	0.49
1:A:79:LEU:HD12	1:A:338:LEU:HD12	1.94	0.49
1:B:312:LEU:HD23	1:B:324:ILE:CD1	2.43	0.48
1:D:195:VAL:HG22	6:D:501:HOH:O	2.14	0.48
1:D:189:THR:O	1:D:236:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:THR:HG22	1:A:102:VAL:N	2.30	0.47
1:A:107:LEU:HD23	1:A:107:LEU:O	2.14	0.47
1:B:138:LEU:HD12	1:B:139:PRO:HD2	1.96	0.47
1:B:186:LYS:HB3	1:B:234:ARG:HG2	1.96	0.47
1:C:183:VAL:O	1:C:229:CYS:HA	2.15	0.47
1:B:22:LEU:HD13	1:B:152:TYR:HD2	1.79	0.47
1:A:266:PHE:O	1:A:271:SER:HB3	2.15	0.46
1:B:184:GLY:HA3	1:B:232:ILE:HD11	1.97	0.46
1:A:39:ALA:O	1:A:43:ILE:HG13	2.15	0.46
1:A:314:SER:HA	6:A:529:HOH:O	2.15	0.45
1:D:144:PHE:HE2	1:D:160:GLY:HA3	1.80	0.45
1:C:186:LYS:HD3	1:C:232:ILE:HB	1.99	0.45
1:A:234:ARG:HD2	1:A:235:GLY:O	2.17	0.45
1:D:20:VAL:CG1	1:D:214:LYS:HE2	2.46	0.45
1:D:144:PHE:CE2	1:D:160:GLY:HA3	2.52	0.45
1:D:159:TRP:CH2	1:D:161:ALA:HB2	2.51	0.45
1:C:297:ILE:HD12	1:C:297:ILE:C	2.38	0.44
1:D:141:ALA:HB1	1:D:159:TRP:HE3	1.82	0.44
1:B:22:LEU:HD13	1:B:152:TYR:CD2	2.51	0.44
1:A:166:THR:HG21	1:A:172:HIS:CE1	2.53	0.44
1:D:75:ARG:HB3	1:D:331:TRP:CZ2	2.53	0.43
1:D:96:GLU:CG	1:D:97:LYS:N	2.81	0.43
1:D:130:LEU:HD12	1:D:153:LEU:HD22	2.00	0.43
1:D:79:LEU:HD23	1:D:338:LEU:HD12	2.00	0.43
1:A:166:THR:HG22	1:B:169:SER:HB2	2.01	0.43
1:B:183:VAL:O	1:B:229:CYS:HA	2.19	0.43
1:A:289:ILE:O	1:A:348:ARG:HB2	2.19	0.43
1:B:73:ALA:HB1	1:B:138:LEU:HD23	2.01	0.42
1:D:113:MET:HB3	1:D:312:LEU:HD21	2.00	0.42
1:A:349:ARG:O	1:A:349:ARG:HG3	2.20	0.42
1:C:165:ARG:HG2	1:D:168:GLU:HG2	2.02	0.42
1:D:312:LEU:HD13	1:D:318:LEU:HD11	2.01	0.42
1:D:104:TRP:CH2	1:D:106:GLY:HA2	2.55	0.42
1:D:303:SER:HA	1:D:328:CYS:HB3	2.01	0.42
1:D:187:ASN:OD1	1:D:233:LEU:HA	2.20	0.41
1:A:18:PRO:HA	1:A:19:PRO:HD3	1.89	0.41
1:D:114:ASP:O	1:D:115:ASN:HB2	2.20	0.41
1:A:316:GLU:HA	1:A:317:PRO:HD3	1.93	0.41
1:A:339:ARG:HH11	1:A:339:ARG:HG2	1.85	0.41
1:B:148:ILE:C	1:B:150:PRO:HD2	2.41	0.41
1:A:119:ILE:HG21	1:B:210:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:O	1:B:298:GLY:HA2	2.21	0.41
1:B:309:ASN:HB3	1:B:327:ALA:HA	2.03	0.41
1:D:241:TYR:CE2	1:D:281:VAL:HG22	2.56	0.41
1:D:297:ILE:HD12	1:D:297:ILE:C	2.41	0.40
1:C:81:GLU:O	1:C:84:LYS:HD3	2.22	0.40
1:D:23:LEU:HD23	1:D:127:ARG:CZ	2.51	0.40
1:C:55:LEU:HD12	1:C:56:VAL:N	2.36	0.40
1:D:183:VAL:O	1:D:229:CYS:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/351 (98%)	336 (98%)	7 (2%)	0	100	100
1	B	336/351 (96%)	328 (98%)	8 (2%)	0	100	100
1	C	342/351 (97%)	334 (98%)	8 (2%)	0	100	100
1	D	339/351 (97%)	320 (94%)	17 (5%)	2 (1%)	25	31
All	All	1360/1404 (97%)	1318 (97%)	40 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	189	THR
1	D	349	ARG

### 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	264/283 (93%)	260 (98%)	4 (2%)	65	79
1	B	262/283 (93%)	258 (98%)	4 (2%)	65	79
1	C	263/283 (93%)	262 (100%)	1 (0%)	91	96
1	D	255/283 (90%)	253 (99%)	2 (1%)	81	91
All	All	1044/1132 (92%)	1033 (99%)	11 (1%)	73	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	187	ASN
1	A	234	ARG
1	A	349	ARG
1	B	187	ASN
1	B	234	ARG
1	B	312	LEU
1	B	320	TYR
1	C	234	ARG
1	D	234	ARG
1	D	303	SER

