



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2020 – 01:09 PM EDT

PDB ID : 6BHT  
Title : HIV-1 CA hexamer in complex with IP6, orthorhombic crystal form  
Authors : Zadrozny, K.; Wagner, J.M.; Ganser-Pornillos, B.K.; Pornillos, O.  
Deposited on : 2017-10-31  
Resolution : 2.69 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](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.

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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 : 2.14.6  
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) : 2.14.6

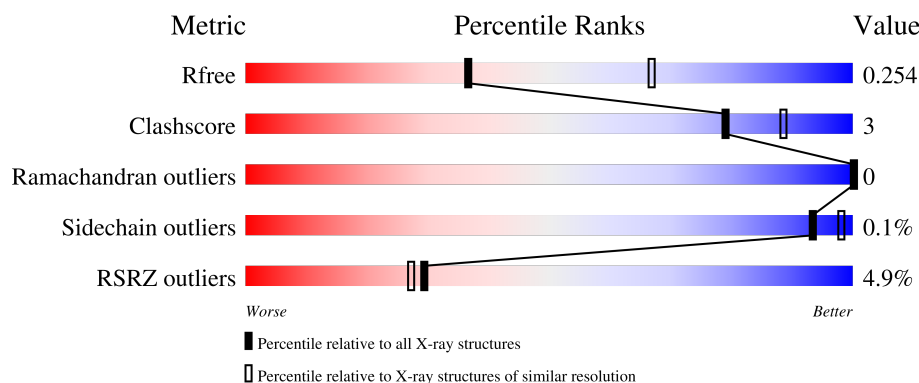
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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  $\geq 3$ , 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	231	 3% 84% 10% 5%
1	B	231	 3% 84% 6% 10%
1	C	231	 4% 86% 9% 5%
1	D	231	 2% 83% 8% 10%
1	E	231	 2% 88% 9% 5%

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Mol	Chain	Length	Quality of chain
1	F	231	<p>2% 90% 6%</p>
1	G	231	<p>10% 89% 5% 6%</p>
1	H	231	<p>6% 92% . .</p>
1	I	231	<p>5% 87% 6% 6%</p>
1	J	231	<p>3% 84% 5% 10%</p>
1	K	231	<p>6% 82% 5% 13%</p>
1	L	231	<p>9% 85% . 13%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19794 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 Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1659	1042	291	312	14			
1	B	209	Total	C	N	O	S	0	0	0
			1612	1016	280	302	14			
1	C	219	Total	C	N	O	S	0	0	0
			1661	1043	291	313	14			
1	D	209	Total	C	N	O	S	0	0	0
			1599	1004	281	300	14			
1	E	211	Total	C	N	O	S	0	0	0
			1632	1026	286	307	13			
1	F	221	Total	C	N	O	S	0	0	0
			1707	1074	300	319	14			
1	G	216	Total	C	N	O	S	0	0	0
			1604	1010	279	301	14			
1	H	221	Total	C	N	O	S	0	0	0
			1662	1046	289	313	14			
1	I	216	Total	C	N	O	S	0	0	0
			1643	1037	287	305	14			
1	J	207	Total	C	N	O	S	0	0	0
			1603	1005	280	304	14			
1	K	201	Total	C	N	O	S	0	0	0
			1532	967	266	285	14			
1	L	202	Total	C	N	O	S	0	0	0
			1527	965	265	284	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12493
A	45	CYS	GLU	engineered mutation	UNP P12493
A	184	ALA	TRP	engineered mutation	UNP P12493
A	185	ALA	MET	engineered mutation	UNP P12493
B	14	CYS	ALA	engineered mutation	UNP P12493

