



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:33 PM EDT

PDB ID : 2I5C / pdb_00002i5c
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 Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

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

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

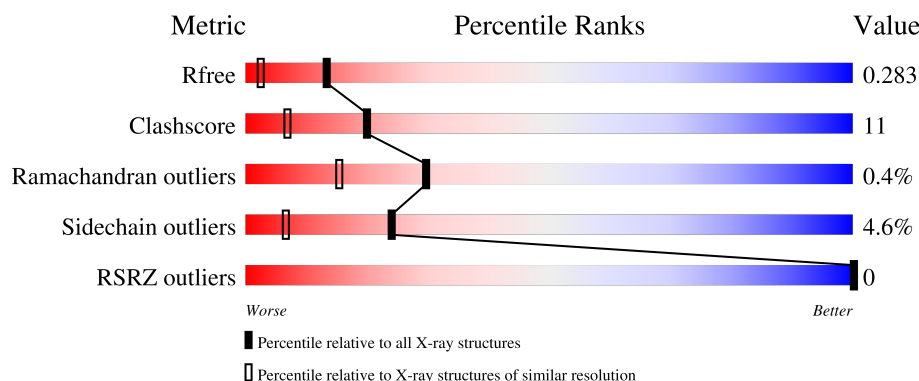
1 Overall quality at a glance i

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 of 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 $\leq 5\%$. 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	109	66% 17% • 14%
1	B	109	63% 19% • 14%
1	C	109	62% 20% • 14%

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.

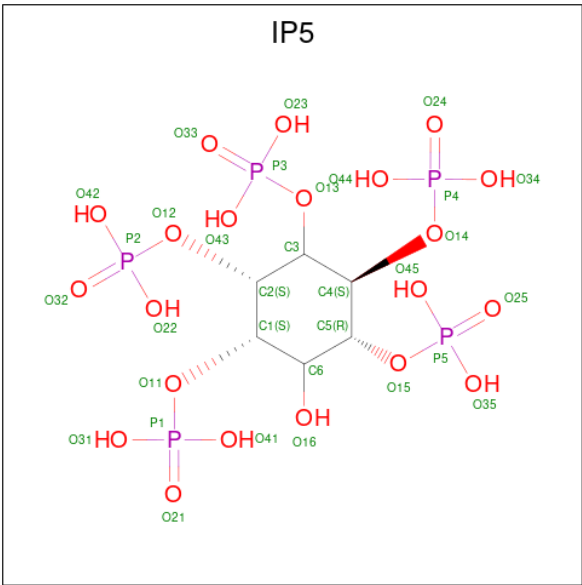
- Molecule 1 is a protein called Pleckstrin.

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)] (CCD ID: 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.

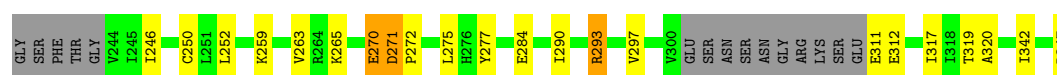
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	102	Total	O	0	0
			102	102		
3	C	98	Total	O	0	0
			98	98		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Pleckstrin

Chain A: 



• Molecule 1: Pleckstrin

Chain B: 



• Molecule 1: Pleckstrin

Chain C: 



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 30.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.75) 98.4 (30.00-1.75)	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 (7.56%)	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)	0.35 , 36.6	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	0.98	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	1.27	2/816 (0.2%)	1.18	4/1101 (0.4%)
1	B	1.32	5/808 (0.6%)	1.11	1/1090 (0.1%)
1	C	1.40	9/825 (1.1%)	1.12	2/1112 (0.2%)
All	All	1.33	16/2449 (0.7%)	1.14	7/3303 (0.2%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	271	ASP	CA-C	8.11	1.59	1.53
1	B	271	ASP	CA-C	6.69	1.58	1.53
1	C	320	ALA	CA-CB	6.21	1.63	1.53
1	C	328	GLN	CD-NE2	-6.05	1.20	1.33
1	B	289	ALA	C-O	5.97	1.30	1.23
1	C	271	ASP	N-CA	5.92	1.50	1.46
1	A	250	CYS	C-O	5.88	1.30	1.23
1	B	253	LYS	C-O	5.37	1.30	1.24
1	C	320	ALA	C-O	5.36	1.30	1.24
1	A	320	ALA	C-O	5.25	1.30	1.24
1	B	284	GLU	C-O	5.23	1.30	1.24
1	C	273	ALA	N-CA	-5.21	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	334	GLU	CD-OE1	5.15	1.35	1.25
1	B	273	ALA	N-CA	-5.12	1.40	1.46
1	C	245	ILE	C-O	5.03	1.29	1.24
1	C	251	LEU	C-O	-5.01	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	ALA	N-CA-C	-9.79	99.14	112.94
1	A	270	GLU	CA-C-N	-8.50	112.70	123.16
1	A	270	GLU	C-N-CA	-8.50	112.70	123.16
1	A	271	ASP	N-CA-C	6.80	122.67	108.39
1	B	259	LYS	N-CA-C	5.66	120.00	113.38
1	A	259	LYS	N-CA-C	5.61	119.95	113.38
1	C	285	ASP	N-CA-C	5.12	116.14	109.64

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 [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	787	0	812	17	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	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	102	0	0	5	0
3	C	98	0	0	0	0
All	All	2771	0	2459	56	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.