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

Mol	Chain	Res	Type
1	D	151	GLN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
3	GAL	A	403	-	12,12,12	1.25	0	17,17,17	1.51	4 (23%)
3	GAL	C	404	-	12,12,12	0.44	0	17,17,17	0.67	0
3	GAL	A	402	-	12,12,12	0.51	0	17,17,17	0.60	0
4	PEP	B	402	-	9,9,9	3.17	3 (33%)	11,13,13	1.90	4 (36%)
5	PO4	B	403	-	4,4,4	0.89	0	6,6,6	0.24	0
4	PEP	C	402	-	9,9,9	2.97	3 (33%)	11,13,13	1.83	3 (27%)
5	PO4	C	403	-	4,4,4	0.64	0	6,6,6	1.07	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
3	GAL	A	403	-	-	1/2/22/22	0/1/1/1
3	GAL	C	404	-	-	2/2/22/22	0/1/1/1
3	GAL	A	402	-	-	0/2/22/22	0/1/1/1
4	PEP	B	402	-	-	0/9/9/9	-
4	PEP	C	402	-	-	0/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	PEP	C2-C1	-8.40	1.41	1.49
4	C	402	PEP	C2-C1	-7.79	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	PEP	C3-C2	3.16	1.40	1.31
4	C	402	PEP	C3-C2	3.12	1.40	1.31
4	C	402	PEP	O2'-C1	-2.43	1.23	1.30
4	B	402	PEP	O2'-C1	-2.43	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	PEP	O2-C2-C3	-4.52	116.08	124.79
4	B	402	PEP	O2-C2-C3	-4.05	116.98	124.79
3	A	403	GAL	C3-C4-C5	3.19	115.92	110.24
4	B	402	PEP	O1-C1-C2	-2.75	117.64	121.79
4	B	402	PEP	O2'-C1-C2	2.68	118.48	113.91
4	B	402	PEP	C3-C2-C1	2.45	127.26	122.73
3	A	403	GAL	O3-C3-C4	-2.30	105.02	110.35
4	C	402	PEP	C3-C2-C1	2.15	126.70	122.73
3	A	403	GAL	O2-C2-C3	-2.14	105.41	110.35
3	A	403	GAL	O5-C5-C4	-2.09	105.90	109.69
4	C	402	PEP	O1-C1-C2	-2.06	118.69	121.79

There are no chirality outliers.

All (3) torsion outliers are listed below:

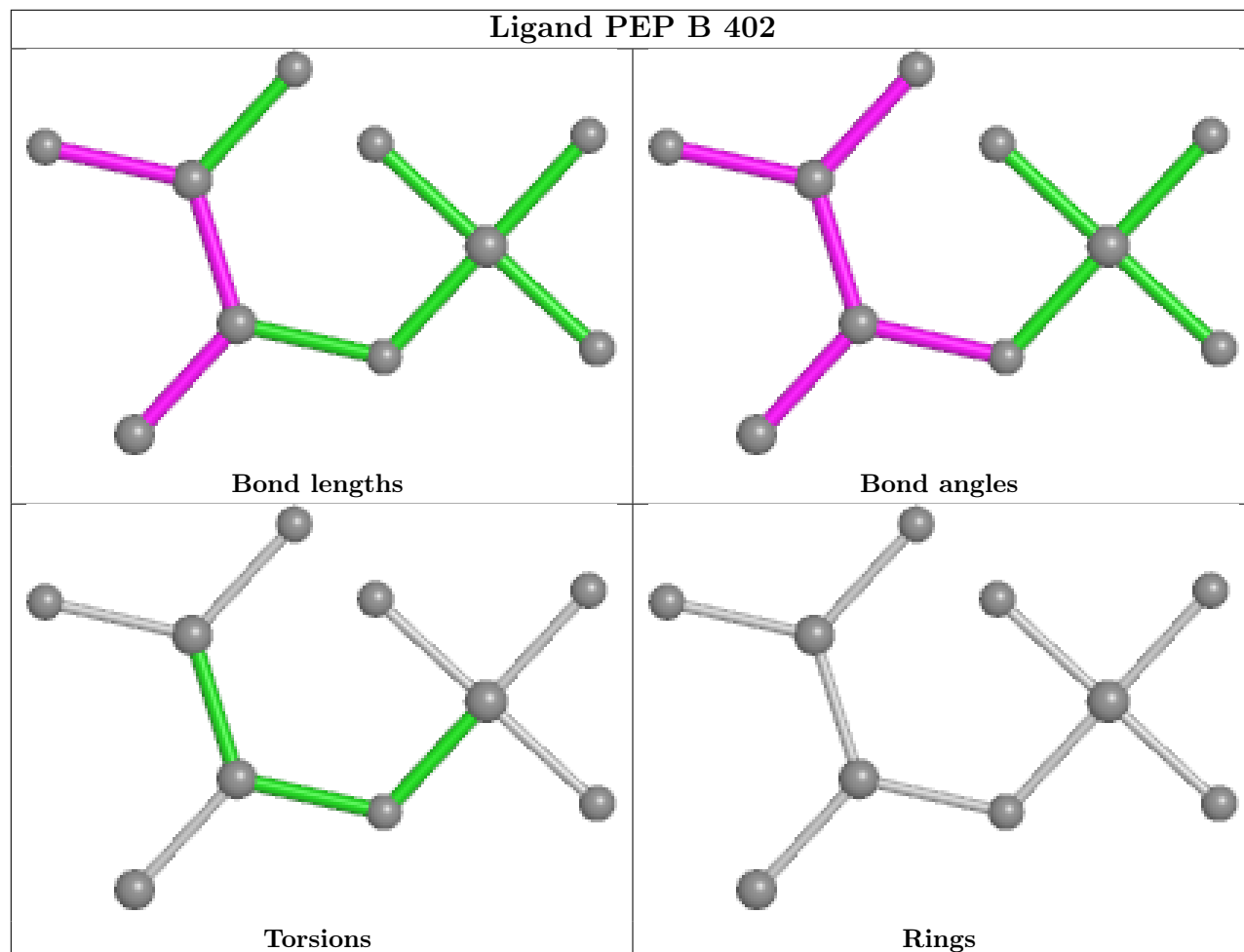
Mol	Chain	Res	Type	Atoms
3	C	404	GAL	C4-C5-C6-O6
3	C	404	GAL	O5-C5-C6-O6
3	A	403	GAL	O5-C5-C6-O6

There are no ring outliers.

