



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 04:16 am BST

PDB ID : 2I5C
Title : Crystal structure of the C-terminal PH domain of pleckstrin in complex with D-myo-Ins(1,2,3,4,5)P5
Authors : Jackson, S.G.; Haslam, R.J.; Junop, M.S.
Deposited on : 2006-08-24
Resolution : 1.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

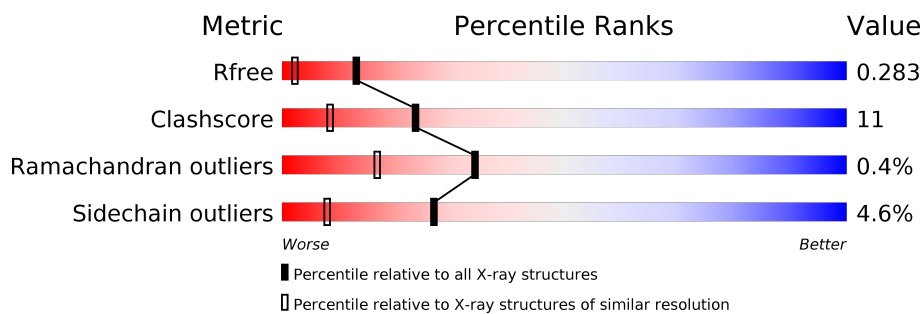
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	109	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>67% 18% • 14%</div>
1	B	109	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>67% 17% •• 14%</div>
1	C	109	<div> <div style="width: 67%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>67% 17% • 14%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2771 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.

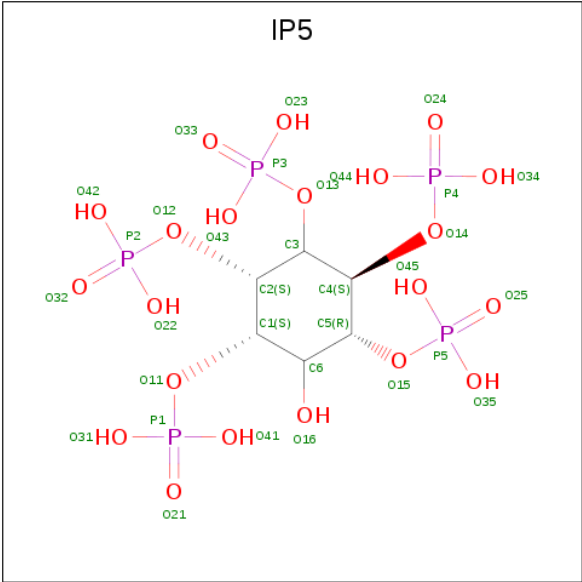
- Molecule 1 is a protein called Pleckstrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	4	0
			787	510	138	136	3			
1	B	94	Total	C	N	O	S	0	3	0
			782	505	138	136	3			
1	C	94	Total	C	N	O	S	0	5	0
			793	515	139	136	3			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLY	-	CLONING ARTIFACT	UNP P08567
A	240	SER	-	CLONING ARTIFACT	UNP P08567
A	241	PHE	-	CLONING ARTIFACT	UNP P08567
A	242	THR	-	CLONING ARTIFACT	UNP P08567
A	243	GLY	-	CLONING ARTIFACT	UNP P08567
B	239	GLY	-	CLONING ARTIFACT	UNP P08567
B	240	SER	-	CLONING ARTIFACT	UNP P08567
B	241	PHE	-	CLONING ARTIFACT	UNP P08567
B	242	THR	-	CLONING ARTIFACT	UNP P08567
B	243	GLY	-	CLONING ARTIFACT	UNP P08567
C	239	GLY	-	CLONING ARTIFACT	UNP P08567
C	240	SER	-	CLONING ARTIFACT	UNP P08567
C	241	PHE	-	CLONING ARTIFACT	UNP P08567
C	242	THR	-	CLONING ARTIFACT	UNP P08567
C	243	GLY	-	CLONING ARTIFACT	UNP P08567

- Molecule 2 is (1R,2S,3R,4S,5S,6R)-6-HYDROXYCYCLOHEXANE-1,2,3,4,5-PENTAYL PENTAKIS[DIHYDROGEN (PHOSPHATE)] (three-letter code: IP5) (formula: C₆H₁₇O₂₁P₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			32	6	21	5		
2	B	1	Total	C	O	P	0	0
			32	6	21	5		
2	C	1	Total	C	O	P	0	0
			32	6	21	5		