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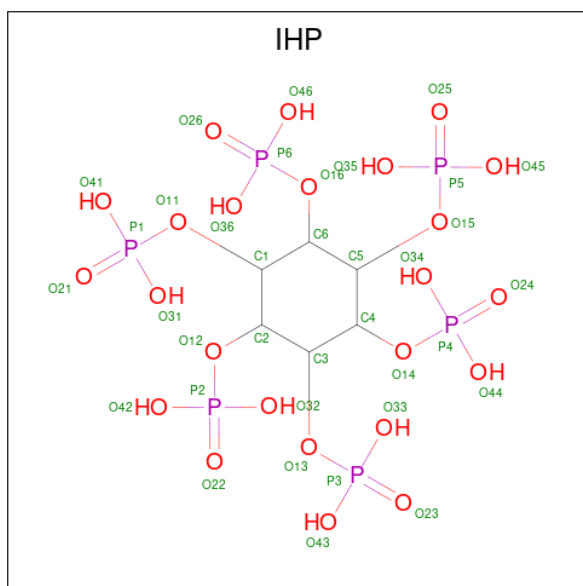
Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12493
B	184	ALA	TRP	engineered mutation	UNP P12493
B	185	ALA	MET	engineered mutation	UNP P12493
C	14	CYS	ALA	engineered mutation	UNP P12493
C	45	CYS	GLU	engineered mutation	UNP P12493
C	184	ALA	TRP	engineered mutation	UNP P12493
C	185	ALA	MET	engineered mutation	UNP P12493
D	14	CYS	ALA	engineered mutation	UNP P12493
D	45	CYS	GLU	engineered mutation	UNP P12493
D	184	ALA	TRP	engineered mutation	UNP P12493
D	185	ALA	MET	engineered mutation	UNP P12493
E	14	CYS	ALA	engineered mutation	UNP P12493
E	45	CYS	GLU	engineered mutation	UNP P12493
E	184	ALA	TRP	engineered mutation	UNP P12493
E	185	ALA	MET	engineered mutation	UNP P12493
F	14	CYS	ALA	engineered mutation	UNP P12493
F	45	CYS	GLU	engineered mutation	UNP P12493
F	184	ALA	TRP	engineered mutation	UNP P12493
F	185	ALA	MET	engineered mutation	UNP P12493
G	14	CYS	ALA	engineered mutation	UNP P12493
G	45	CYS	GLU	engineered mutation	UNP P12493
G	184	ALA	TRP	engineered mutation	UNP P12493
G	185	ALA	MET	engineered mutation	UNP P12493
H	14	CYS	ALA	engineered mutation	UNP P12493
H	45	CYS	GLU	engineered mutation	UNP P12493
H	184	ALA	TRP	engineered mutation	UNP P12493
H	185	ALA	MET	engineered mutation	UNP P12493
I	14	CYS	ALA	engineered mutation	UNP P12493
I	45	CYS	GLU	engineered mutation	UNP P12493
I	184	ALA	TRP	engineered mutation	UNP P12493
I	185	ALA	MET	engineered mutation	UNP P12493
J	14	CYS	ALA	engineered mutation	UNP P12493
J	45	CYS	GLU	engineered mutation	UNP P12493
J	184	ALA	TRP	engineered mutation	UNP P12493
J	185	ALA	MET	engineered mutation	UNP P12493
K	14	CYS	ALA	engineered mutation	UNP P12493
K	45	CYS	GLU	engineered mutation	UNP P12493
K	184	ALA	TRP	engineered mutation	UNP P12493
K	185	ALA	MET	engineered mutation	UNP P12493
L	14	CYS	ALA	engineered mutation	UNP P12493
L	45	CYS	GLU	engineered mutation	UNP P12493
L	184	ALA	TRP	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12493

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	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	K	1	Total	C	O	P	0	0
			36	6	24	6		
2	K	1	Total	C	O	P	0	1
			72	12	48	12		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	12	Total	O	0	0
			12	12		
3	C	13	Total	O	0	0
			13	13		
3	D	16	Total	O	0	0
			16	16		
3	E	18	Total	O	0	0
			18	18		

