



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 01:58 PM EDT

PDB ID : 4Y94  
Title : Crystal structure of the PH-TH module of Bruton's tyrosine kinase bound to inositol hexakisphosphate  
Authors : Wang, Q.; Kuriyan, J.  
Deposited on : 2015-02-16  
Resolution : 2.40 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	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

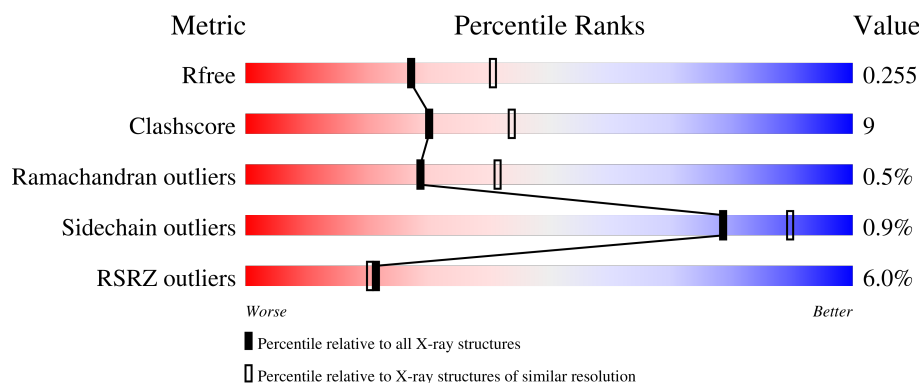
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	171	<div> <div>8%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>• 8%</div> </div> </div>
1	B	171	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>• 13%</div> </div> </div>
1	C	171	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div> </div>
1	D	171	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>• 11%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IHP	D	201	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5393 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.

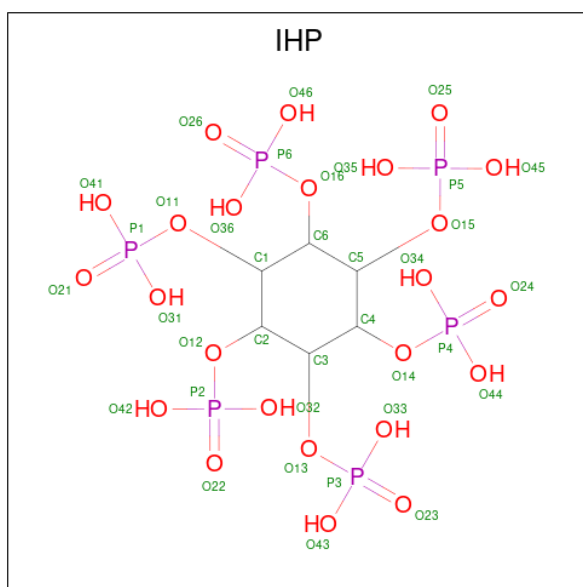
- Molecule 1 is a protein called Non-specific protein-tyrosine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	149	Total	C	N	O	S	0	0	0
			1242	804	211	220	7			
1	C	157	Total	C	N	O	S	0	0	0
			1306	841	220	239	6			
1	A	158	Total	C	N	O	S	0	0	0
			1310	844	220	240	6			
1	D	153	Total	C	N	O	S	0	0	0
			1272	823	216	226	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q3ZC95
C	0	GLY	-	expression tag	UNP Q3ZC95
A	0	GLY	-	expression tag	UNP Q3ZC95
D	0	GLY	-	expression tag	UNP Q3ZC95

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			36	6	24	6		
2	C	1	Total	C	O	P	0	0
			36	6	24	6		
2	A	1	Total	C	O	P	0	0
			36	6	24	6		
2	A	1	Total	C	O	P	0	0
			36	6	24	6		
2	D	1	Total	C	O	P	0	0
			36	6	24	6		
2	D	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

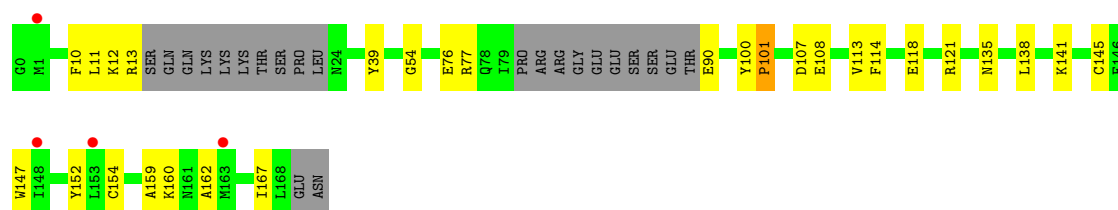
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total 8	O 8	0	0
4	C	15	Total 15	O 15	0	0
4	A	11	Total 11	O 11	0	0
4	D	9	Total 9	O 9	0	0

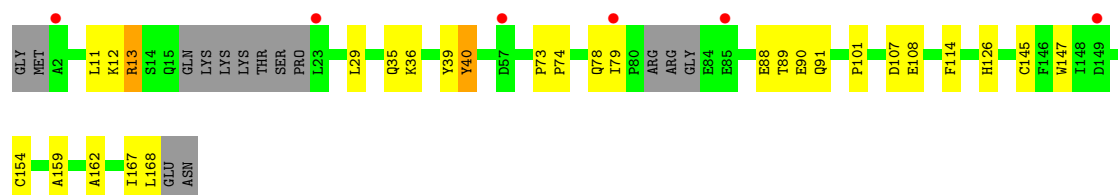
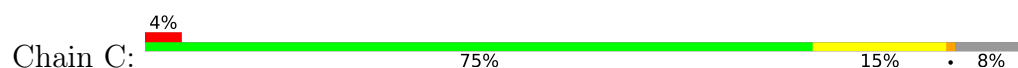
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

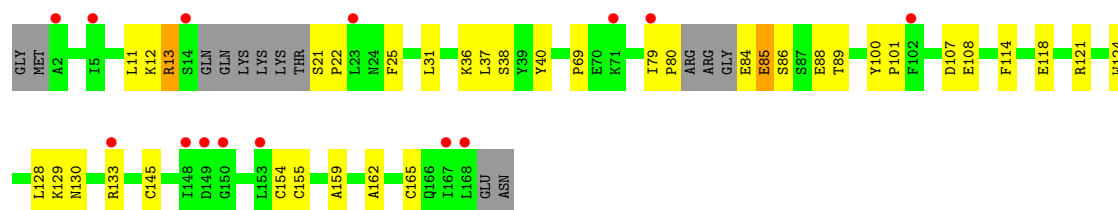
- Molecule 1: Non-specific protein-tyrosine kinase



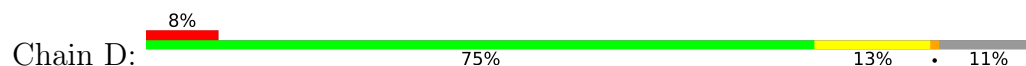
- Molecule 1: Non-specific protein-tyrosine kinase



- Molecule 1: Non-specific protein-tyrosine kinase



- Molecule 1: Non-specific protein-tyrosine kinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.20Å 64.01Å 80.03Å 82.08° 88.79° 89.89°	Depositor
Resolution (Å)	46.48 – 2.40 46.48 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.48-2.40) 88.6 (46.48-2.31)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.229 , 0.255 0.230 , 0.255	Depositor DCC
$R_{free}$ test set	2025 reflections (6.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: ZN, IHP

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	0.53	0/1341	0.68	4/1811 (0.2%)
1	B	0.30	0/1271	0.49	1/1713 (0.1%)
1	C	0.30	0/1336	0.48	0/1803
1	D	0.28	0/1302	0.47	0/1755
All	All	0.37	0/5250	0.54	5/7082 (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	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	85	GLU	CB-CA-C	-7.16	96.09	110.40
1	A	86	SER	N-CA-CB	6.99	120.99	110.50
1	A	86	SER	N-CA-C	-6.76	92.73	111.00
1	B	100	TYR	C-N-CD	5.32	139.56	128.40
1	A	21	SER	C-N-CD	5.24	139.40	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	49	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	1310	0	1306	31	0
1	B	1242	0	1251	18	0
1	C	1306	0	1302	21	2
1	D	1272	0	1283	23	0
2	A	72	0	12	4	0
2	B	36	0	6	0	0
2	C	36	0	6	3	1
2	D	72	0	12	11	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	0	1	0
4	B	8	0	0	0	0
4	C	15	0	0	2	0
4	D	9	0	0	0	0
All	All	5393	0	5178	98	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 9.