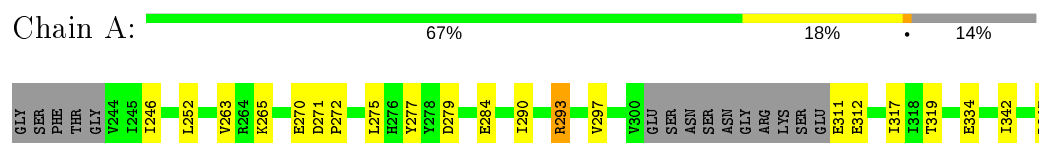
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	102	Total	O	0	0
			102	102		
3	C	98	Total	O	0	0
			98	98		

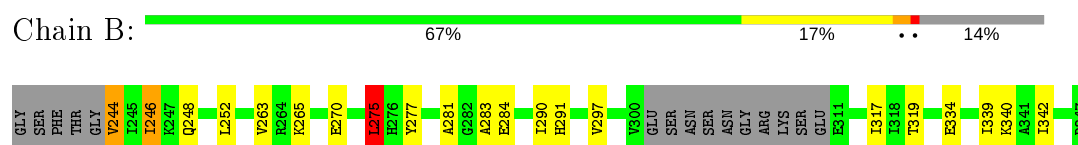
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

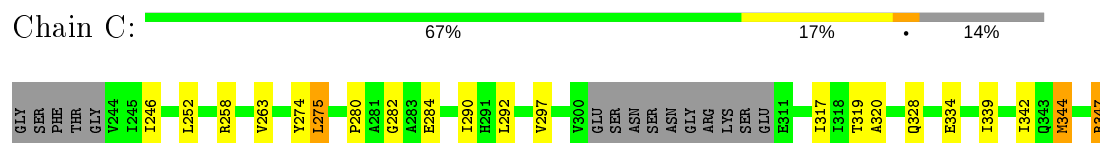
• Molecule 1: Pleckstrin



• Molecule 1: Pleckstrin



• Molecule 1: Pleckstrin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.50Å 47.60Å 87.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 30.03 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.75) 98.4 (30.03-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.176 , 0.243 0.264 , 0.283	Depositor DCC
R_{free} test set	2609 reflections (7.67%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.037 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.038 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.487 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.487 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2771	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: IP5

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	1.15	1/816 (0.1%)	0.99	1/1101 (0.1%)
1	B	1.15	2/808 (0.2%)	0.98	1/1090 (0.1%)
1	C	1.20	4/825 (0.5%)	0.97	0/1112
All	All	1.17	7/2449 (0.3%)	0.98	2/3303 (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	1
1	B	0	2
1	C	0	2
All	All	0	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	334	GLU	CD-OE1	8.62	1.35	1.25
1	A	334	GLU	CD-OE1	7.07	1.33	1.25
1	B	334	GLU	CD-OE1	6.29	1.32	1.25
1	C	334	GLU	CG-CD	5.62	1.60	1.51
1	C	274	TYR	CD2-CE2	5.47	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	275	LEU	CA-CB-CG	5.11	127.04	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	GLU	Peptide
1	B	281	ALA	Peptide
1	B	283	ALA	Peptide
1	C	280	PRO	Peptide
1	C	282	GLY	Peptide

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	787	0	812	16	0
1	B	782	0	801	21	0
1	C	793	0	825	19	0
2	A	32	0	7	0	0
2	B	32	0	7	1	0
2	C	32	0	7	0	0
3	A	113	0	0	2	0
3	B	102	0	0	5	0
3	C	98	0	0	0	0
All	All	2771	0	2459	55	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 11.

The worst 5 of 55 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:297[B]:VAL:HG11	1:A:342:ILE:CG2	2.13	0.79
1:B:340:LYS:CE	3:B:579:HOH:O	2.35	0.75
1:B:246:ILE:N	1:B:246:ILE:HD13	2.02	0.73
1:C:297[B]:VAL:HG11	1:C:342:ILE:CG2	2.20	0.71
1:B:290[B]:ILE:HD11	1:B:319:THR:HG22	1.73	0.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	94/109 (86%)	94 (100%)	0	0	100	100
1	B	93/109 (85%)	92 (99%)	0	1 (1%)	14	3
1	C	95/109 (87%)	94 (99%)	1 (1%)	0	100	100
All	All	282/327 (86%)	280 (99%)	1 (0%)	1 (0%)	34	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/92 (91%)	80 (95%)	4 (5%)	25	7
1	B	83/92 (90%)	80 (96%)	3 (4%)	35	13
1	C	85/92 (92%)	81 (95%)	4 (5%)	26	7
All	All	252/276 (91%)	241 (96%)	11 (4%)	27	8