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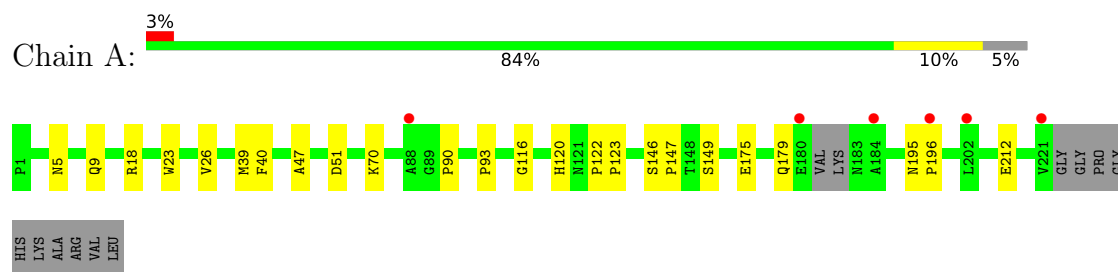
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	20	Total 20	O 20	0	0
3	G	2	Total 2	O 2	0	0
3	H	8	Total 8	O 8	0	0
3	I	17	Total 17	O 17	0	0
3	J	26	Total 26	O 26	0	0
3	K	8	Total 8	O 8	0	0
3	L	6	Total 6	O 6	0	0

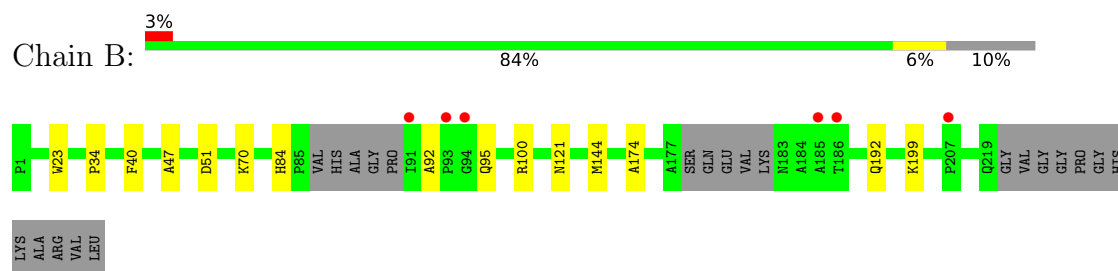
### 3 Residue-property plots [i](#)

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.

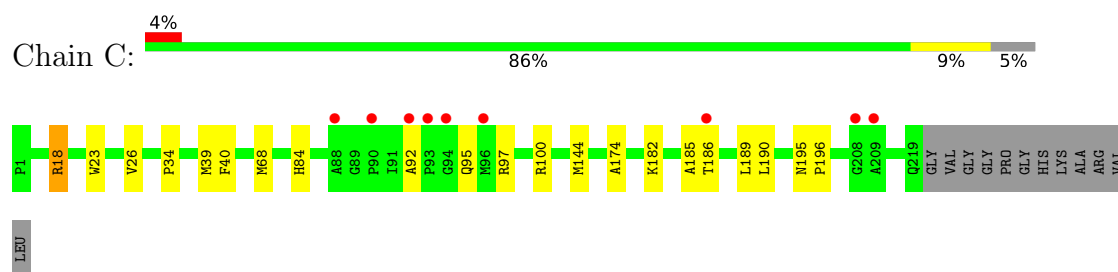
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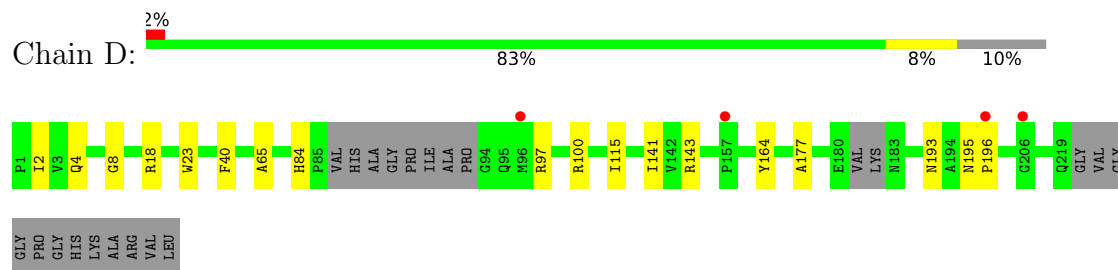
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