All (98) 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:C:13:ARG:HG2	1:C:13:ARG:HH11	1.17	1.07
1:A:12:LYS:HE2	2:A:502:IHP:O36	1.70	0.90
1:A:12:LYS:CE	2:A:502:IHP:O36	2.21	0.88
1:C:13:ARG:HG2	1:C:13:ARG:NH1	1.91	0.78
1:A:89:THR:HG21	1:D:120:LEU:CD1	2.23	0.69
1:B:11:LEU:HB3	1:B:114:PHE:HB2	1.76	0.67
1:A:145:CYS:SG	1:A:154:CYS:HB3	2.34	0.66
1:A:159:ALA:HB3	1:A:162:ALA:HB2	1.77	0.66
1:C:159:ALA:HB3	1:C:162:ALA:HB2	1.76	0.66
1:A:13:ARG:CG	1:A:13:ARG:HH11	2.09	0.66
2:D:202:IHP:O26	2:D:202:IHP:H5	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ALA:HB3	1:D:162:ALA:HB2	1.79	0.64
1:C:89:THR:HG22	1:C:90:GLU:N	2.12	0.63
1:C:13:ARG:NH2	1:C:147:TRP:O	2.31	0.63
1:A:89:THR:HG21	1:D:120:LEU:HD11	1.79	0.63
2:D:202:IHP:H6	2:D:202:IHP:O35	1.99	0.63
2:D:201:IHP:O26	2:D:201:IHP:H5	1.97	0.62
1:A:145:CYS:HB2	1:A:154:CYS:SG	2.39	0.62
1:C:11:LEU:HB3	1:C:114:PHE:HB2	1.82	0.61
1:A:84:GLU:O	1:A:88:GLU:HG2	2.01	0.60
1:A:85:GLU:O	1:A:85:GLU:HG2	2.02	0.60
1:A:13:ARG:HH11	1:A:13:ARG:HG2	1.67	0.59
1:A:36:LYS:NZ	2:A:501:IHP:O14	2.35	0.59
1:A:12:LYS:NZ	2:A:502:IHP:O36	2.36	0.58
1:A:13:ARG:HG2	1:A:13:ARG:NH1	2.18	0.58
1:D:39:TYR:CZ	1:D:54:GLY:HA3	2.39	0.58
2:C:201:IHP:O34	4:C:301:HOH:O	2.17	0.58
1:B:101:PRO:HB3	1:B:114:PHE:CD2	2.39	0.57
1:D:101:PRO:HB3	1:D:114:PHE:CE2	2.39	0.57
1:A:155:CYS:HB3	1:A:165:CYS:SG	2.43	0.57
1:A:85:GLU:HA	1:A:88:GLU:HG2	1.88	0.56
1:A:129:LYS:O	1:A:133:ARG:HG3	2.05	0.56
1:D:15:GLN:N	2:D:201:IHP:O42	2.37	0.56
1:A:124:TRP:O	1:A:128:LEU:HG	2.05	0.56
1:C:35:GLN:HG3	1:C:36:LYS:HG3	1.87	0.56
1:A:85:GLU:HA	1:A:88:GLU:CG	2.37	0.55
2:C:201:IHP:H2	4:C:302:HOH:O	2.07	0.54
1:D:34:VAL:HG23	1:D:35:GLN:N	2.23	0.54
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.04	0.54
1:D:107:ASP:OD1	1:D:108:GLU:N	2.41	0.53
1:C:88:GLU:O	1:C:89:THR:HB	2.08	0.53
1:C:167:ILE:HG22	1:C:168:LEU:HG	1.91	0.53
1:C:89:THR:CG2	1:C:90:GLU:N	2.72	0.53
1:B:147:TRP:CE2	1:B:160:LYS:HG2	2.44	0.53
1:A:13:ARG:HD3	1:A:25:PHE:CE2	2.44	0.52
1:D:11:LEU:HB3	1:D:114:PHE:HB2	1.90	0.52
1:B:101:PRO:HB3	1:B:114:PHE:CE2	2.44	0.52
1:A:11:LEU:HB3	1:A:114:PHE:HB2	1.91	0.52
1:D:68:VAL:O	1:D:146:PHE:HE1	1.92	0.52
1:B:12:LYS:HE3	1:B:39:TYR:CE2	2.46	0.51
1:D:12:LYS:CE	2:D:201:IHP:O21	2.59	0.51
1:A:107:ASP:OD1	1:A:108:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASP:OD1	1:B:108:GLU:N	2.44	0.51
1:B:118:GLU:OE1	1:B:121:ARG:NH2	2.40	0.50
1:D:101:PRO:HB3	1:D:114:PHE:CD2	2.47	0.50
1:C:101:PRO:HB3	1:C:114:PHE:CE2	2.47	0.50
1:D:34:VAL:O	1:D:58:VAL:HG21	2.11	0.49
1:A:118:GLU:OE1	1:A:121:ARG:NH2	2.46	0.49
1:D:12:LYS:HE2	2:D:201:IHP:O21	2.13	0.49
1:A:79:ILE:HD11	1:A:100:TYR:OH	2.13	0.48
1:A:31:LEU:O	1:A:37:LEU:HA	2.12	0.48
1:A:101:PRO:HB3	1:A:114:PHE:CE2	2.48	0.48
1:B:147:TRP:CZ2	1:B:160:LYS:HG2	2.48	0.48
1:D:90:GLU:N	1:D:90:GLU:OE1	2.47	0.48
1:B:141:LYS:HG2	1:B:167:ILE:HD13	1.96	0.47
1:B:159:ALA:HB3	1:B:162:ALA:HB2	1.96	0.47
1:C:40:TYR:N	1:C:40:TYR:CD1	2.81	0.47
1:C:107:ASP:OD1	1:C:108:GLU:N	2.48	0.47
1:C:29:LEU:O	1:C:39:TYR:HA	2.15	0.47
1:A:89:THR:HG21	1:D:120:LEU:HD13	1.95	0.47
1:D:12:LYS:NZ	2:D:201:IHP:O21	2.48	0.46
1:D:40:TYR:CD1	1:D:40:TYR:N	2.83	0.46
1:A:69:PRO:HD3	4:A:611:HOH:O	2.15	0.46
1:C:89:THR:HG22	1:C:91:GLN:H	1.81	0.46
1:A:79:ILE:HG23	1:A:80:PRO:HD2	1.97	0.46
1:D:35:GLN:HG2	1:D:36:LYS:HG3	1.98	0.46
1:C:101:PRO:HB3	1:C:114:PHE:CD2	2.51	0.45
1:D:24:ASN:ND2	2:D:201:IHP:O35	2.49	0.45
1:C:12:LYS:HE3	2:C:201:IHP:O46	2.16	0.44
1:B:90:GLU:N	1:B:90:GLU:OE1	2.50	0.44
1:A:40:TYR:CD1	1:A:40:TYR:N	2.85	0.44
1:C:145:CYS:SG	1:C:154:CYS:HB3	2.58	0.44
1:A:130:ASN:HA	1:A:133:ARG:HD2	2.00	0.43
1:D:68:VAL:O	1:D:146:PHE:CE1	2.70	0.43
2:D:201:IHP:H6	2:D:201:IHP:O45	2.19	0.43
1:B:13:ARG:NH2	1:B:147:TRP:O	2.38	0.43
1:C:78:GLN:HG2	1:C:79:ILE:O	2.19	0.42
1:B:145:CYS:SG	1:B:154:CYS:HB3	2.59	0.42
1:B:147:TRP:HB2	1:B:152:TYR:CE1	2.55	0.42
1:B:39:TYR:CZ	1:B:54:GLY:HA3	2.54	0.42
1:D:65:GLU:O	1:D:103:GLN:N	2.39	0.42
2:D:201:IHP:O45	2:D:201:IHP:C6	2.68	0.42
1:B:76:GLU:HG3	1:B:77:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:PRO:HA	1:C:74:PRO:HD2	1.91	0.41
1:D:34:VAL:CG2	1:D:35:GLN:N	2.84	0.41
2:D:201:IHP:O25	2:D:201:IHP:P6	2.79	0.41
1:B:135:ASN:HB2	1:B:138:LEU:HD21	2.03	0.41
1:B:10:PHE:HB3	1:B:113:VAL:HG13	2.02	0.40

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:C:36:LYS:NZ	2:D:202:IHP:O33[1_565]	2.07	0.13
1:C:126:HIS:CE1	2:C:201:IHP:O23[1_455]	2.16	0.04

## 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	152/171 (89%)	149 (98%)	2 (1%)	1 (1%)	22	32
1	B	143/171 (84%)	140 (98%)	2 (1%)	1 (1%)	22	32
1	C	151/171 (88%)	148 (98%)	3 (2%)	0	100	100
1	D	147/171 (86%)	145 (99%)	1 (1%)	1 (1%)	22	32
All	All	593/684 (87%)	582 (98%)	8 (1%)	3 (0%)	29	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	101	PRO
1	A	22	PRO
1	B	101	PRO

### 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	149/160 (93%)	147 (99%)	2 (1%)	69	84
1	B	139/160 (87%)	139 (100%)	0	100	100
1	C	148/160 (92%)	146 (99%)	2 (1%)	67	82
1	D	143/160 (89%)	142 (99%)	1 (1%)	84	92
All	All	579/640 (90%)	574 (99%)	5 (1%)	78	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	ARG
1	C	40	TYR
1	A	13	ARG
1	A	38	SER
1	D	40	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
2	IHP	A	501	-	36,36,36	1.65	9 (25%)	54,60,60	1.22	4 (7%)
2	IHP	A	502	-	36,36,36	1.45	5 (13%)	54,60,60	1.46	12 (22%)
2	IHP	B	201	-	36,36,36	1.66	9 (25%)	54,60,60	1.29	6 (11%)
2	IHP	D	201	-	36,36,36	1.48	7 (19%)	54,60,60	1.49	9 (16%)
2	IHP	D	202	-	36,36,36	1.42	5 (13%)	54,60,60	1.63	11 (20%)
2	IHP	C	201	-	36,36,36	1.65	9 (25%)	54,60,60	1.12	3 (5%)