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

Mol	Chain	Res	Type
1	B	244	VAL
1	B	246	ILE

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Mol	Chain	Res	Type
1	C	284	GLU
1	A	347	ARG
1	C	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	B	291	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IP5	A	550	-	32,32,32	1.04	3 (9%)	48,53,53	1.21	5 (10%)
2	IP5	C	552	-	32,32,32	1.09	2 (6%)	48,53,53	1.00	5 (10%)
2	IP5	B	551	-	32,32,32	1.06	1 (3%)	48,53,53	1.18	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IP5	A	550	-	-	4/25/49/49	0/1/1/1
2	IP5	C	552	-	-	6/25/49/49	0/1/1/1
2	IP5	B	551	-	-	5/25/49/49	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	IP5	P4-O44	-2.31	1.45	1.54
2	B	551	IP5	P5-O15	2.29	1.63	1.59
2	A	550	IP5	C4-C5	2.26	1.56	1.52
2	C	552	IP5	P5-O15	2.17	1.63	1.59
2	A	550	IP5	P5-O15	2.15	1.63	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	IP5	O35-P5-O25	3.12	122.90	110.68
2	A	550	IP5	O35-P5-O45	2.99	119.07	107.64
2	B	551	IP5	O13-P3-O33	-2.96	97.98	109.39
2	A	550	IP5	O15-P5-O25	-2.73	98.84	109.39
2	A	550	IP5	O31-P1-O41	2.62	117.63	107.64

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

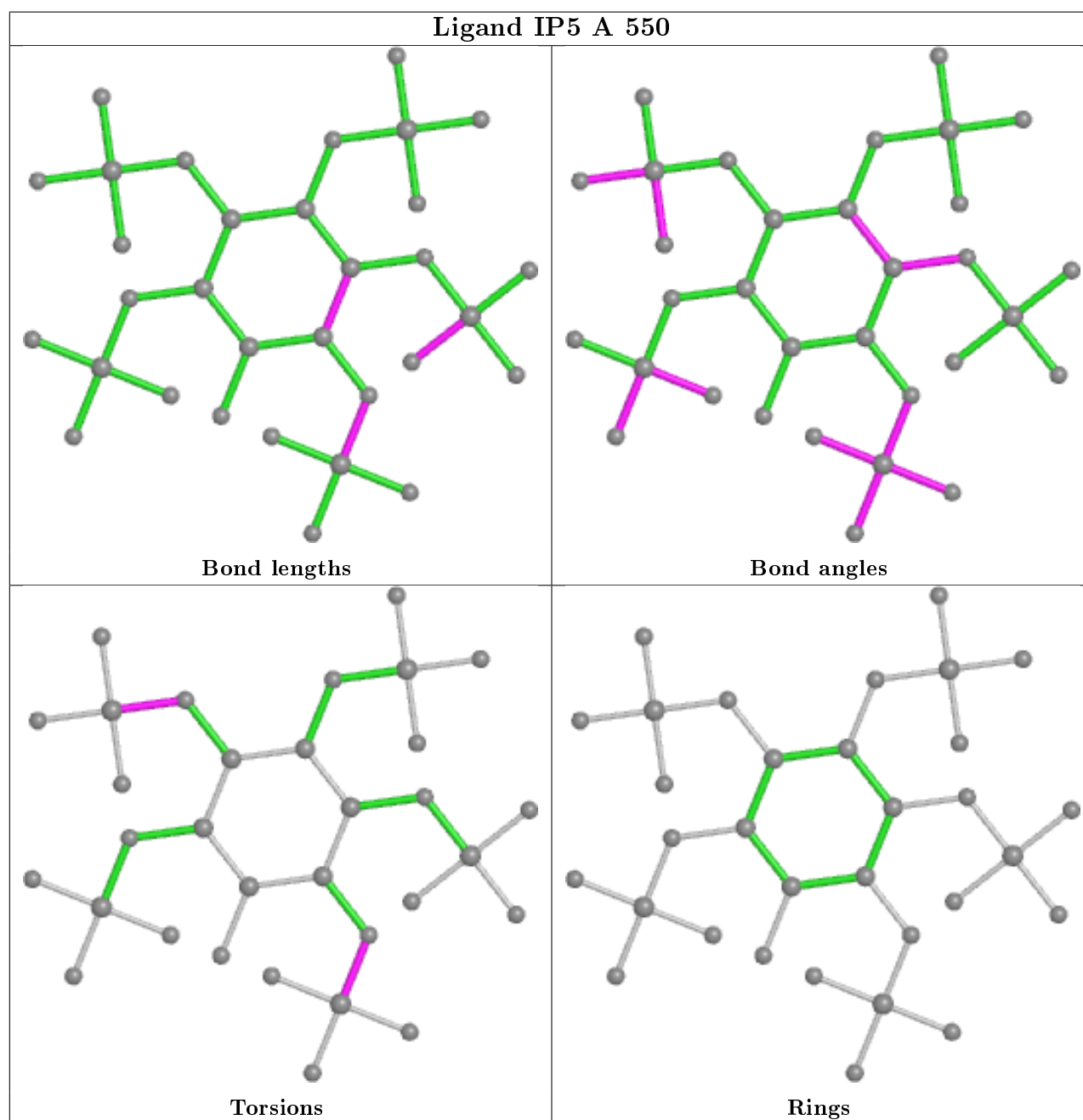
Mol	Chain	Res	Type	Atoms
2	C	552	IP5	C4-O14-P4-O24
2	B	551	IP5	C4-O14-P4-O24
2	C	552	IP5	C1-O11-P1-O41
2	C	552	IP5	C5-O15-P5-O45
2	C	552	IP5	C4-O14-P4-O44