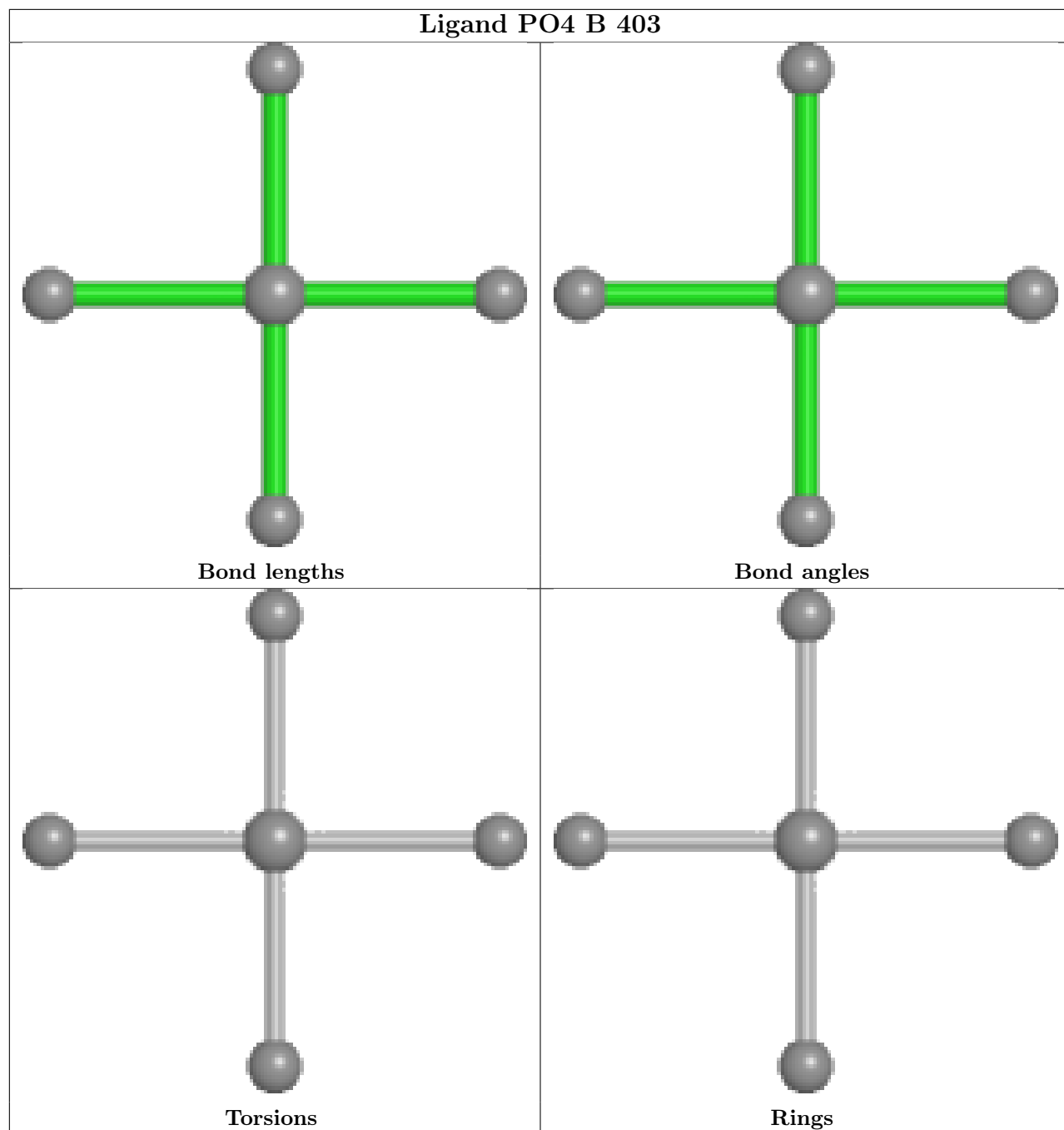
No monomer is involved in short contacts.

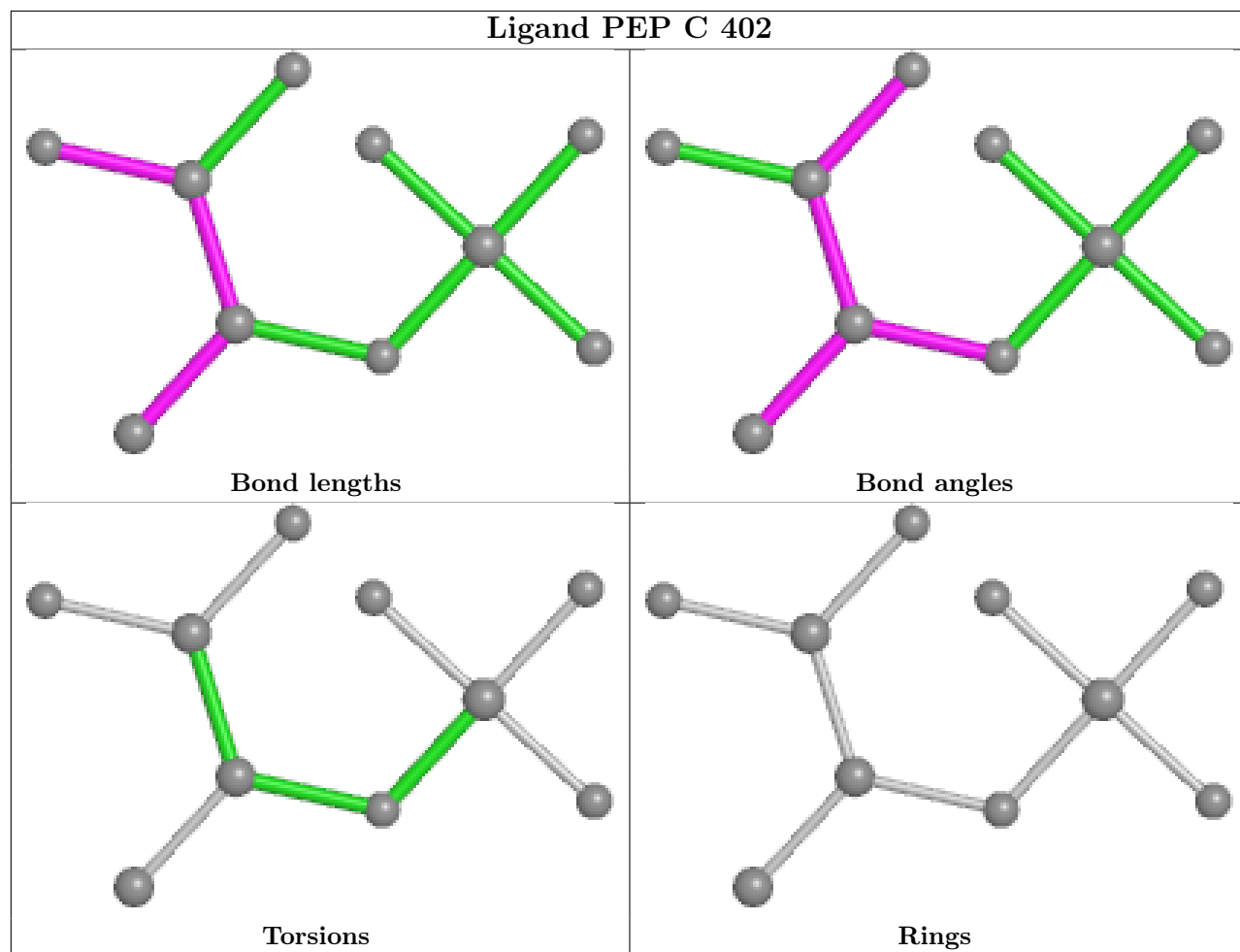
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