All (56) 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
1:A:275:LEU:HB3	1:A:290[B]:ILE:CG2	2.22	0.70
1:A:293:ARG:HG2	3:A:551:HOH:O	1.92	0.69
1:B:246:ILE:N	1:B:246:ILE:CD1	2.57	0.68
1:C:297[B]:VAL:HG11	1:C:342:ILE:HG21	1.77	0.67
1:A:297[B]:VAL:HG11	1:A:342:ILE:HG22	1.76	0.66
1:B:244:VAL:HG13	3:B:575:HOH:O	1.95	0.66
1:A:297[B]:VAL:HG11	1:A:342:ILE:HG21	1.78	0.65
1:A:290[B]:ILE:HD11	1:A:319:THR:HG22	1.80	0.62
1:A:275:LEU:HB3	1:A:290[B]:ILE:HG23	1.81	0.62
1:A:272:PRO:HG3	1:B:252:LEU:HD11	1.83	0.60
1:B:340:LYS:HE3	3:B:579:HOH:O	2.03	0.58
1:C:275:LEU:HB3	1:C:290[B]:ILE:HG22	1.84	0.58
1:B:297[B]:VAL:HG11	1:B:342:ILE:CG2	2.33	0.58
1:B:270:GLU:HG2	3:B:575:HOH:O	2.06	0.56
1:C:290[B]:ILE:HD11	1:C:319:THR:HG22	1.89	0.55
1:B:275:LEU:HB3	1:B:290[B]:ILE:HG22	1.89	0.54
1:B:290[B]:ILE:HD11	1:B:319:THR:CG2	2.37	0.54
1:B:297[B]:VAL:HG23	1:B:339:ILE:HG23	1.91	0.53
1:C:252:LEU:CD2	1:C:263:VAL:HG22	2.40	0.51
1:B:270:GLU:OE2	3:B:647:HOH:O	2.20	0.50
1:C:297[B]:VAL:HG11	1:C:342:ILE:HG22	1.94	0.49
1:B:297[B]:VAL:HG11	1:B:342:ILE:HG22	1.96	0.48
1:A:246[A]:ILE:HG13	1:A:270:GLU:HG3	1.95	0.47
1:A:290[B]:ILE:CD1	1:A:317:ILE:HG21	2.45	0.47
2:B:551:IP5:O45	2:B:551:IP5:O44	2.33	0.47
1:C:275:LEU:CB	1:C:290[B]:ILE:CG2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:HIS:CD2	1:B:291:HIS:N	2.84	0.45
1:C:290[B]:ILE:CD1	1:C:317:ILE:HG21	2.46	0.45
1:C:275:LEU:HB3	1:C:290[B]:ILE:CG2	2.46	0.45
1:A:271:ASP:C	1:A:271:ASP:OD2	2.60	0.44
1:C:252:LEU:HB2	1:C:328:GLN:HB3	2.00	0.44
1:C:297[B]:VAL:HG23	1:C:339:ILE:HG23	1.98	0.44
1:C:252:LEU:HD23	1:C:263:VAL:HG22	2.00	0.44
1:B:252:LEU:CD2	1:B:263:VAL:HG22	2.48	0.43
1:C:275:LEU:HB2	1:C:290[B]:ILE:HG23	1.98	0.43
1:A:252:LEU:CD2	1:A:263:VAL:HG22	2.49	0.42
1:A:293:ARG:NH1	3:A:574:HOH:O	2.44	0.42
1:A:265:LYS:O	1:A:277:TYR:HA	2.19	0.42
1:C:297[B]:VAL:CG2	1:C:339:ILE:HG23	2.51	0.41
1:B:265:LYS:O	1:B:277:TYR:HA	2.20	0.41
1:B:297[B]:VAL:HG11	1:B:342:ILE:HG21	2.01	0.41
1:C:344:MET:O	1:C:347:ARG:NH1	2.48	0.41
1:B:290[B]:ILE:CD1	1:B:317:ILE:HG21	2.51	0.41
1:B:248:GLN:HG3	1:C:258:ARG:NH2	2.35	0.41
1:A:271:ASP:CG	3:A:644:HOH:O	2.64	0.41
1:A:271:ASP:OD2	1:A:271:ASP:O	2.40	0.40
1:B:297[B]:VAL:CG2	1:B:339:ILE:HG23	2.51	0.40
1:C:290[A]:ILE:HG22	1:C:292:LEU:HD23	2.03	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	94/109 (86%)	94 (100%)	0	0	100	100
1	B	93/109 (85%)	92 (99%)	0	1 (1%)	11	2
1	C	95/109 (87%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	282/327 (86%)	280 (99%)	1 (0%)	1 (0%)	30 15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	GLU