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	IHP	A	501	-	-	6/30/54/54	0/1/1/1
2	IHP	A	502	-	-	4/30/54/54	0/1/1/1
2	IHP	B	201	-	-	3/30/54/54	0/1/1/1
2	IHP	D	201	-	-	5/30/54/54	0/1/1/1
2	IHP	D	202	-	-	7/30/54/54	0/1/1/1
2	IHP	C	201	-	-	3/30/54/54	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IHP	P3-O43	4.32	1.71	1.54
2	C	201	IHP	P3-O43	4.31	1.71	1.54
2	B	201	IHP	P3-O43	4.31	1.71	1.54
2	D	201	IHP	P3-O43	3.92	1.70	1.54
2	D	202	IHP	P3-O43	3.78	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IHP	P3-O33	3.70	1.69	1.54
2	B	201	IHP	P3-O33	3.69	1.69	1.54
2	C	201	IHP	P3-O33	3.68	1.69	1.54
2	A	502	IHP	P3-O43	3.62	1.68	1.54
2	D	201	IHP	P3-O33	3.28	1.67	1.54
2	B	201	IHP	P4-O14	3.20	1.65	1.59
2	A	501	IHP	P2-O32	3.20	1.67	1.54
2	C	201	IHP	P2-O32	3.19	1.67	1.54
2	D	202	IHP	P3-O33	3.19	1.67	1.54
2	B	201	IHP	P2-O32	3.18	1.67	1.54
2	A	501	IHP	P4-O14	3.06	1.65	1.59
2	A	502	IHP	P3-O33	3.05	1.66	1.54
2	C	201	IHP	P4-O14	3.03	1.65	1.59
2	D	201	IHP	P2-O32	2.88	1.65	1.54
2	D	202	IHP	P5-O15	2.72	1.64	1.59
2	A	501	IHP	P2-O12	2.63	1.64	1.59
2	D	201	IHP	P5-O15	2.63	1.64	1.59
2	D	202	IHP	P2-O32	2.62	1.65	1.54
2	B	201	IHP	P5-O15	2.61	1.64	1.59
2	C	201	IHP	P2-O12	2.59	1.64	1.59
2	A	501	IHP	P5-O15	2.59	1.64	1.59
2	C	201	IHP	P5-O15	2.58	1.64	1.59
2	B	201	IHP	P2-O12	2.56	1.64	1.59
2	A	502	IHP	P2-O32	2.46	1.64	1.54
2	D	201	IHP	P4-O14	2.44	1.63	1.59
2	A	502	IHP	C5-C4	-2.43	1.47	1.52
2	B	201	IHP	P1-O31	2.30	1.63	1.54
2	C	201	IHP	P1-O31	2.27	1.63	1.54
2	A	501	IHP	P1-O31	2.27	1.63	1.54
2	B	201	IHP	P2-O42	2.12	1.63	1.54
2	A	501	IHP	P2-O42	2.11	1.63	1.54
2	D	202	IHP	P1-O31	2.10	1.63	1.54
2	C	201	IHP	P2-O42	2.09	1.62	1.54
2	A	501	IHP	P1-O41	2.04	1.62	1.54
2	D	201	IHP	P2-O42	2.04	1.62	1.54
2	C	201	IHP	P1-O41	2.03	1.62	1.54
2	B	201	IHP	P1-O41	2.02	1.62	1.54
2	D	201	IHP	P1-O31	2.00	1.62	1.54
2	A	502	IHP	P6-O26	-2.00	1.44	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	IHP	O14-C4-C5	-5.52	95.68	108.69
2	D	201	IHP	O11-C1-C6	-4.39	98.33	108.69
2	D	201	IHP	C5-C6-C1	4.39	120.02	110.41
2	B	201	IHP	O13-C3-C2	-4.31	98.52	108.69
2	A	501	IHP	O13-C3-C2	-3.91	99.48	108.69
2	D	202	IHP	O11-C1-C6	-3.79	99.76	108.69
2	D	201	IHP	O13-C3-C4	-3.29	100.93	108.69
2	D	202	IHP	O31-P1-O21	3.06	122.68	110.68
2	D	201	IHP	O43-P3-O23	3.06	122.64	110.68
2	A	502	IHP	O43-P3-O23	3.05	122.62	110.68
2	A	502	IHP	O14-C4-C3	2.99	115.73	108.69
2	A	502	IHP	O45-P5-O15	-2.93	92.86	105.99
2	D	202	IHP	O43-P3-O23	2.86	121.86	110.68
2	D	202	IHP	O16-P6-O26	2.84	120.36	109.39
2	D	202	IHP	C6-C1-C2	2.84	116.63	110.41
2	C	201	IHP	O13-C3-C2	-2.79	102.10	108.69
2	A	502	IHP	O41-P1-O31	-2.68	97.40	107.64
2	A	502	IHP	O41-P1-O21	2.68	121.16	110.68
2	D	202	IHP	O15-C5-C6	2.62	114.87	108.69
2	C	201	IHP	O43-P3-O23	2.62	120.94	110.68
2	A	501	IHP	O43-P3-O23	2.62	120.93	110.68
2	B	201	IHP	O43-P3-O23	2.60	120.86	110.68
2	B	201	IHP	O14-C4-C5	-2.54	102.70	108.69
2	A	502	IHP	O44-P4-O14	-2.45	95.02	105.99
2	A	502	IHP	O46-P6-O26	2.41	120.13	110.68
2	B	201	IHP	O31-P1-O21	2.38	120.01	110.68
2	C	201	IHP	O31-P1-O21	2.38	119.99	110.68
2	A	501	IHP	O31-P1-O21	2.37	119.96	110.68
2	D	201	IHP	C6-C1-C2	2.36	115.58	110.41
2	A	502	IHP	O13-C3-C2	-2.35	103.14	108.69
2	D	202	IHP	C5-C6-C1	2.35	115.55	110.41
2	D	201	IHP	O31-P1-O21	2.35	119.87	110.68
2	B	201	IHP	O12-C2-C3	-2.32	103.23	108.69
2	A	502	IHP	O45-P5-O25	2.26	119.53	110.68
2	D	202	IHP	O34-P4-O24	2.23	119.41	110.68
2	D	201	IHP	O16-P6-O26	2.19	117.84	109.39
2	A	502	IHP	C5-C4-C3	-2.15	105.70	110.41
2	A	501	IHP	O14-C4-C5	-2.13	103.67	108.69
2	A	502	IHP	O31-P1-O21	2.09	118.85	110.68
2	A	502	IHP	O46-P6-O36	-2.09	99.67	107.64
2	D	202	IHP	O41-P1-O31	-2.04	99.83	107.64
2	D	201	IHP	O46-P6-O26	2.01	118.56	110.68
2	B	201	IHP	C5-C6-C1	2.01	114.82	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	IHP	O13-C3-C2	-2.01	103.96	108.69
2	D	201	IHP	C4-C3-C2	2.00	114.79	110.41

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	IHP	C1-O11-P1-O21
2	C	201	IHP	C5-O15-P5-O35
2	A	501	IHP	C1-O11-P1-O21
2	A	501	IHP	C4-O14-P4-O24
2	A	502	IHP	C5-O15-P5-O35
2	D	201	IHP	C5-C4-O14-P4
2	D	201	IHP	C6-C5-O15-P5
2	D	201	IHP	C5-C6-O16-P6
2	D	202	IHP	C6-C5-O15-P5
2	D	202	IHP	C5-C6-O16-P6
2	D	202	IHP	C5-O15-P5-O25
2	A	501	IHP	C5-O15-P5-O35
2	A	502	IHP	C2-O12-P2-O42
2	D	201	IHP	C2-O12-P2-O42
2	D	202	IHP	C1-O11-P1-O21
2	B	201	IHP	C2-O12-P2-O32
2	B	201	IHP	C4-O14-P4-O44
2	B	201	IHP	C5-O15-P5-O45
2	C	201	IHP	C3-O13-P3-O43
2	A	501	IHP	C3-O13-P3-O33
2	A	501	IHP	C4-O14-P4-O34
2	A	501	IHP	C6-O16-P6-O46
2	A	502	IHP	C4-O14-P4-O44
2	A	502	IHP	C6-O16-P6-O36
2	D	201	IHP	C3-O13-P3-O33
2	D	202	IHP	C1-O11-P1-O31
2	D	202	IHP	C3-O13-P3-O43
2	D	202	IHP	C4-O14-P4-O44