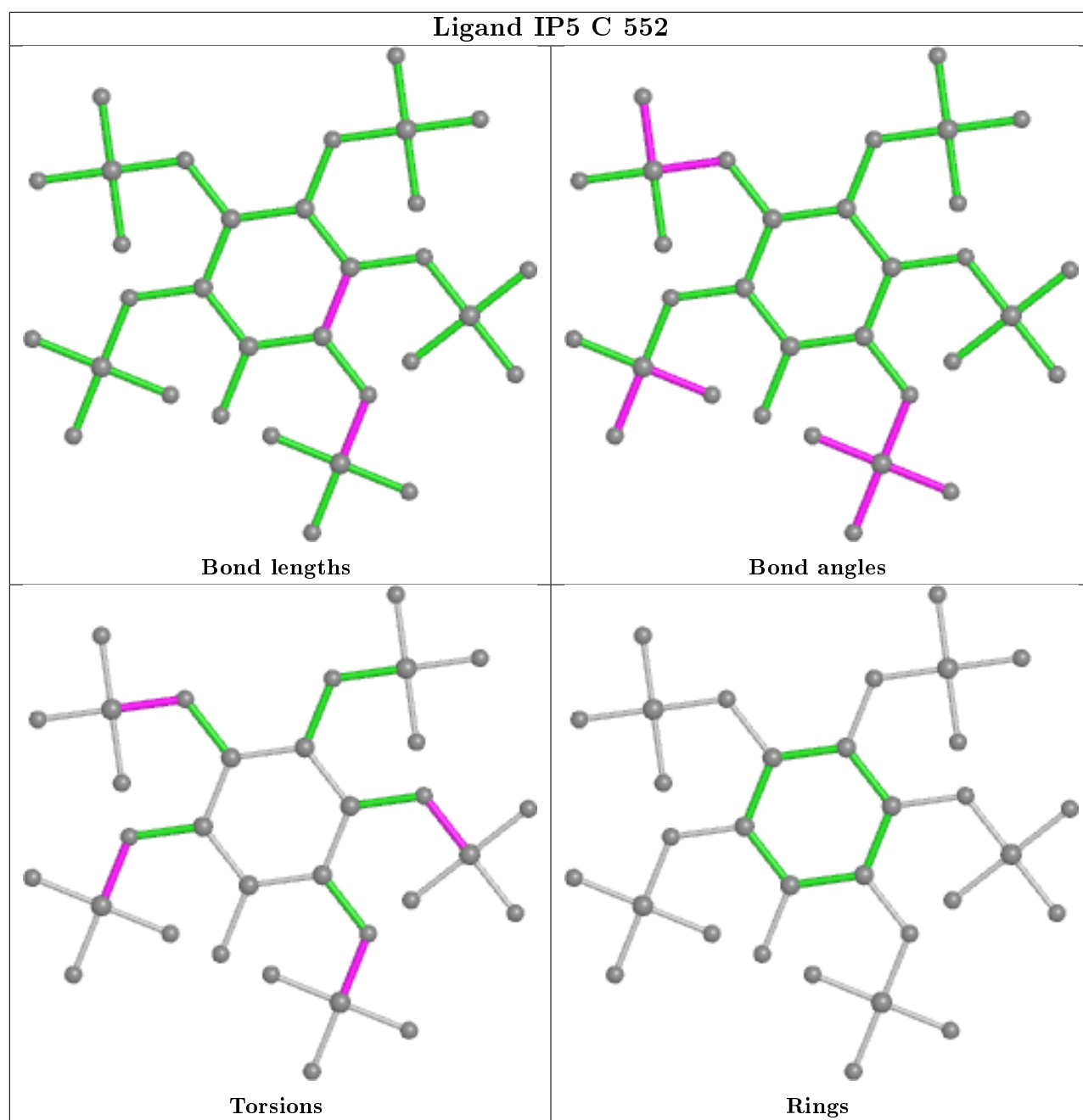
There are no ring outliers.