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	84/92 (91%)	80 (95%)	4 (5%)	23 6
1	B	83/92 (90%)	80 (96%)	3 (4%)	31 11
1	C	85/92 (92%)	81 (95%)	4 (5%)	23 6
All	All	252/276 (91%)	241 (96%)	11 (4%)	24 7

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

Mol	Chain	Res	Type
1	A	284	GLU
1	A	293	ARG
1	A	312	GLU
1	A	347	ARG
1	B	244	VAL
1	B	246	ILE
1	B	275	LEU
1	C	275	LEU
1	C	284	GLU
1	C	344	MET
1	C	347	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	313	ASN
1	A	328	GLN
1	B	291	HIS
1	B	313	ASN
1	B	343	GLN
1	C	254	GLN
1	C	313	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	552	-	32,32,32	1.11	2 (6%)	53,53,53	1.04	5 (9%)
2	IP5	B	551	-	32,32,32	1.08	1 (3%)	53,53,53	1.21	6 (11%)
2	IP5	A	550	-	32,32,32	1.05	3 (9%)	53,53,53	1.22	6 (11%)

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	C	552	-	-	3/25/49/49	0/1/1/1
2	IP5	B	551	-	-	3/25/49/49	0/1/1/1
2	IP5	A	550	-	-	2/25/49/49	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	550	IP5	P4-O44	-2.39	1.45	1.54
2	B	551	IP5	P5-O15	2.35	1.63	1.59
2	A	550	IP5	C4-C5	2.28	1.56	1.52
2	C	552	IP5	P5-O15	2.22	1.63	1.59
2	A	550	IP5	P5-O15	2.20	1.63	1.59
2	C	552	IP5	C4-C5	2.15	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	IP5	O13-P3-O33	-3.19	97.98	109.33
2	B	551	IP5	O35-P5-O25	3.10	122.90	110.83
2	A	550	IP5	O35-P5-O45	3.00	119.07	107.80
2	A	550	IP5	O15-P5-O25	-2.94	98.84	109.33
2	A	550	IP5	O31-P1-O41	2.62	117.63	107.80
2	A	550	IP5	O14-C4-C3	-2.51	103.43	108.76
2	B	551	IP5	O22-P2-O12	2.49	115.54	105.85
2	C	552	IP5	O22-P2-O12	2.37	115.08	105.85
2	A	550	IP5	O22-P2-O12	2.29	114.79	105.85
2	C	552	IP5	O15-P5-O25	-2.29	101.17	109.33
2	B	551	IP5	O14-P4-O24	-2.26	101.29	109.33
2	C	552	IP5	O35-P5-O25	2.15	119.21	110.83
2	A	550	IP5	O42-P2-O32	2.08	118.94	110.83
2	B	551	IP5	O23-P3-O33	2.07	118.91	110.83
2	C	552	IP5	O35-P5-O45	2.07	115.57	107.80
2	B	551	IP5	O34-P4-O44	2.05	115.50	107.80
2	C	552	IP5	O31-P1-O41	2.05	115.50	107.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	552	IP5	C5-O15-P5-O45
2	A	550	IP5	C5-O15-P5-O25
2	C	552	IP5	C4-O14-P4-O24
2	A	550	IP5	C5-O15-P5-O45
2	B	551	IP5	C5-O15-P5-O35
2	B	551	IP5	C4-O14-P4-O34
2	C	552	IP5	C1-O11-P1-O41
2	B	551	IP5	C4-O14-P4-O24

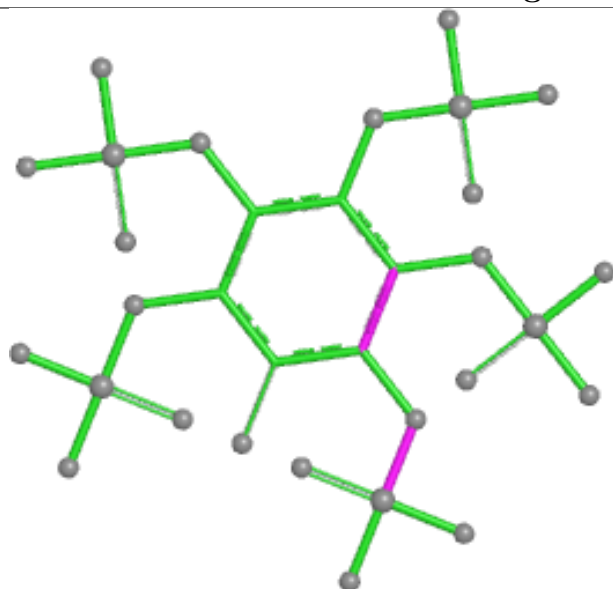
There are no ring outliers.