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IHP	1	0

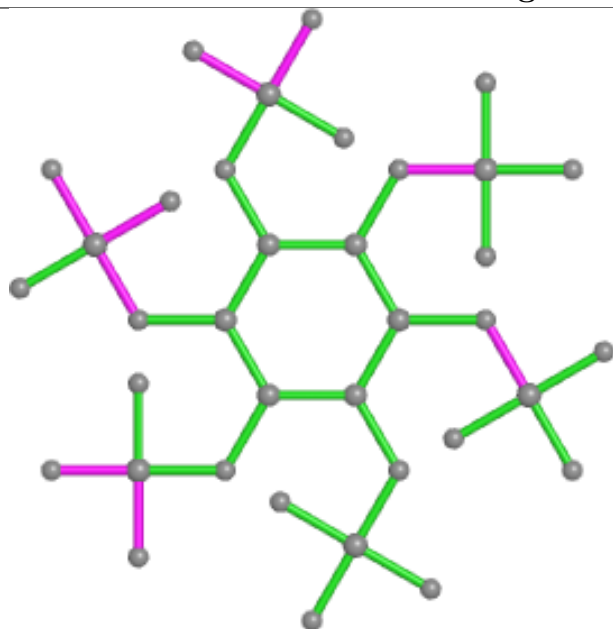
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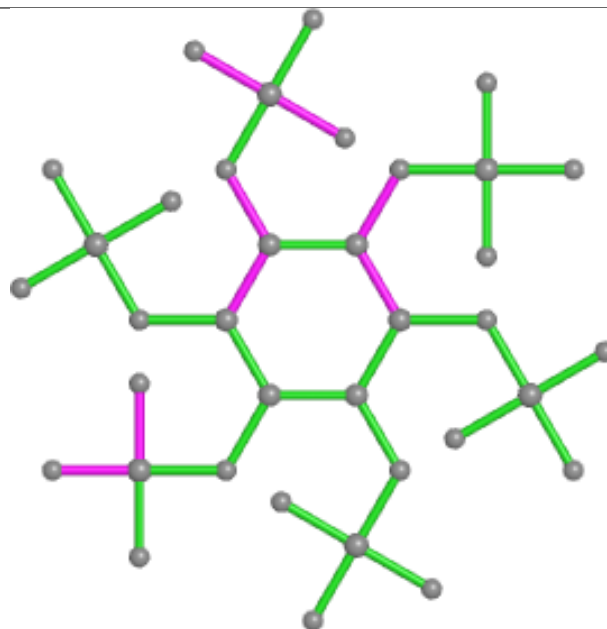
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	IHP	3	0
2	D	201	IHP	9	0
2	D	202	IHP	2	1
2	C	201	IHP	3	1

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.

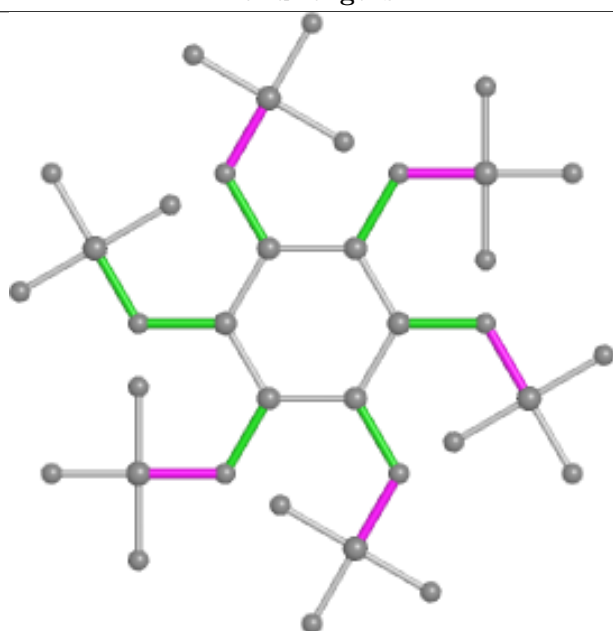
## Ligand IHP A 501



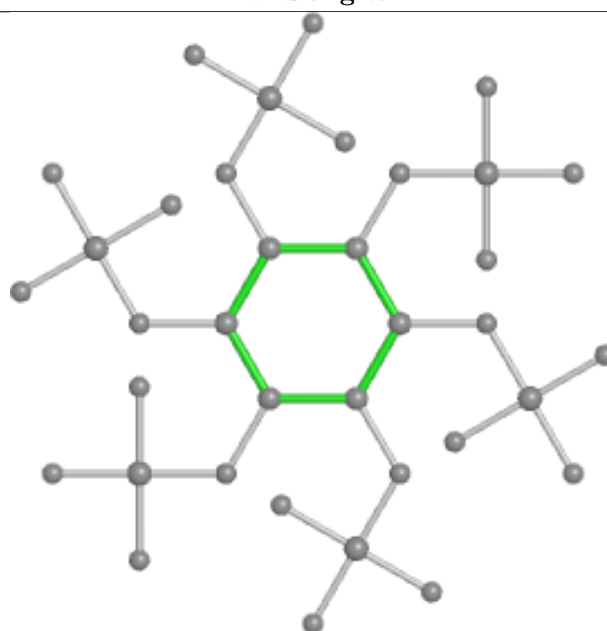
Bond lengths



Bond angles

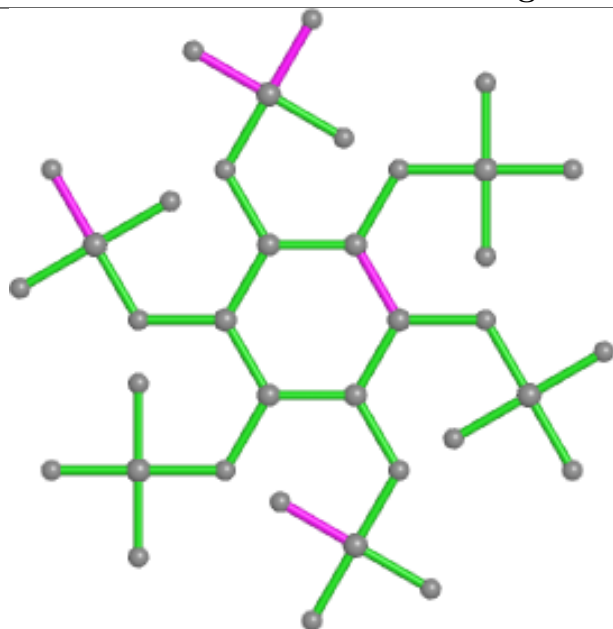


Torsions

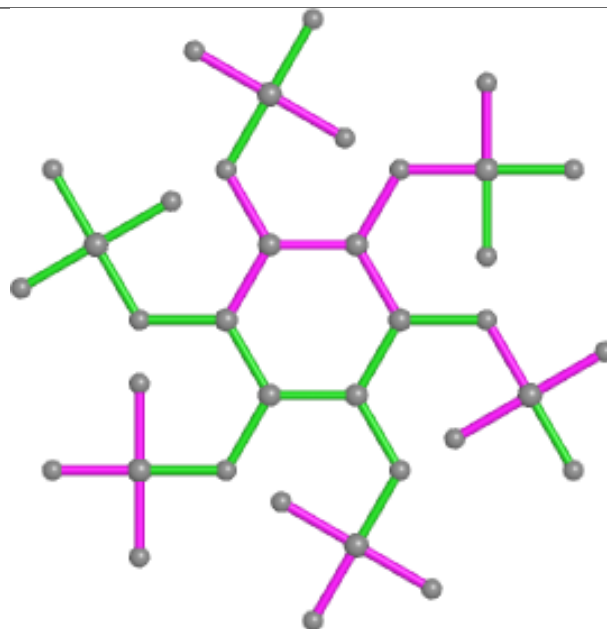


Rings

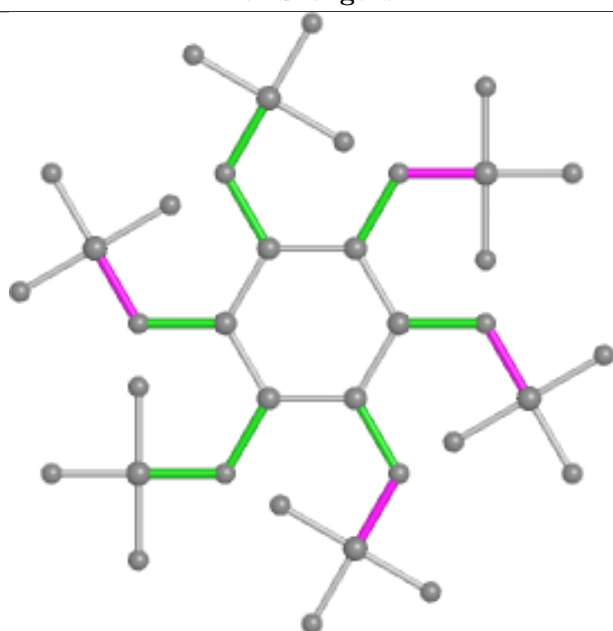
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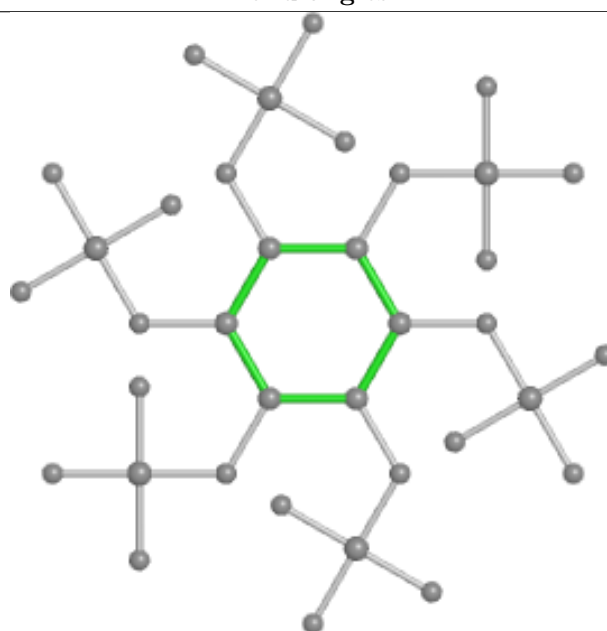
Bond lengths