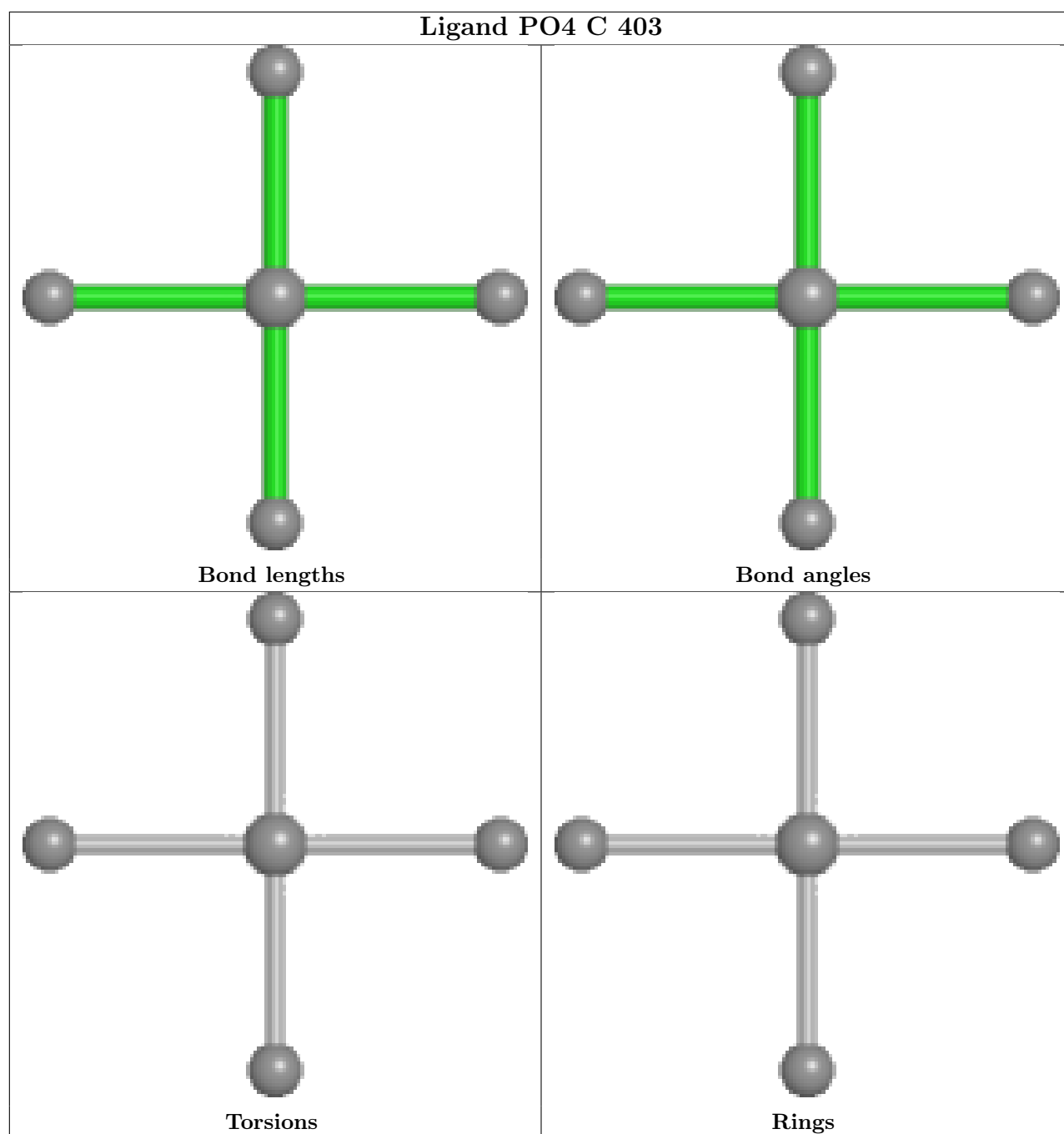
equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	344/351 (98%)	0.09	16 (4%) 31 38	19, 28, 38, 44	0
1	B	340/351 (96%)	-0.11	7 (2%) 63 70	24, 32, 38, 43	0
1	C	344/351 (98%)	-0.42	1 (0%) 94 96	16, 22, 27, 34	0
1	D	343/351 (97%)	0.25	33 (9%) 8 10	20, 30, 37, 42	0
All	All	1371/1404 (97%)	-0.05	57 (4%) 36 43	16, 28, 37, 44	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLY	7.3
1	D	315	GLY	7.0
1	D	350	GLY	6.2
1	D	236	GLY	6.0
1	D	317	PRO	5.4
1	D	6	ASP	5.2
1	D	269	ALA	5.0
1	D	237	LYS	4.9
1	D	103	GLY	4.8
1	D	100	THR	4.8
1	C	350	GLY	4.7
1	A	269	ALA	4.6
1	A	315	GLY	4.5
1	D	102	VAL	4.4
1	D	101	THR	4.3
1	A	314	SER	4.1
1	D	235	GLY	4.0
1	D	314	SER	4.0
1	A	271	SER	3.9
1	A	237	LYS	3.6
1	B	6	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	235	GLY	3.3
1	D	189	THR	3.3
1	A	272	SER	3.3
1	A	239	PRO	3.3
1	D	99	ARG	3.1
1	D	271	SER	3.1
1	B	290	ALA	3.0
1	D	243	ALA	2.9
1	D	251	GLU	2.9
1	D	192	THR	2.9
1	A	350	GLY	2.9
1	D	191	GLY	2.8
1	D	254	ASN	2.8
1	A	245	HIS	2.8
1	A	268	HIS	2.7
1	D	190	ASP	2.6
1	A	101	THR	2.6
1	B	291	GLY	2.6
1	D	245	HIS	2.5
1	D	240	ASN	2.4
1	D	312	LEU	2.4
1	A	238	GLU	2.3
1	B	251	GLU	2.3
1	D	247	ALA	2.3
1	A	240	ASN	2.3
1	D	241	TYR	2.2
1	D	188	GLY	2.2
1	D	238	GLU	2.2
1	D	313	GLU	2.2
1	D	239	PRO	2.2
1	A	100	THR	2.2
1	B	260	ALA	2.1
1	D	257	GLY	2.1
1	B	254	ASN	2.1
1	B	347	ALA	2.0
1	D	311	SER	2.0