1 monomer is involved in 1 short contact:

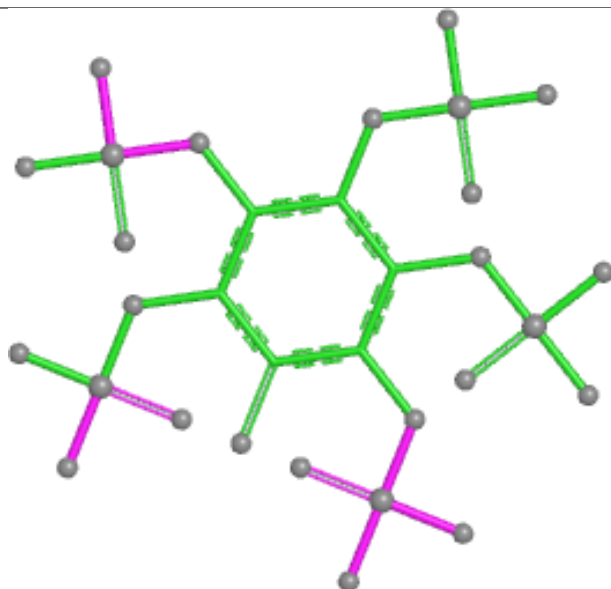
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	551	IP5	1	0

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.