Bond angles

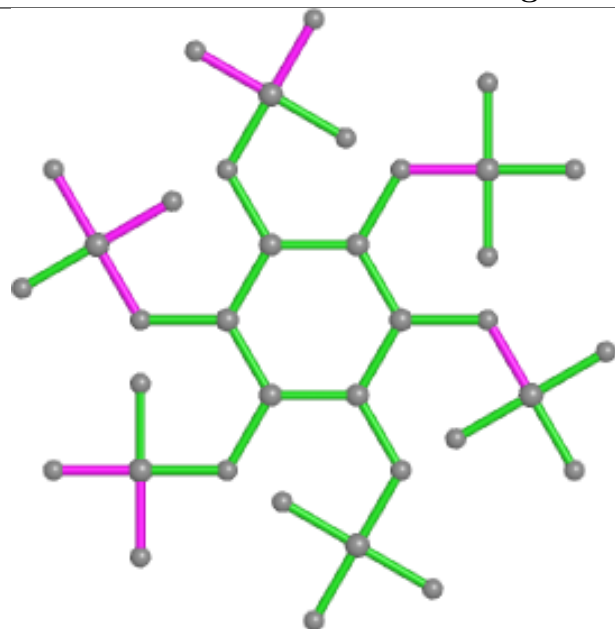


Torsions

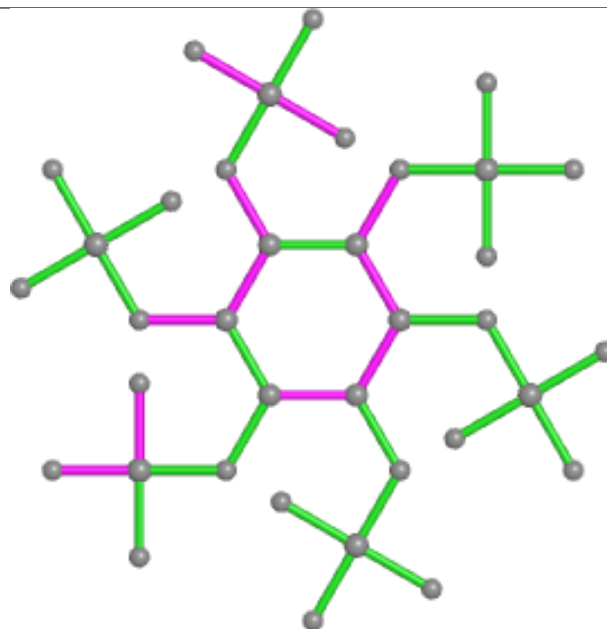


Rings

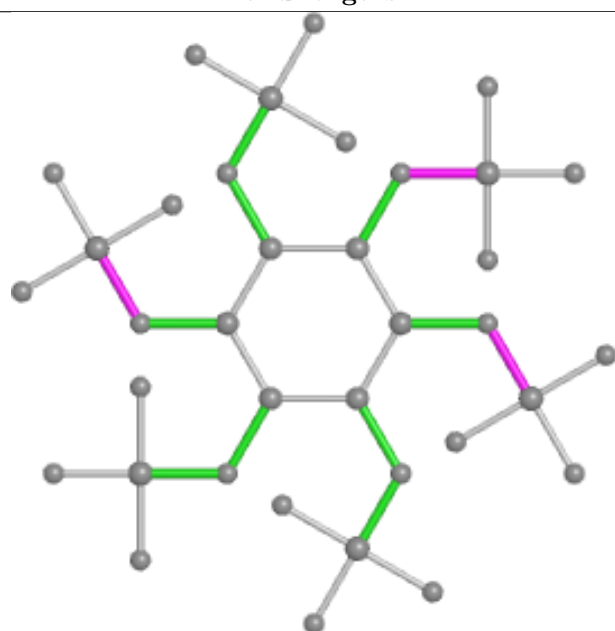
## Ligand IHP B 201



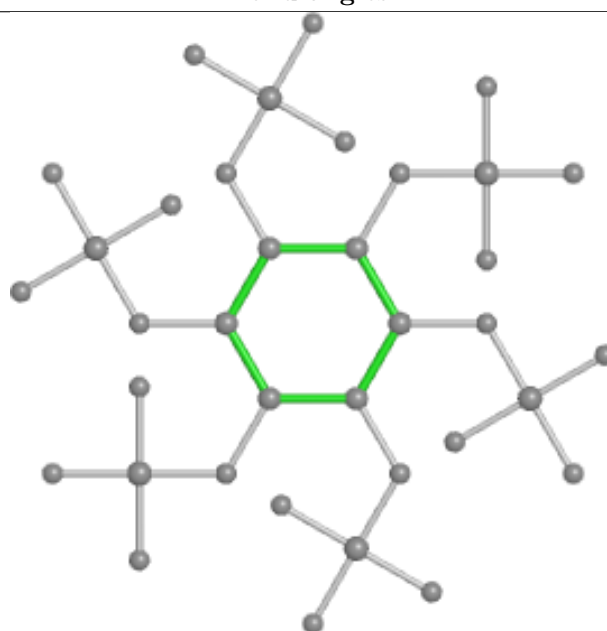
Bond lengths



Bond angles

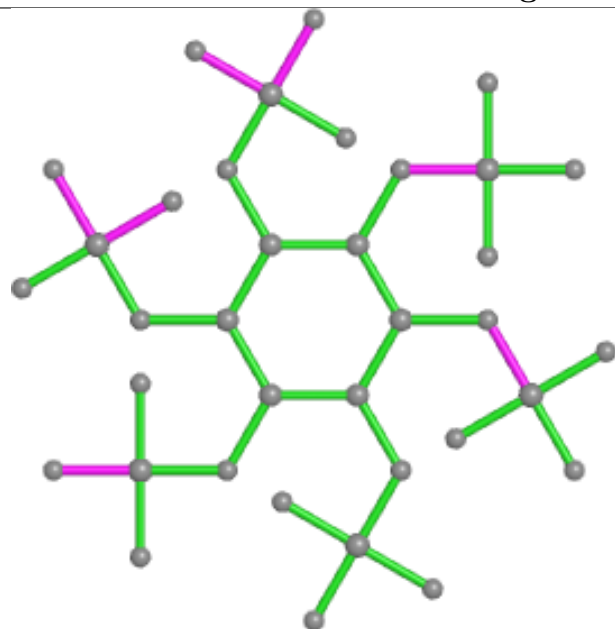


Torsions

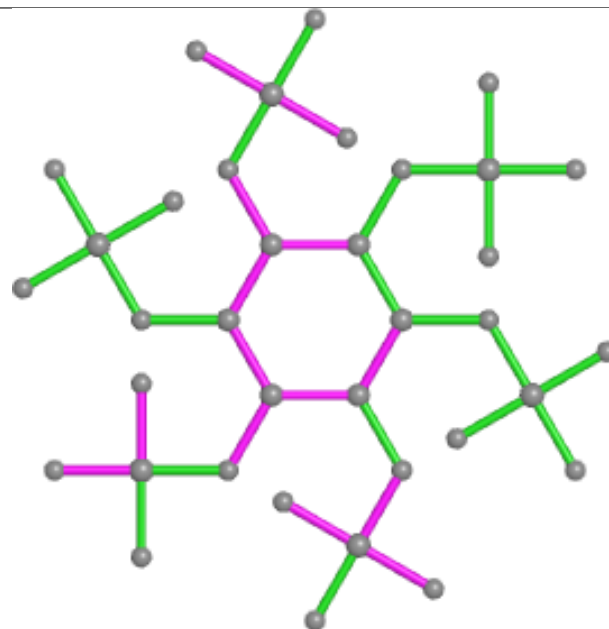


Rings

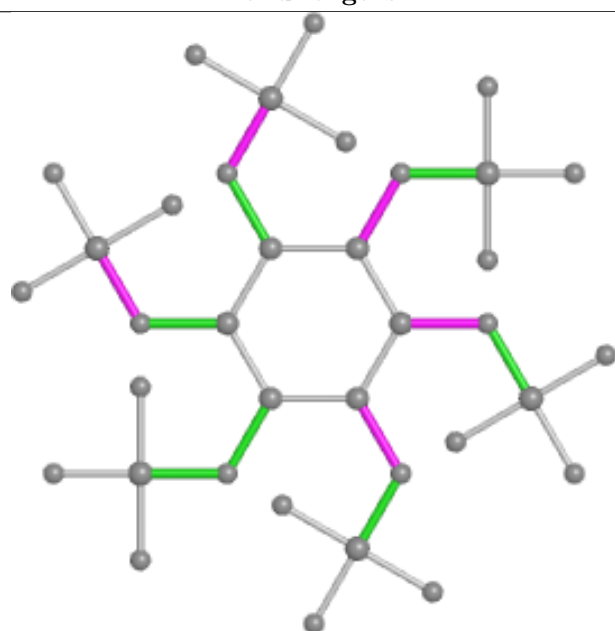
## Ligand IHP D 201



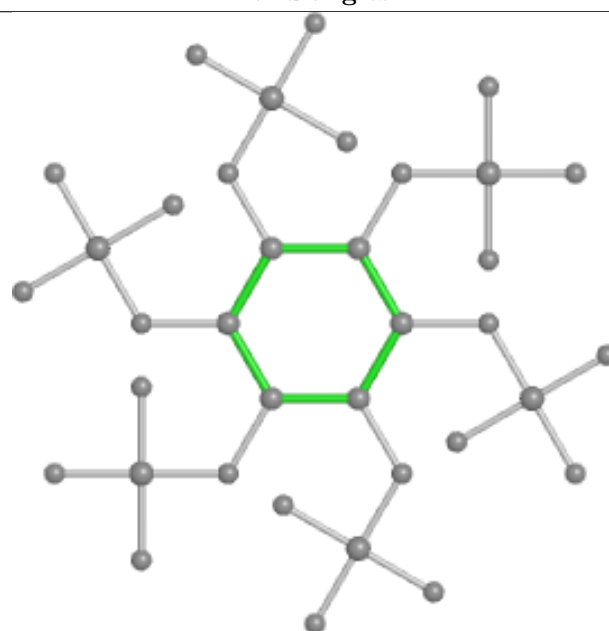
Bond lengths



Bond angles



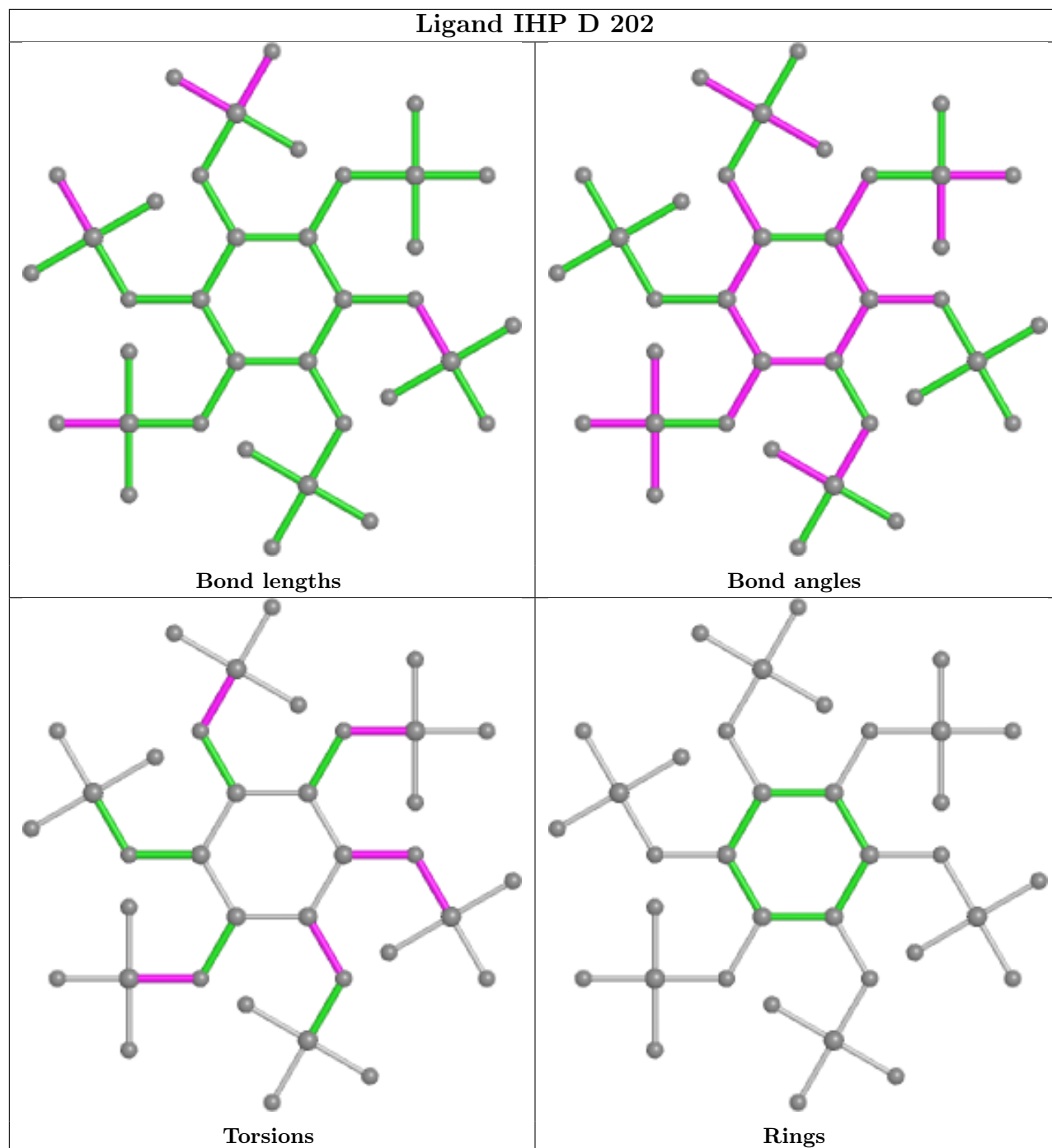
Torsions

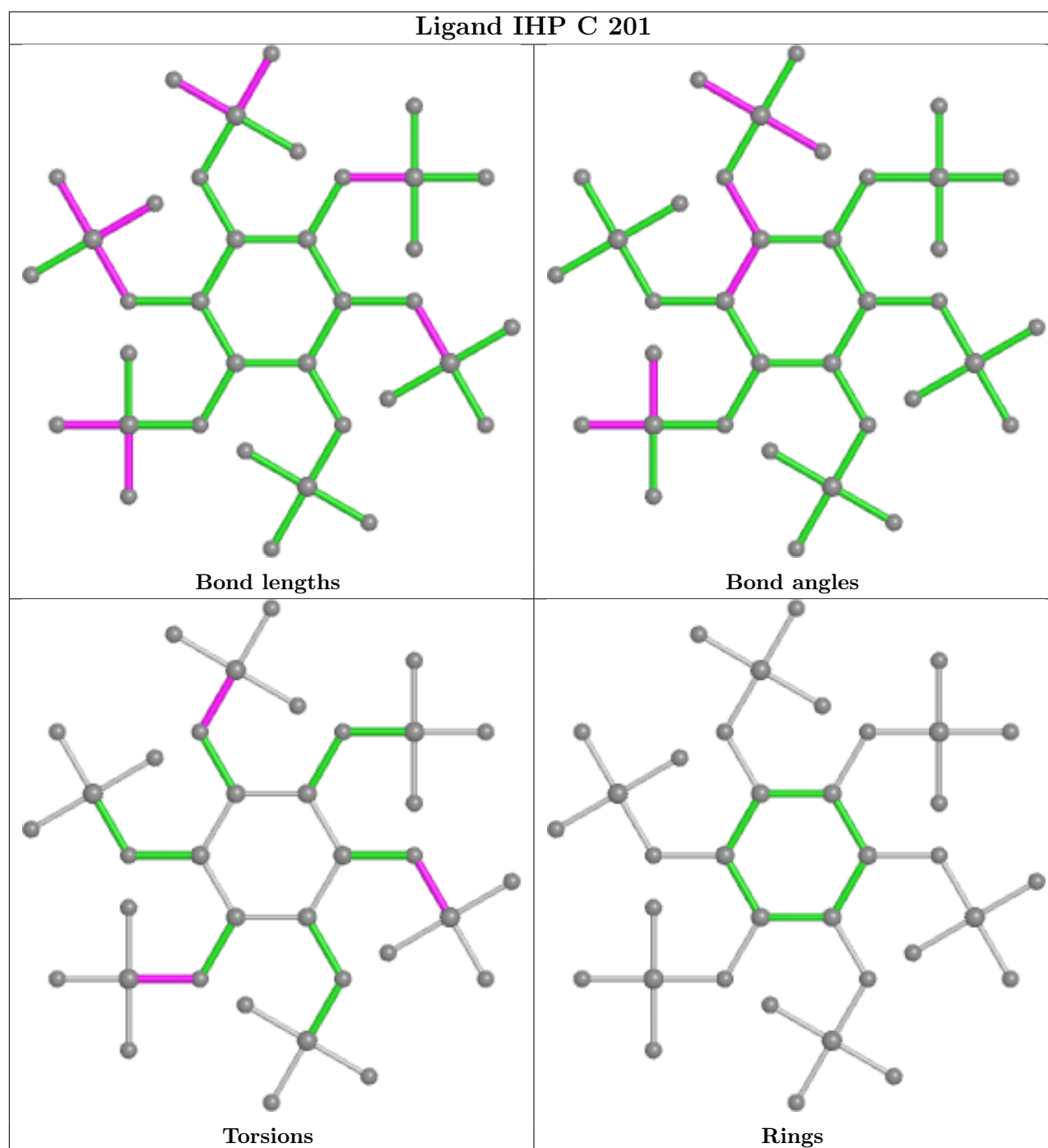


Rings



## Ligand IHP D 202





## 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	158/171 (92%)	0.59	14 (8%) 9 9	34, 54, 83, 100	0
1	B	149/171 (87%)	0.48	4 (2%) 54 52	32, 52, 75, 86	0
1	C	157/171 (91%)	0.39	6 (3%) 40 39	29, 49, 72, 84	0
1	D	153/171 (89%)	0.66	13 (8%) 10 10	34, 60, 91, 99	0
All	All	617/684 (90%)	0.53	37 (5%) 21 20	29, 54, 84, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	147	TRP	5.6