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

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](#)

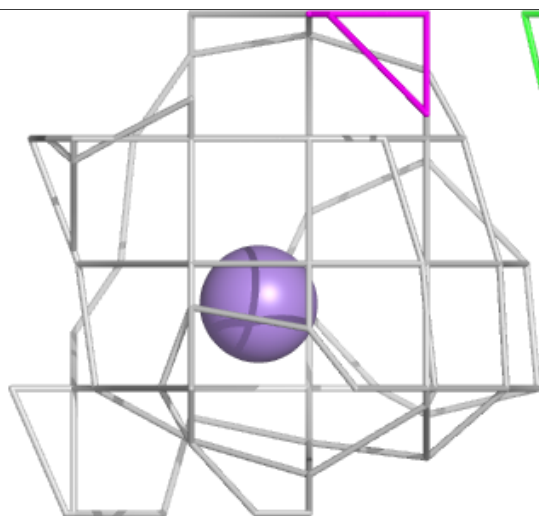
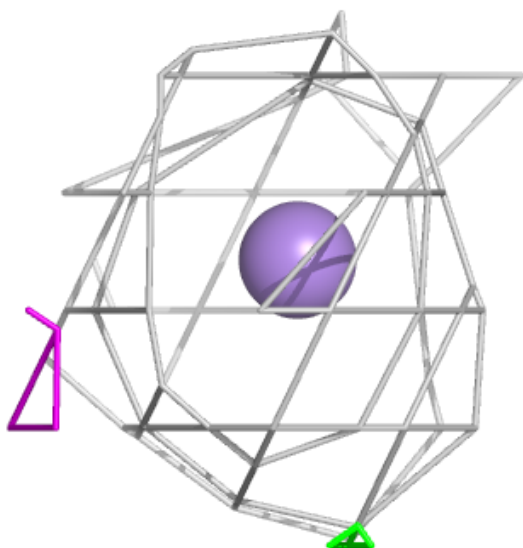
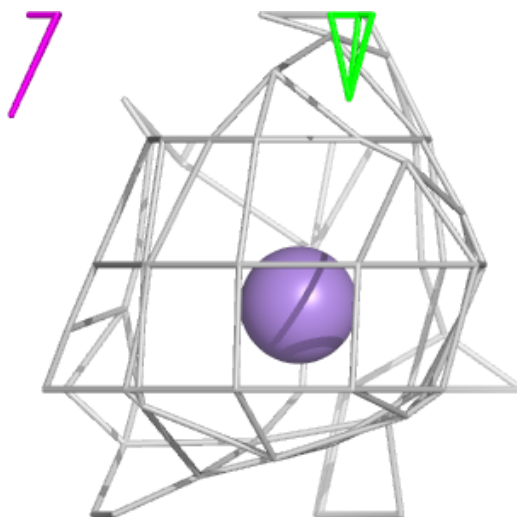
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	A	401	1/1	0.80	0.26	31,31,31,31	1
3	GAL	C	404	12/12	0.89	0.21	24,28,37,42	24
5	PO4	B	403	5/5	0.90	0.15	31,34,35,36	5
3	GAL	A	402	12/12	0.95	0.17	25,28,32,38	24
2	MN	D	401	1/1	0.96	0.26	38,38,38,38	0
4	PEP	B	402	10/10	0.96	0.10	30,31,32,32	0
3	GAL	A	403	12/12	0.96	0.14	22,25,27,28	0
5	PO4	C	403	5/5	0.96	0.14	23,25,26,26	5
2	MN	B	401	1/1	0.97	0.09	32,32,32,32	1
4	PEP	C	402	10/10	0.97	0.08	19,20,21,21	0
2	MN	C	401	1/1	0.98	0.06	20,20,20,20	1

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

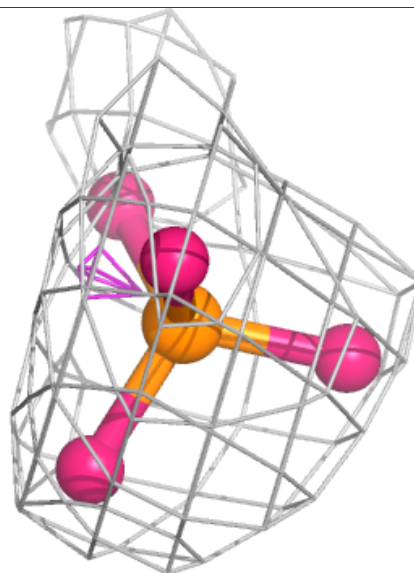
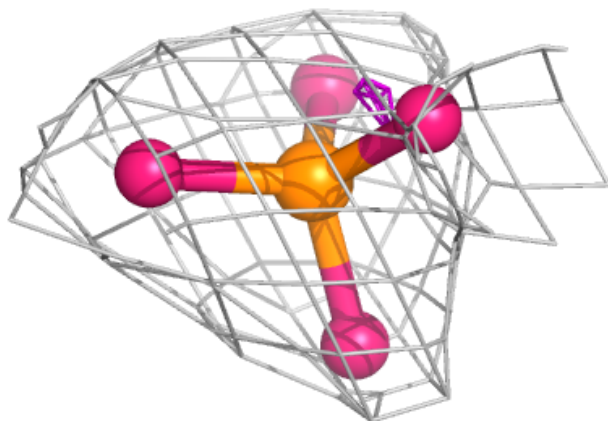
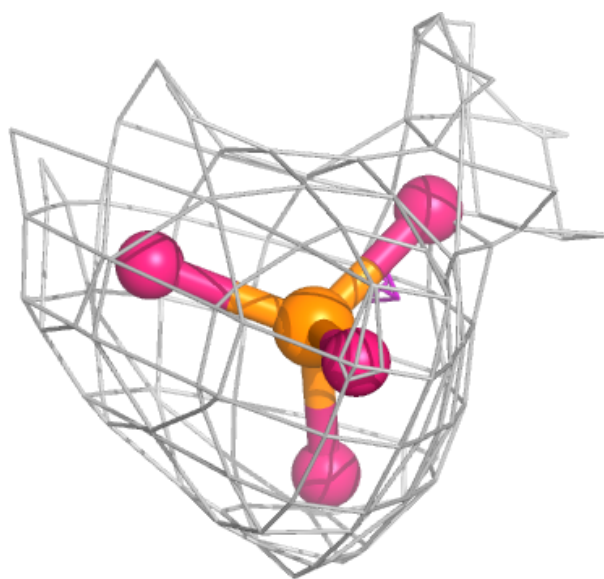
**Electron density around MN A 401:**