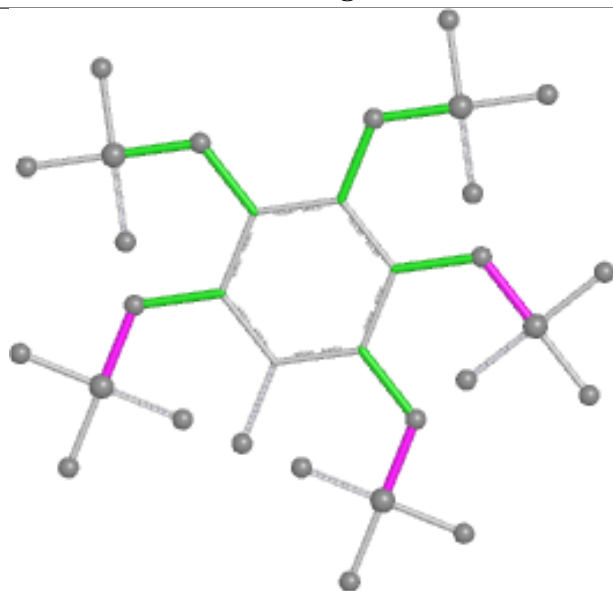
Ligand IP5 C 552



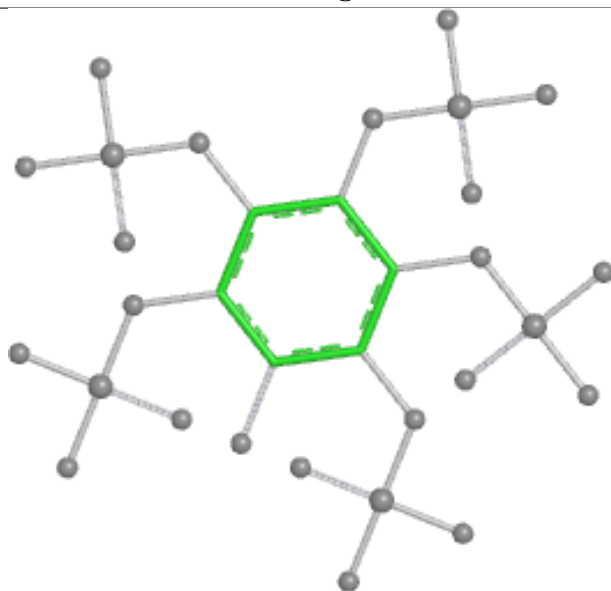
Bond lengths



Bond angles

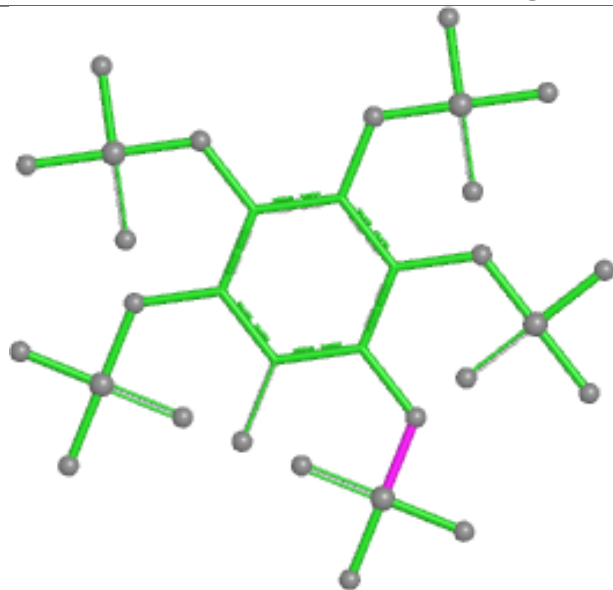


Torsions

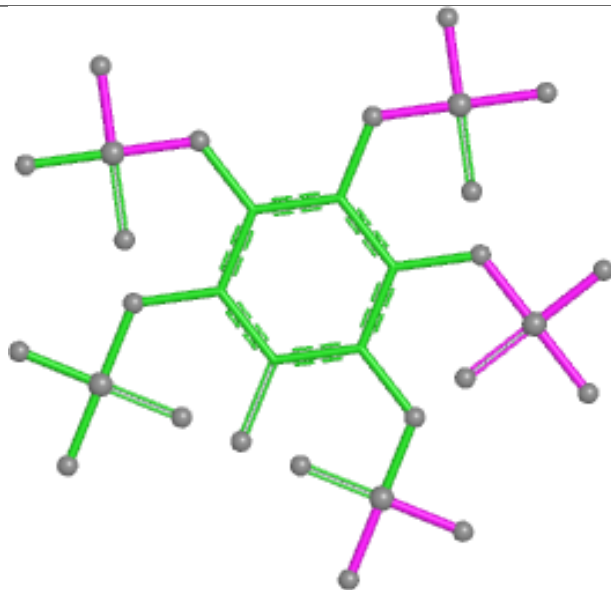


Rings

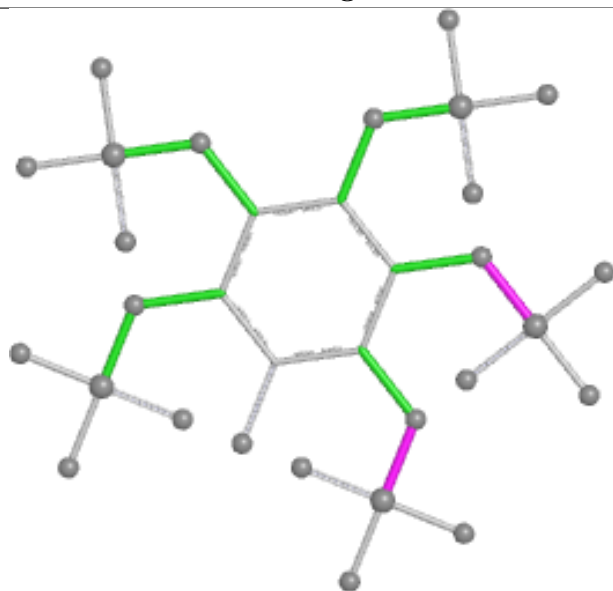
Ligand IP5 B 551



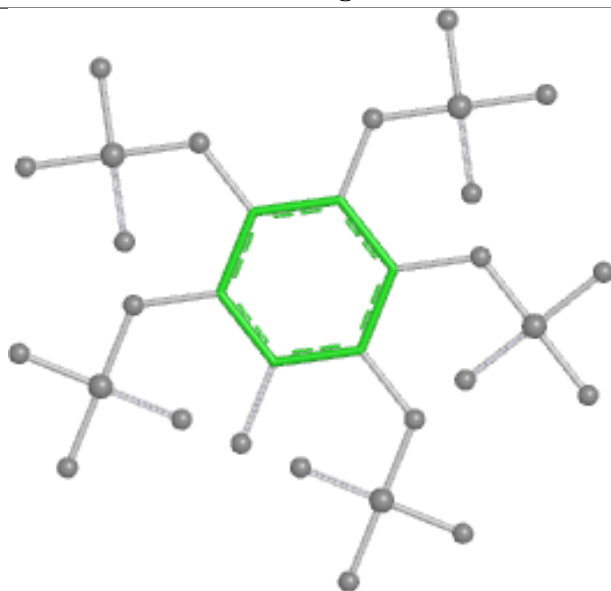
Bond lengths



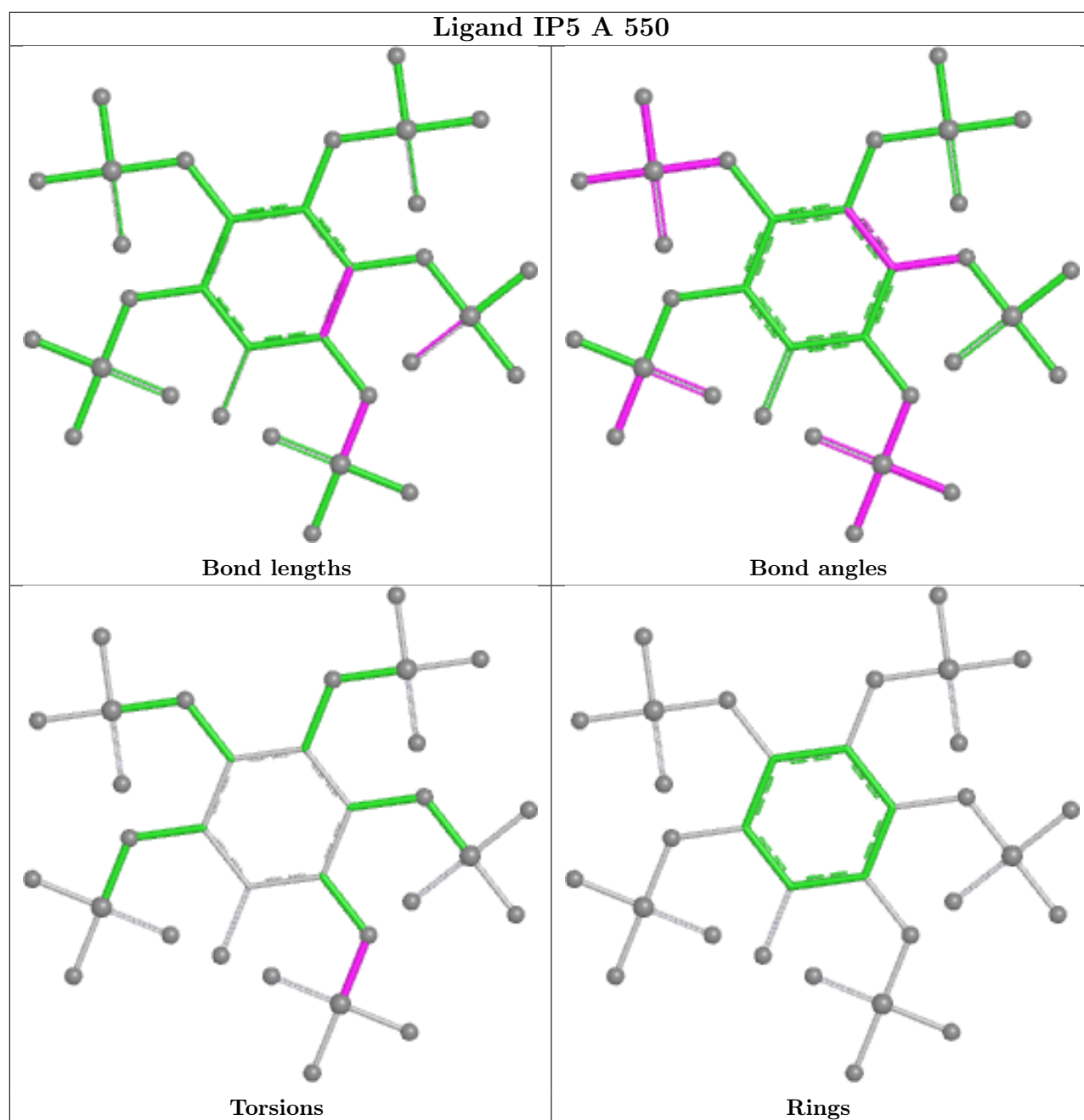
Bond angles



Torsions



Rings



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, 95th 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 ²)	Q<0.9
1	A	94/109 (86%)	-0.93	0 100 100	24, 40, 57, 65	4 (4%)
1	B	94/109 (86%)	-0.98	0 100 100	24, 39, 49, 65	3 (3%)
1	C	94/109 (86%)	-0.99	0 100 100	24, 39, 50, 63	5 (5%)
All	All	282/327 (86%)	-0.97	0 100 100	24, 39, 52, 65	12 (4%)

There are no RSRZ outliers to report.

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, 95th 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.