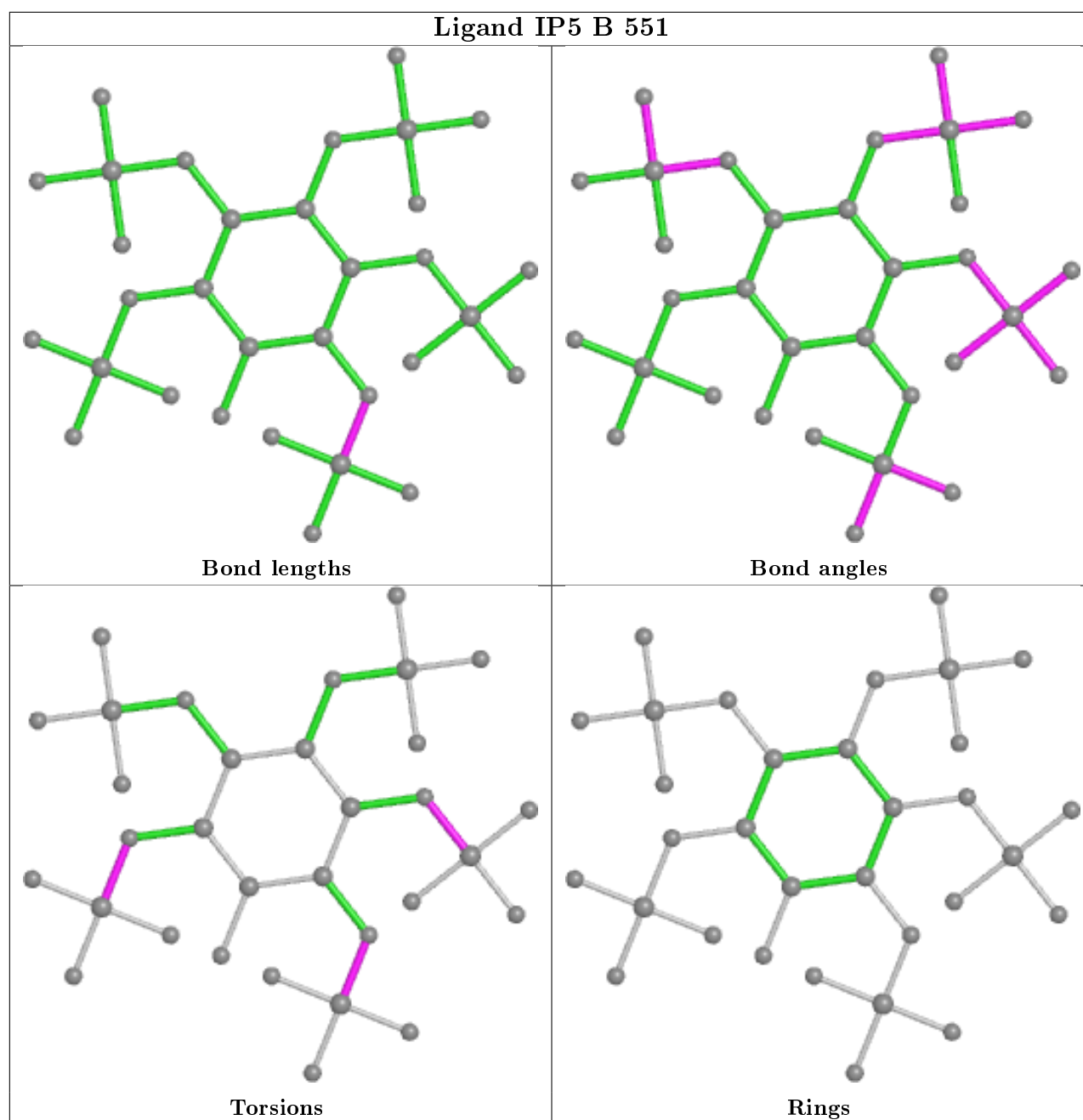
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	551	IP5	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