1	A	149	ASP	4.4
1	B	153	LEU	4.4
1	B	1	MET	3.7
1	C	85	GLU	3.7
1	D	153	LEU	3.6
1	A	168	LEU	3.6
1	A	148	ILE	3.5
1	A	150	GLY	3.4
1	A	2	ALA	3.0
1	D	159	ALA	2.8
1	A	23	LEU	2.8
1	D	158	THR	2.7
1	C	149	ASP	2.6
1	B	148	ILE	2.6
1	D	141	LYS	2.5
1	C	79	ILE	2.5
1	D	168	LEU	2.4
1	D	108	GLU	2.4
1	C	2	ALA	2.3
1	D	46	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	14	SER	2.3
1	D	167	ILE	2.3
1	D	138	LEU	2.3
1	D	151	GLN	2.2
1	A	153	LEU	2.2
1	A	133	ARG	2.2
1	D	157	GLN	2.2
1	A	71	LYS	2.2
1	C	23	LEU	2.2
1	A	5	ILE	2.1
1	A	79	ILE	2.1
1	A	167	ILE	2.0
1	A	102	PHE	2.0
1	D	71	LYS	2.0
1	B	163	MET	2.0
1	C	57	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IHP	C	201	36/36	0.81	0.20	55,82,96,103	0
2	IHP	D	201	36/36	0.84	0.14	68,95,106,120	0
2	IHP	A	502	36/36	0.86	0.12	58,79,91,95	0
2	IHP	A	501	36/36	0.86	0.13	79,96,111,118	0
2	IHP	D	202	36/36	0.86	0.12	76,90,102,109	0
2	IHP	B	201	36/36	0.90	0.13	59,84,99,105	0
3	ZN	A	503	1/1	0.93	0.11	59,59,59,59	0