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



**Electron density around PO4 B 403:**

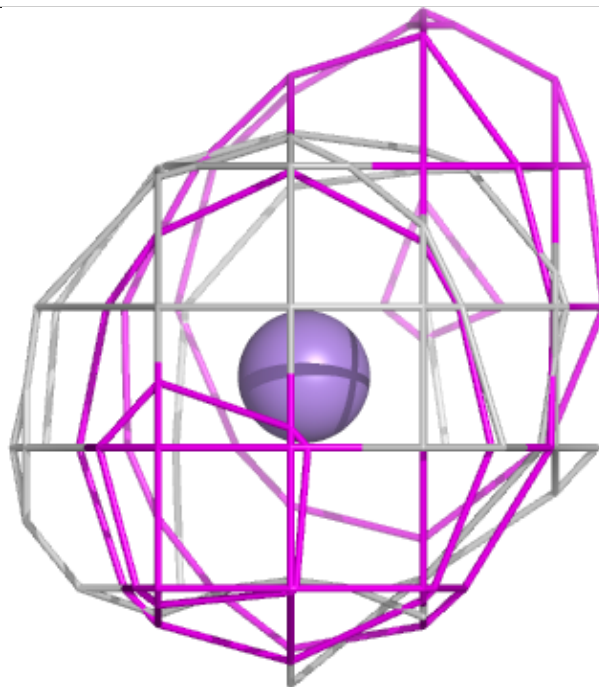
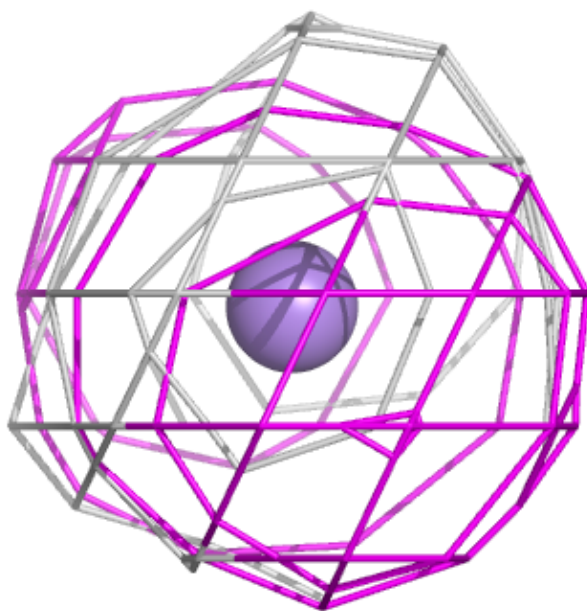
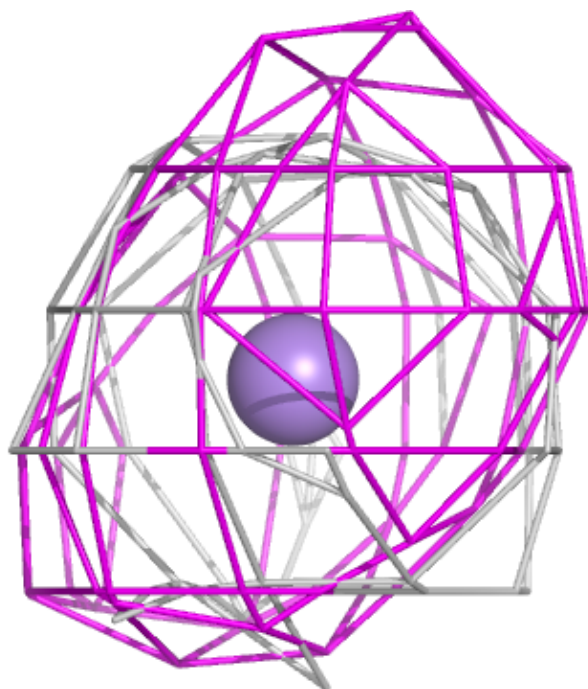
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





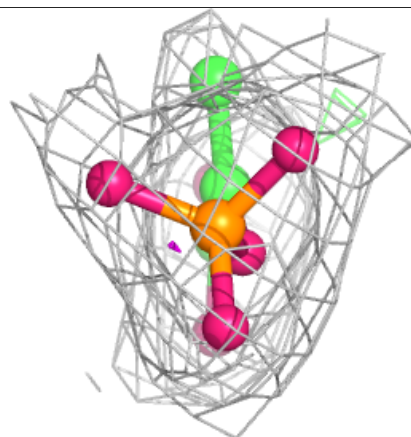
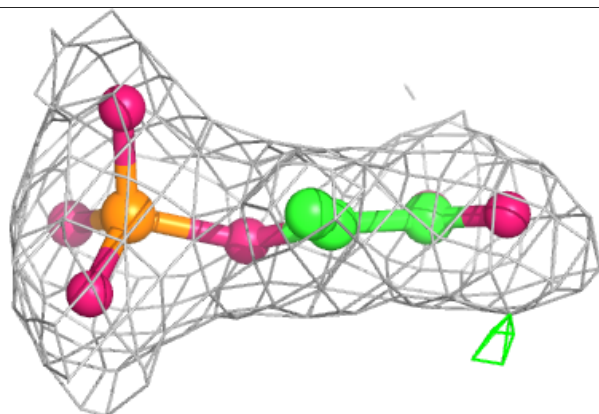
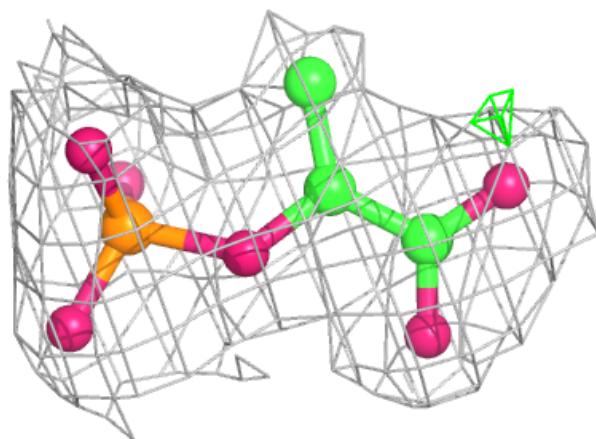
**Electron density around MN D 401:**