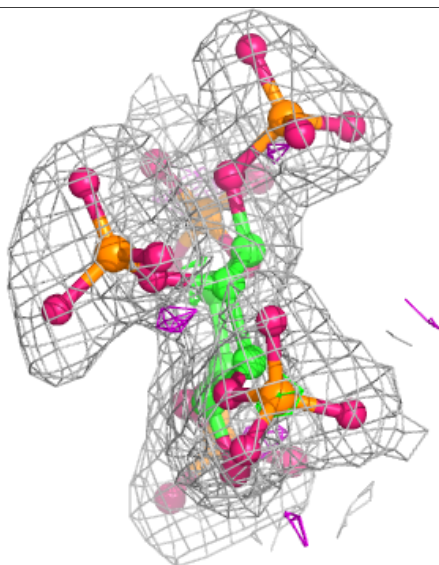
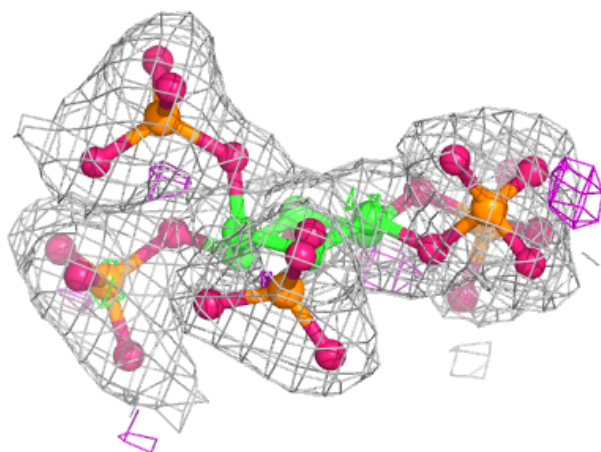
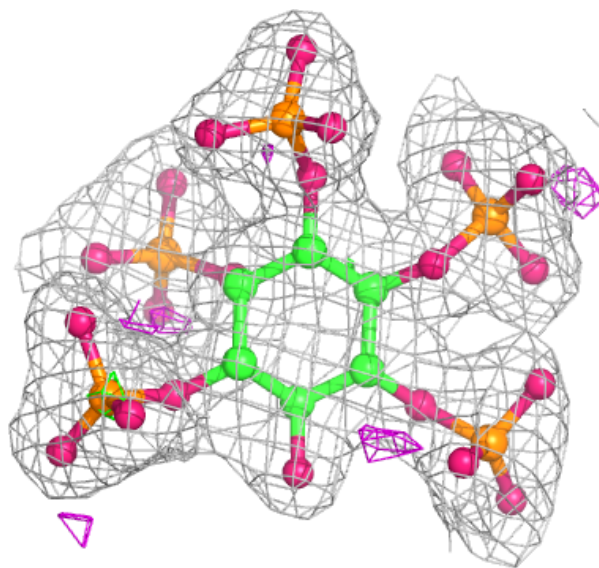
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