*Continued on next page...*

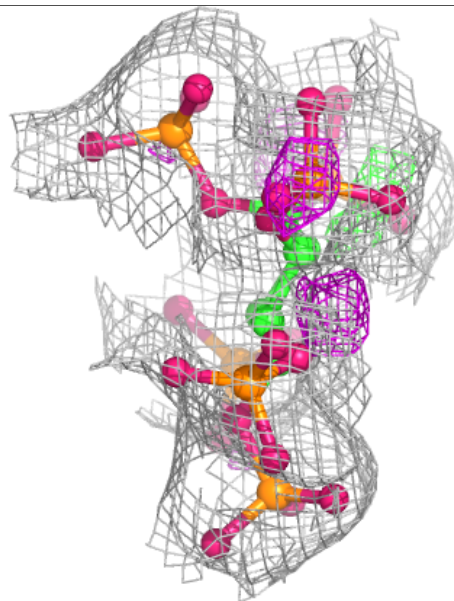
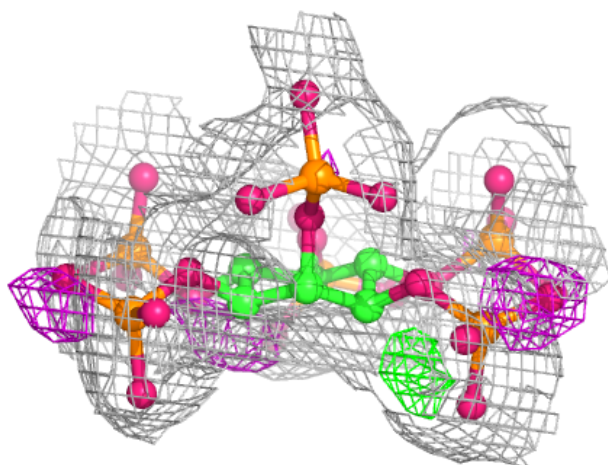
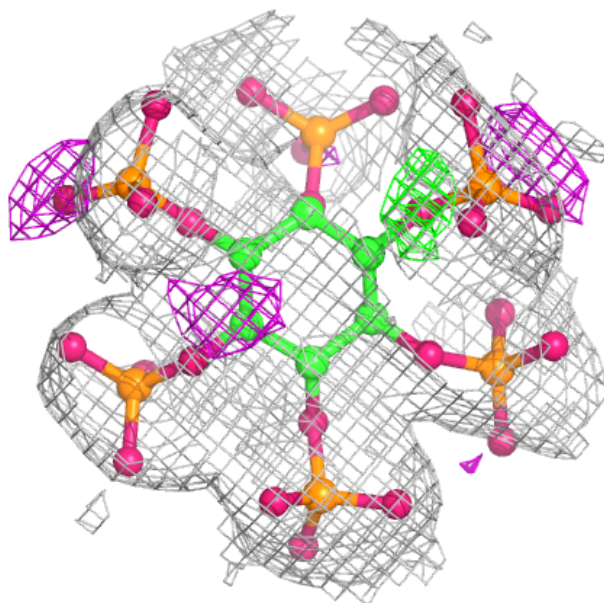
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	D	203	1/1	0.93	0.11	86,86,86,86	0
3	ZN	B	202	1/1	0.98	0.11	54,54,54,54	0
3	ZN	C	202	1/1	0.99	0.14	49,49,49,49	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.

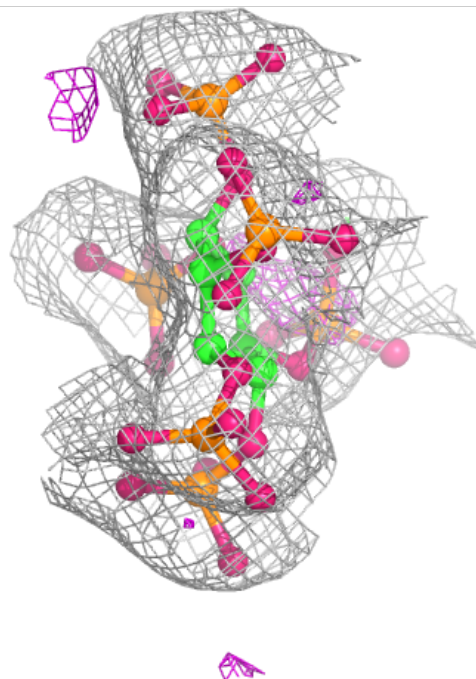
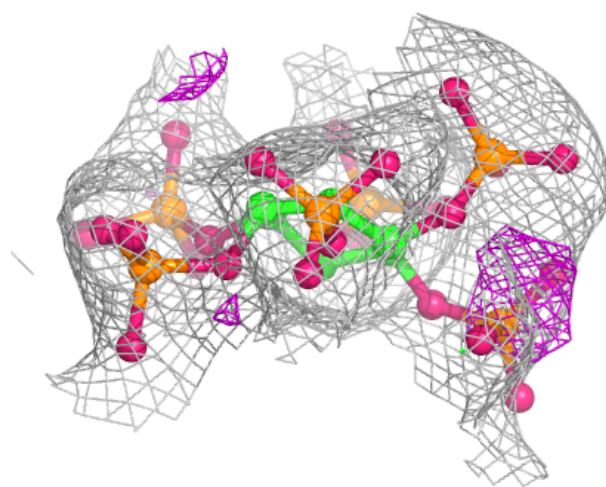
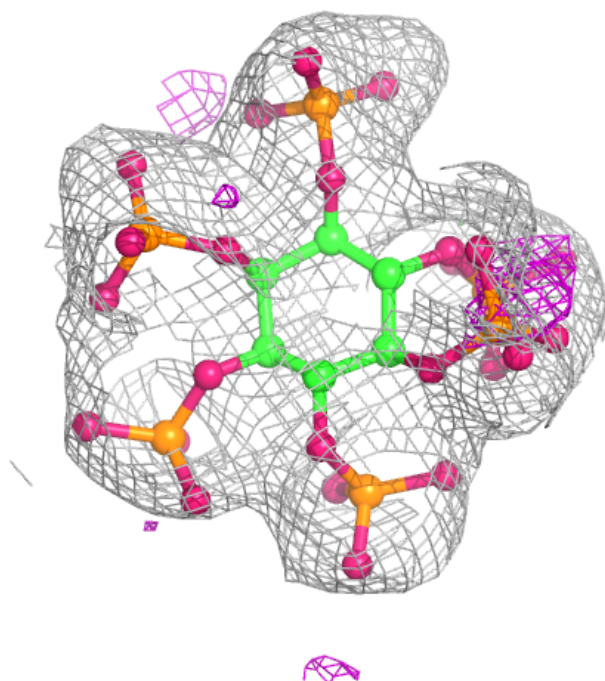
**Electron density around IHP C 201:**

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 IHP D 201:**

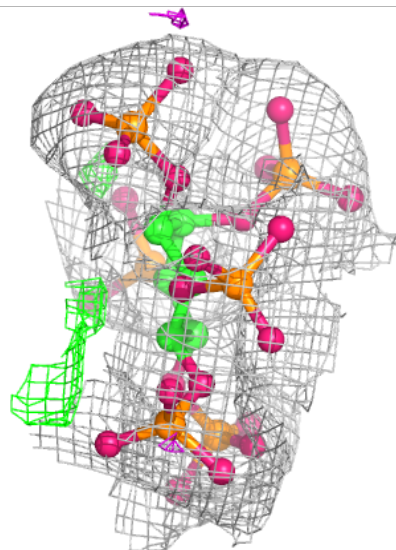
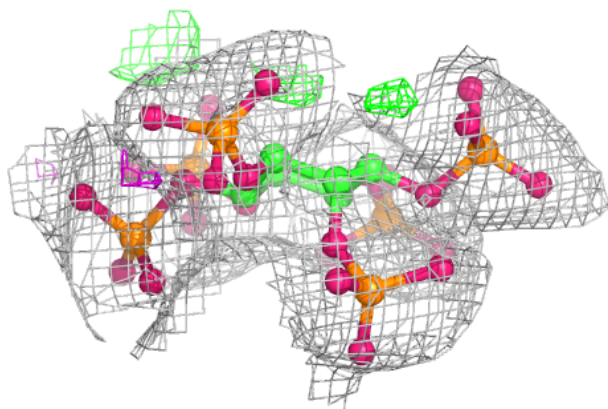
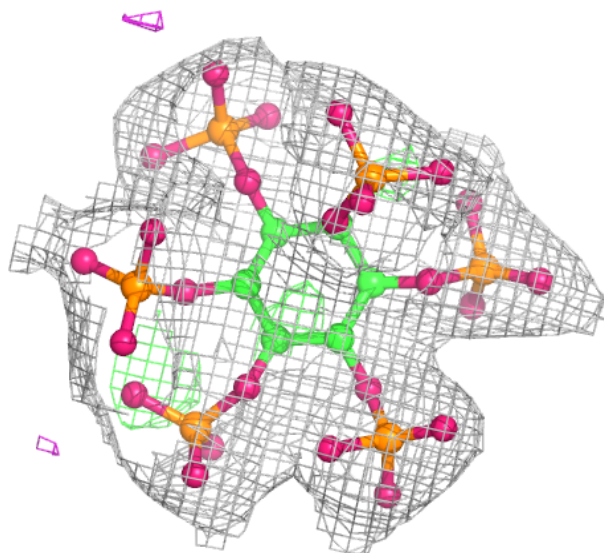
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