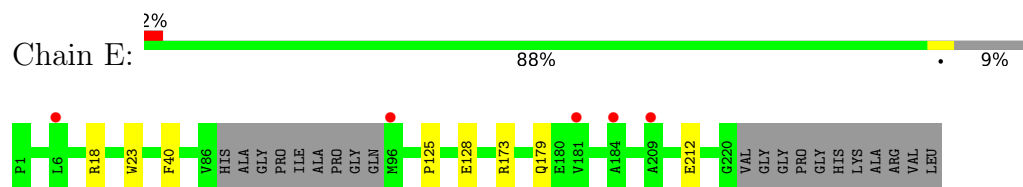


- Molecule 1: Capsid protein p24

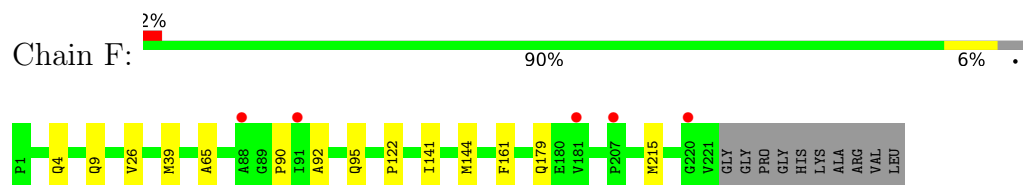




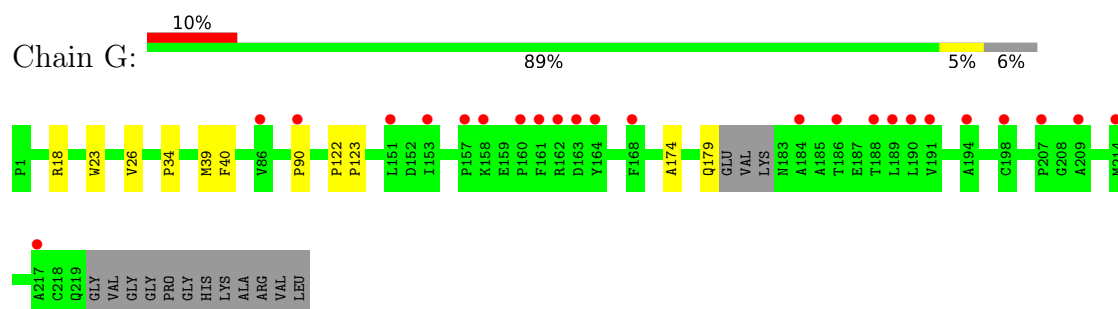
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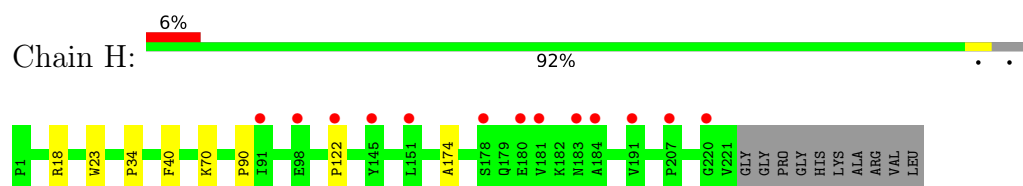
- Molecule 1: Capsid protein p24