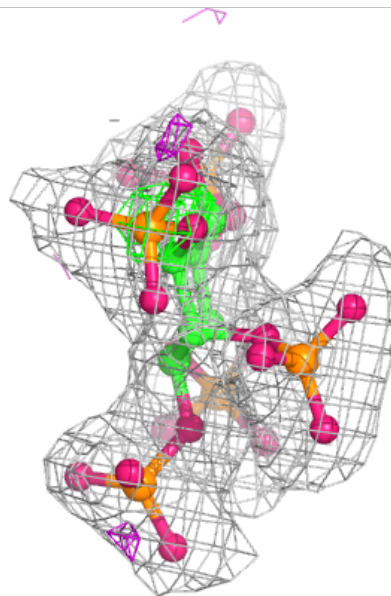
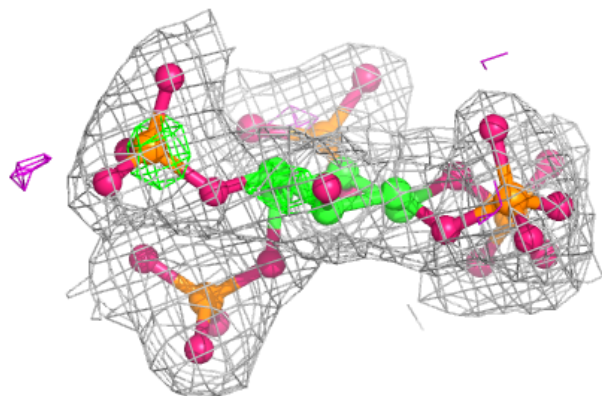
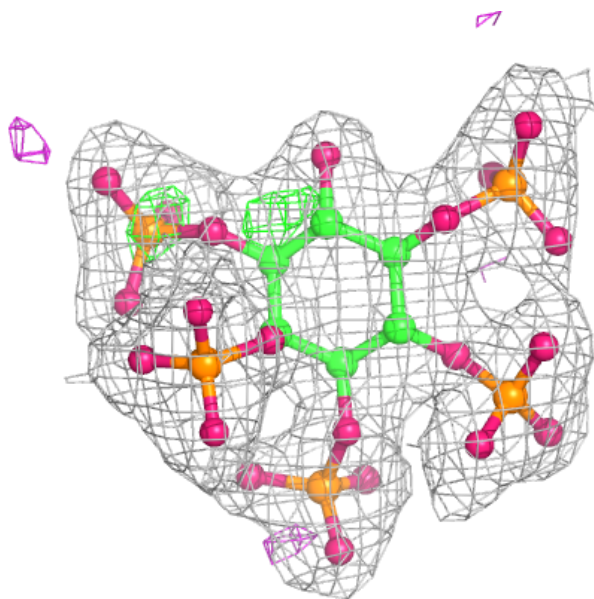
Electron density around IP5 C 552:

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



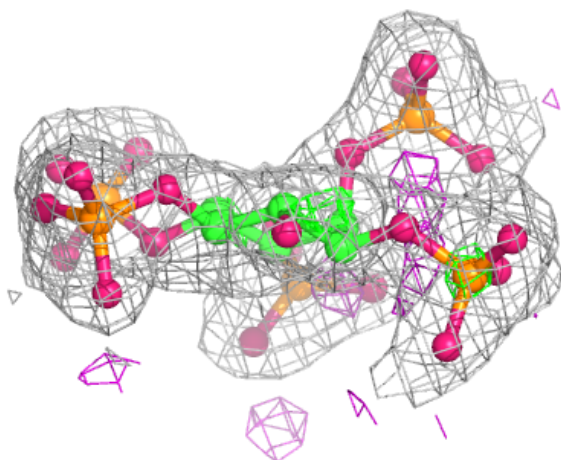
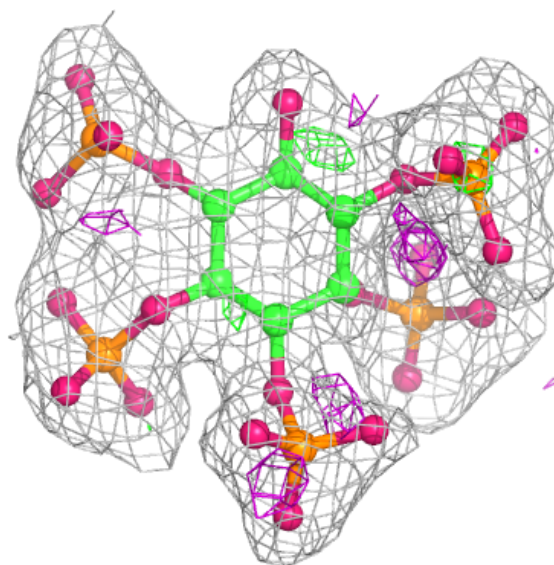
Electron density around IP5 A 550:

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



Electron density around IP5 B 551:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.