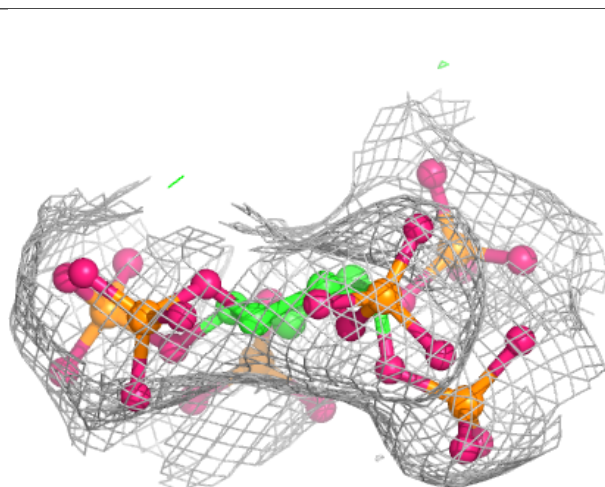
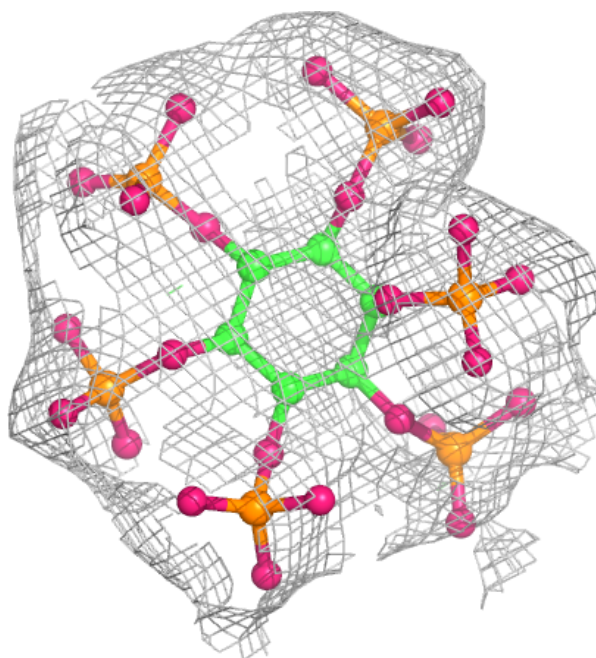
**Electron density around IHP A 502:**

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



**Electron density around IHP A 501:**

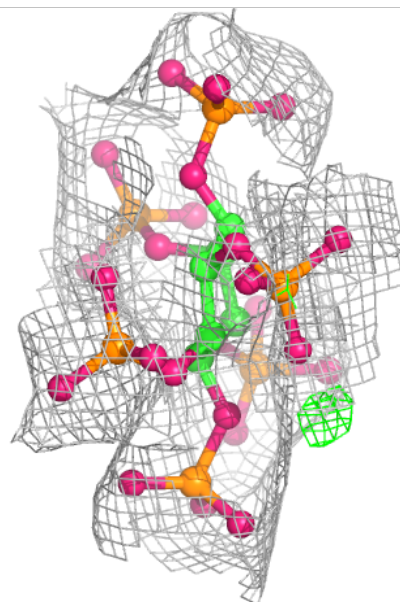
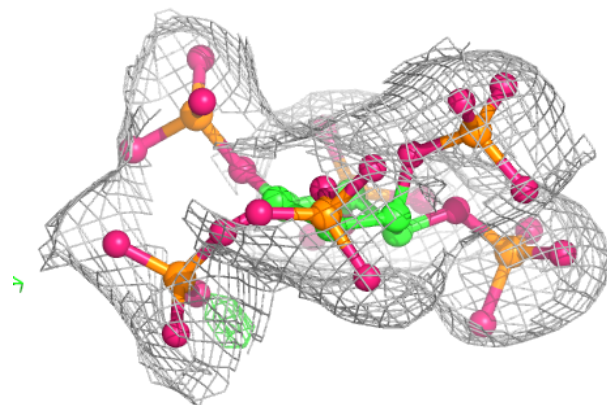
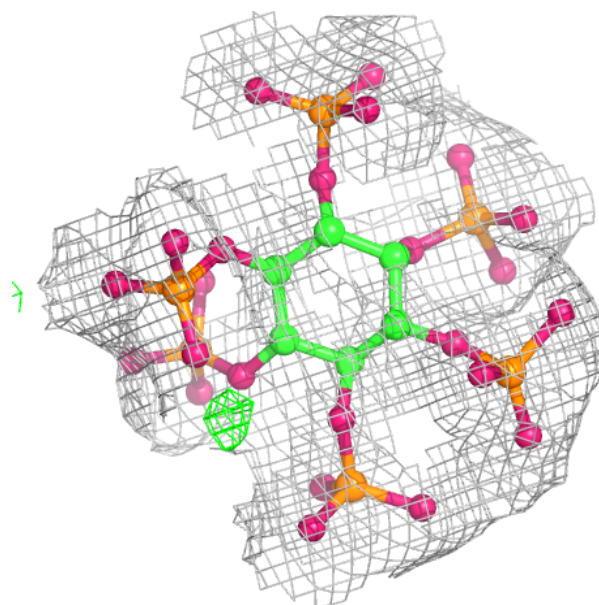
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





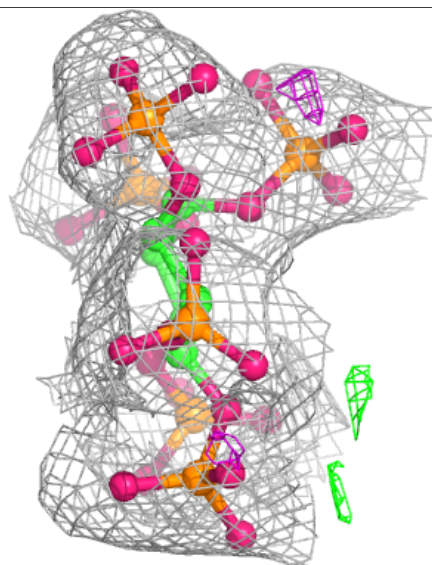
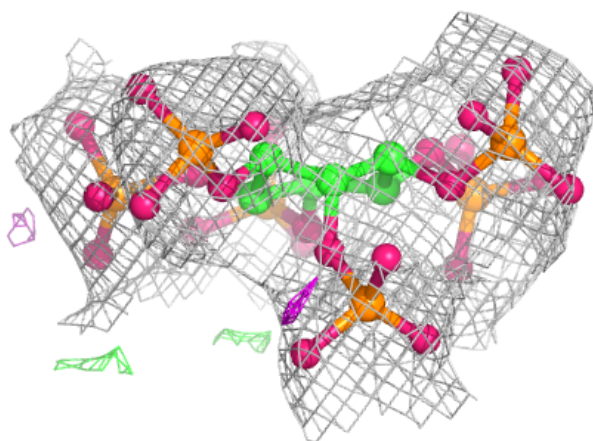
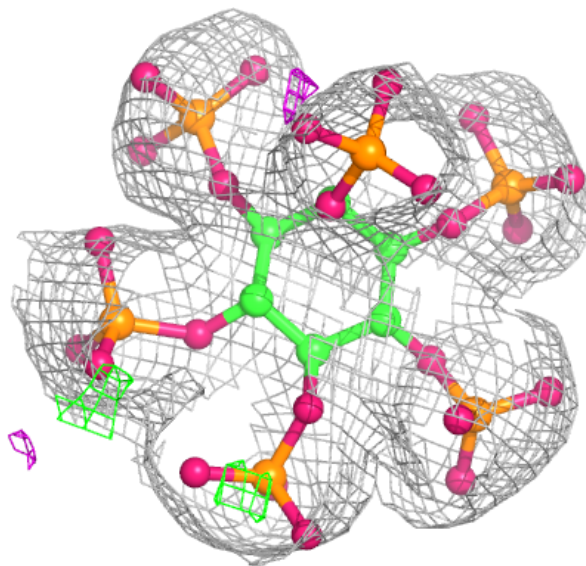
**Electron density around IHP D 202:**

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



**Electron density around IHP B 201:**

$2mF_o-DF_c$  (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.