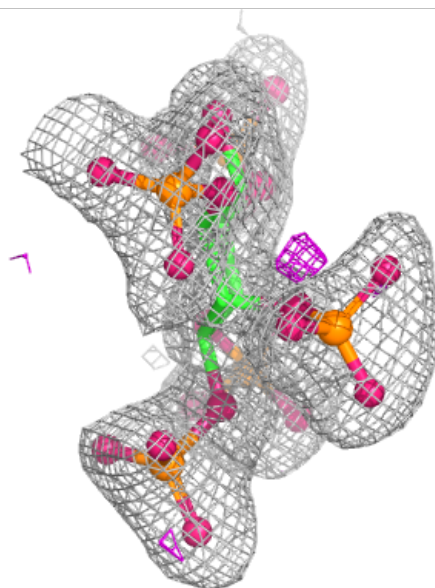
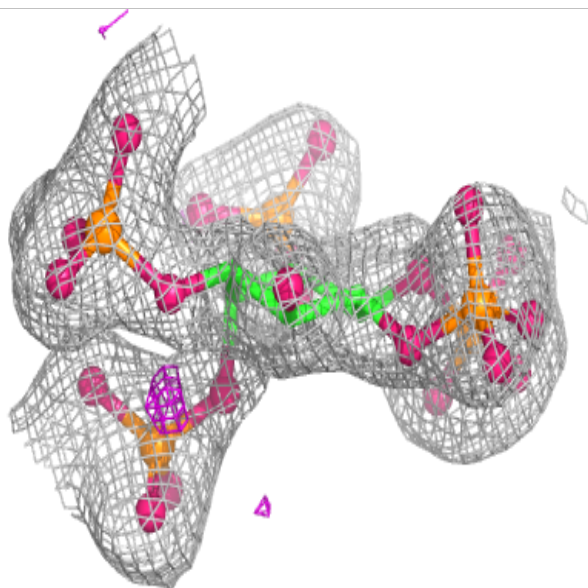
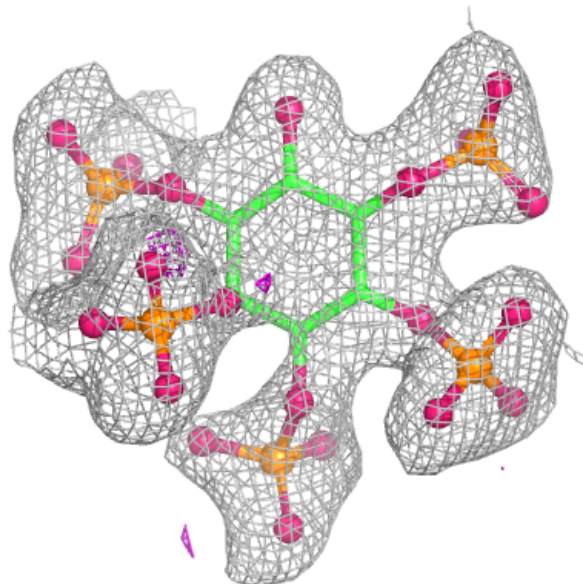
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IP5	B	551	32/32	0.99	0.04	36,41,48,50	0
2	IP5	A	550	32/32	1.00	0.03	37,41,47,49	0
2	IP5	C	552	32/32	1.00	0.03	36,40,48,49	0

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.

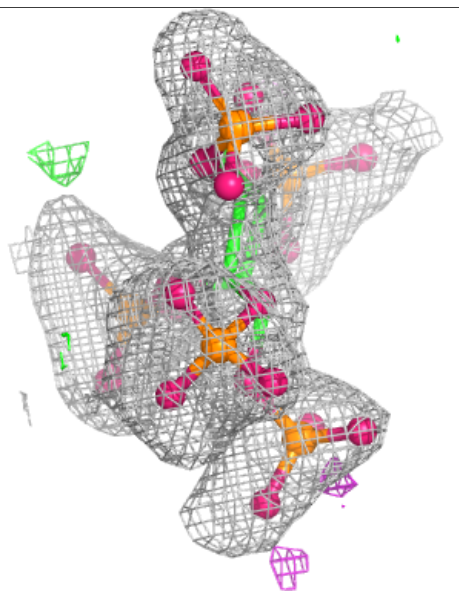
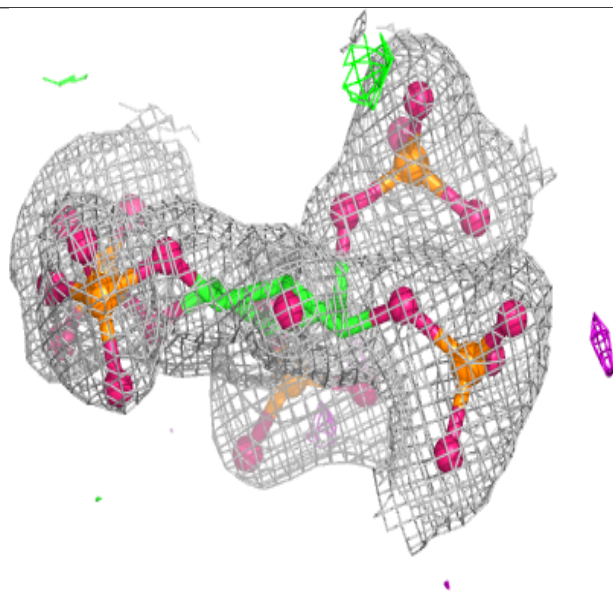
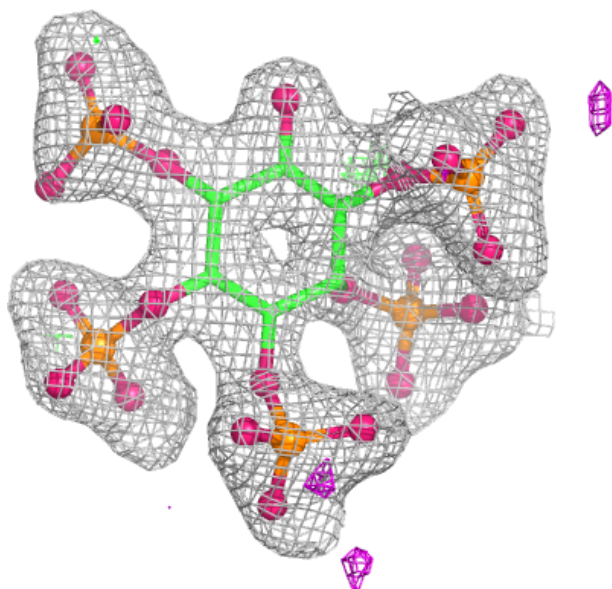
Electron density around IP5 B 551:

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



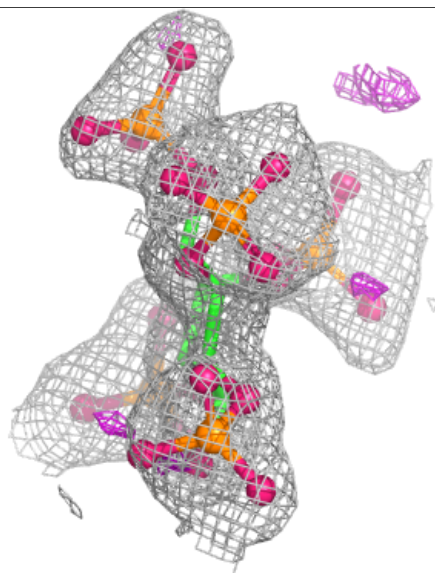
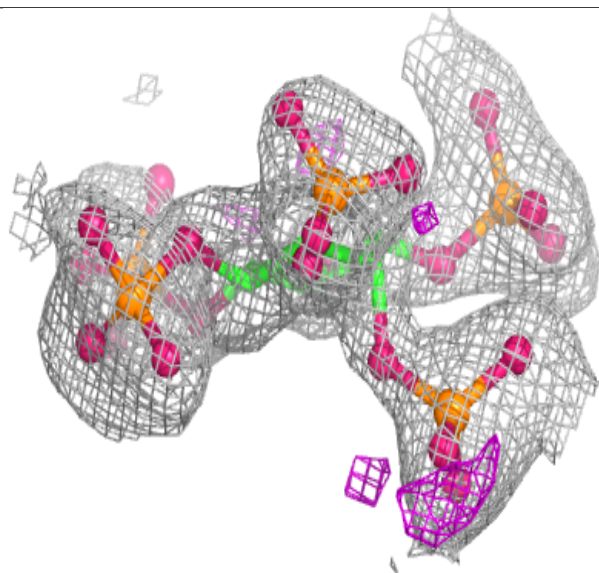
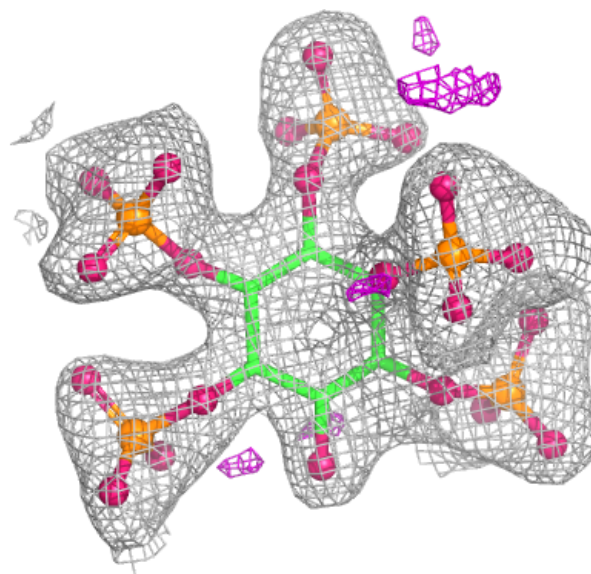
Electron density around IP5 A 550:

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



Electron density around IP5 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.