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



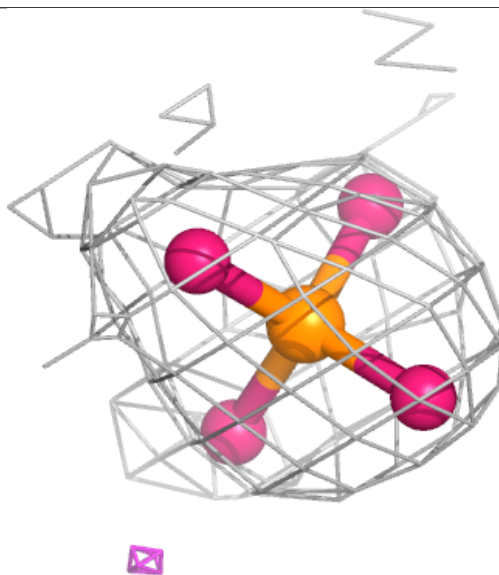
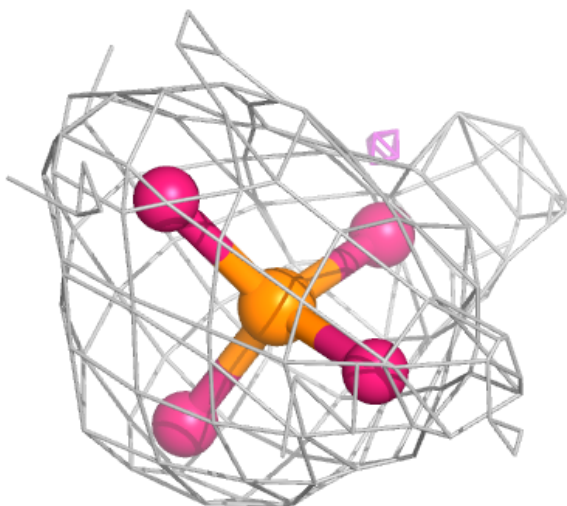
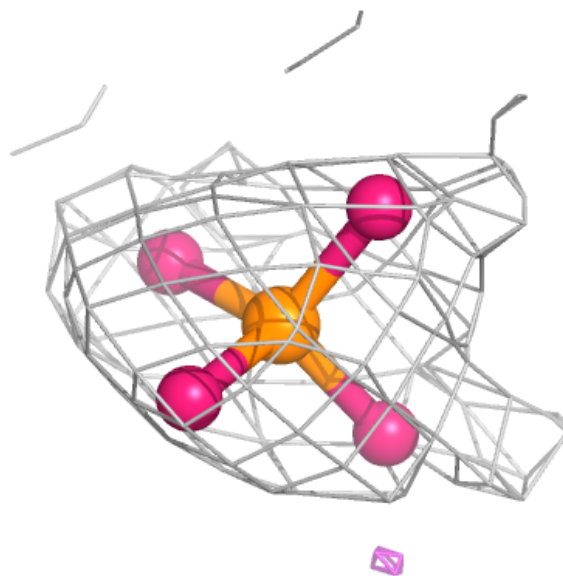
**Electron density around PEP B 402:**

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



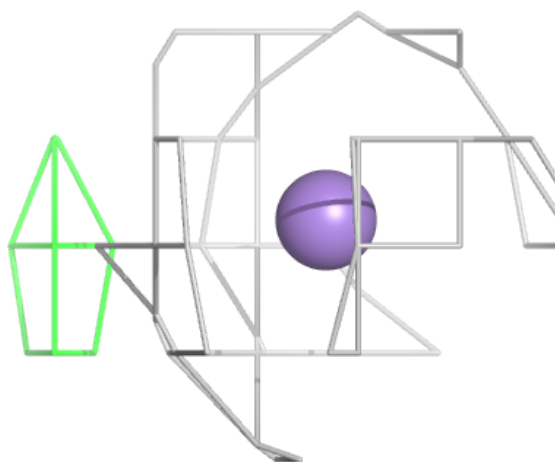
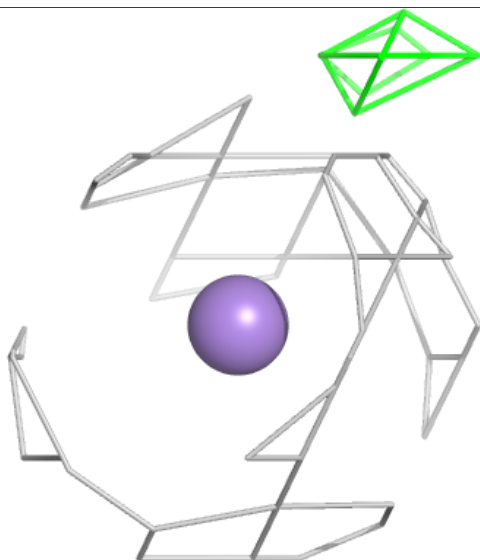
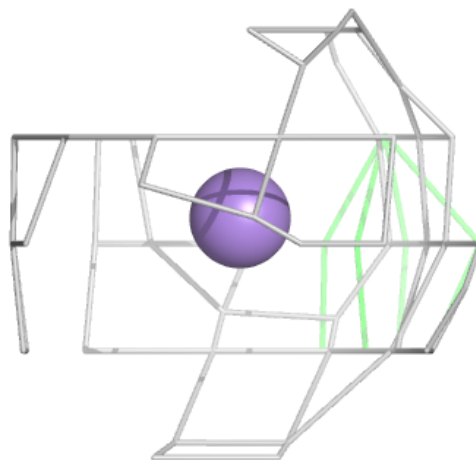
**Electron density around PO4 C 403:**