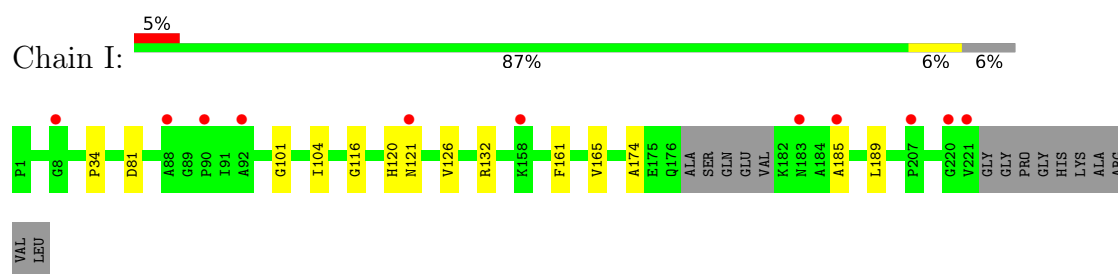
- Molecule 1: Capsid protein p24



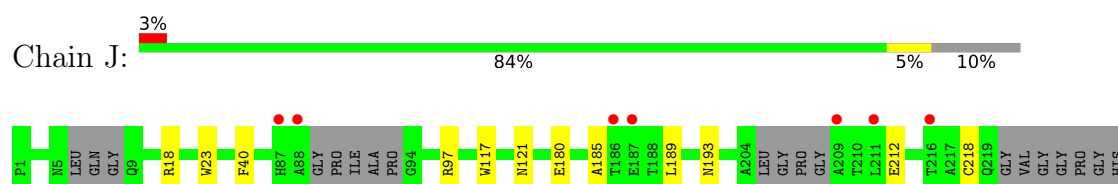
- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

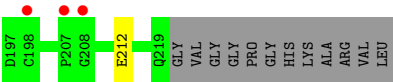
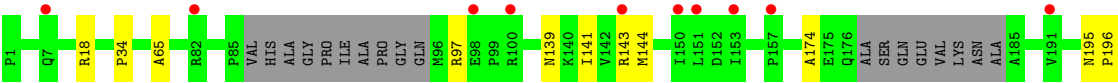
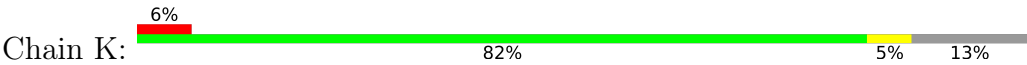


- Molecule 1: Capsid protein p24

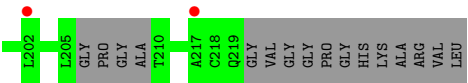
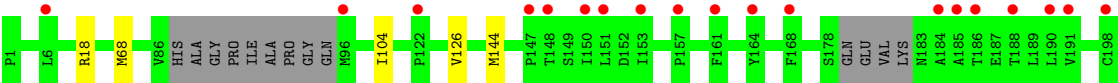
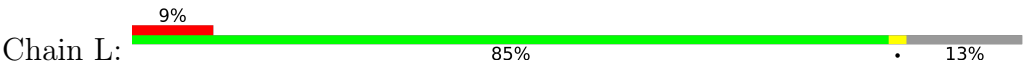


LYS  
ALA  
ARG  
VAL  
LEU

● Molecule 1: Capsid protein p24



● Molecule 1: Capsid protein p24



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.32Å 137.17Å 209.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.77 – 2.69 39.77 – 2.69	Depositor EDS
% Data completeness (in resolution range)	88.2 (39.77-2.69) 88.3 (39.77-2.69)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.227 , 0.255 0.227 , 0.254	Depositor DCC
$R_{free}$ test set	2000 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: 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	0.25	0/1695	0.39	0/2309
1	B	0.24	0/1645	0.38	0/2235
1	C	0.24	0/1697	0.38	0/2313
1	D	0.24	0/1631	0.39	0/2215
1	E	0.24	0/1665	0.39	0/2261
1	F	0.24	0/1744	0.39	0/2371
1	G	0.24	0/1639	0.40	0/2235
1	H	0.24	0/1698	0.39	0/2314
1	I	0.24	0/1679	0.38	0/2284
1	J	0.24	0/1633	0.39	0/2216
1	K	0.24	0/1564	0.39	0/2127
1	L	0.24	0/1557	0.38	0/2119
All	All	0.24	0/19847	0.39	0/26999