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



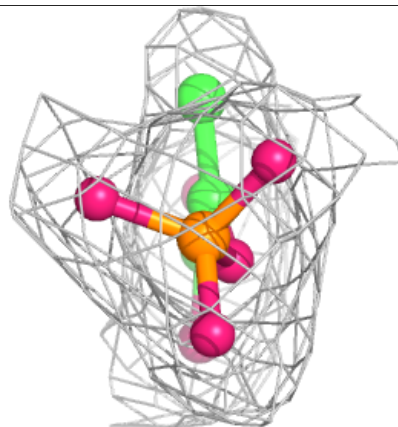
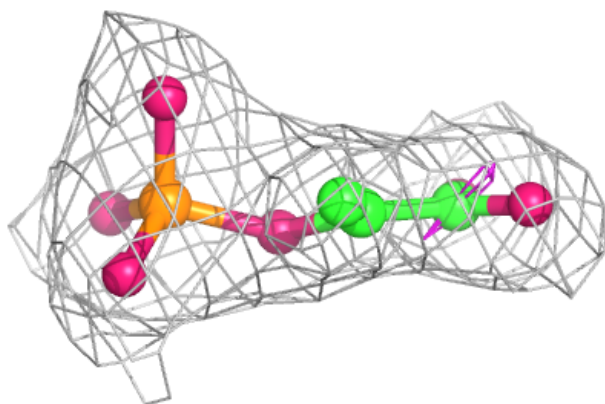
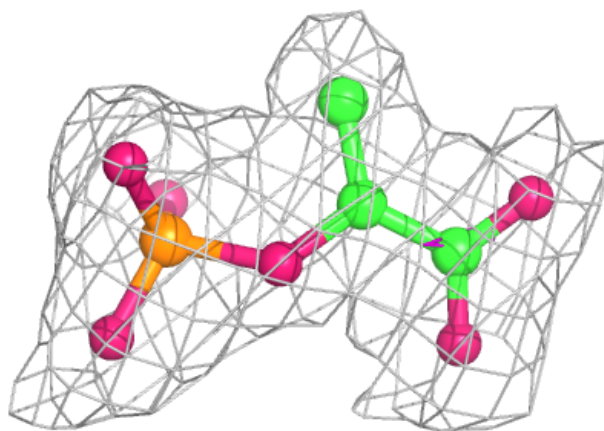
**Electron density around MN B 401:**

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



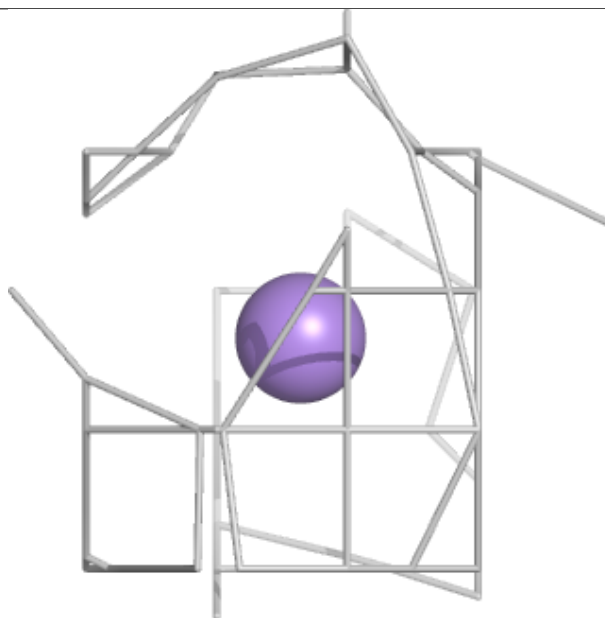
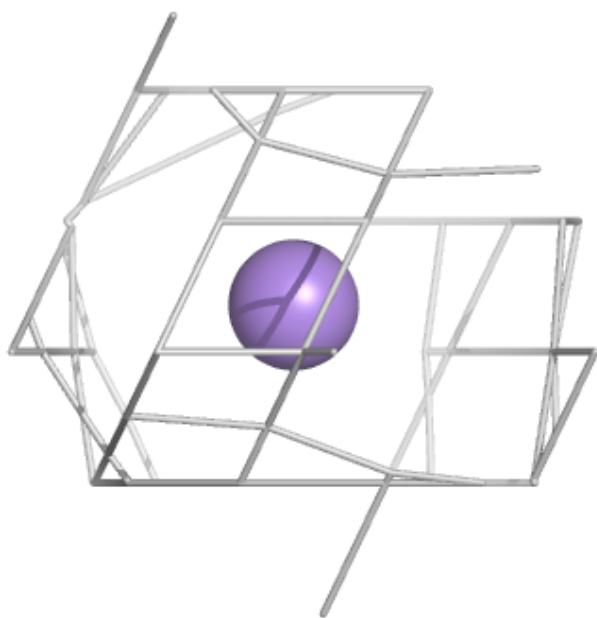
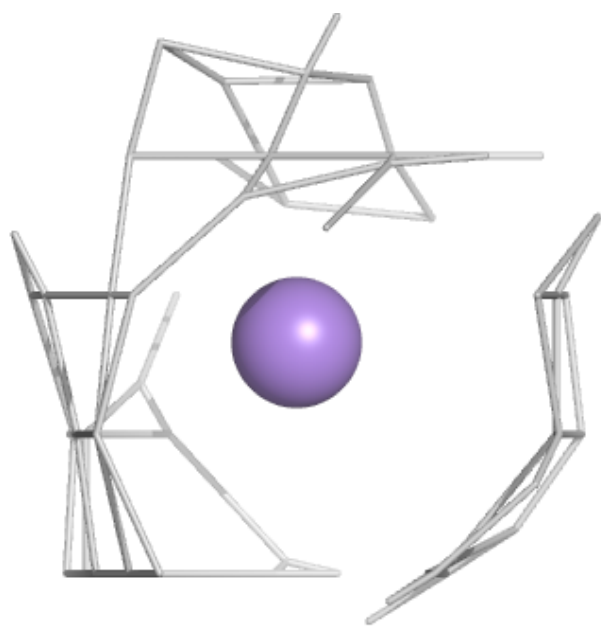
**Electron density around PEP C 402:**

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



**Electron density around MN C 401:**

$2mF_o-DF_c$  (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.