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	1659	0	1619	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1612	0	1602	10	0
1	C	1661	0	1627	16	0
1	D	1599	0	1564	11	0
1	E	1632	0	1625	6	0
1	F	1707	0	1711	9	0
1	G	1604	0	1535	9	0
1	H	1662	0	1618	7	0
1	I	1643	0	1620	8	0
1	J	1603	0	1574	9	0
1	K	1532	0	1497	13	0
1	L	1527	0	1475	6	0
2	C	36	0	6	3	0
2	D	36	0	6	4	0
2	K	108	0	18	12	0
3	A	27	0	0	0	0
3	B	12	0	0	0	0
3	C	13	0	0	0	0
3	D	16	0	0	0	0
3	E	18	0	0	0	0
3	F	20	0	0	0	0
3	G	2	0	0	0	0
3	H	8	0	0	0	0
3	I	17	0	0	1	0
3	J	26	0	0	2	0
3	K	8	0	0	0	0
3	L	6	0	0	0	0
All	All	19794	0	19097	107	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 3.

The worst 5 of 107 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)
2:D:301:IHP:O43	1:E:18:ARG:NH1	1.97	0.97
1:G:18:ARG:NH1	2:K:301:IHP:O42	2.08	0.85
1:C:185:ALA:O	1:C:189:LEU:HB2	1.82	0.79
1:K:18:ARG:NH2	2:K:301:IHP:O32	2.18	0.75
1:K:18:ARG:HH22	2:K:301:IHP:P1	2.11	0.73

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	215/231 (93%)	211 (98%)	4 (2%)	0	100	100
1	B	203/231 (88%)	199 (98%)	4 (2%)	0	100	100
1	C	217/231 (94%)	211 (97%)	6 (3%)	0	100	100
1	D	203/231 (88%)	199 (98%)	4 (2%)	0	100	100
1	E	207/231 (90%)	204 (99%)	3 (1%)	0	100	100
1	F	219/231 (95%)	213 (97%)	6 (3%)	0	100	100
1	G	212/231 (92%)	206 (97%)	6 (3%)	0	100	100
1	H	219/231 (95%)	216 (99%)	3 (1%)	0	100	100
1	I	212/231 (92%)	206 (97%)	6 (3%)	0	100	100
1	J	199/231 (86%)	196 (98%)	3 (2%)	0	100	100
1	K	195/231 (84%)	192 (98%)	3 (2%)	0	100	100
1	L	194/231 (84%)	190 (98%)	4 (2%)	0	100	100
All	All	2495/2772 (90%)	2443 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	175/193 (91%)	174 (99%)	1 (1%)	86	94
1	B	174/193 (90%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	176/193 (91%)	175 (99%)	1 (1%)	86	94
1	D	169/193 (88%)	169 (100%)	0	100	100
1	E	177/193 (92%)	177 (100%)	0	100	100
1	F	186/193 (96%)	186 (100%)	0	100	100
1	G	163/193 (84%)	163 (100%)	0	100	100
1	H	173/193 (90%)	173 (100%)	0	100	100
1	I	174/193 (90%)	174 (100%)	0	100	100
1	J	173/193 (90%)	172 (99%)	1 (1%)	86	94
1	K	162/193 (84%)	162 (100%)	0	100	100
1	L	158/193 (82%)	158 (100%)	0	100	100
All	All	2060/2316 (89%)	2057 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	C	18	ARG
1	J	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	67	GLN
1	J	121	ASN
1	G	63	GLN
1	D	4	GLN
1	F	63	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](#)

5 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	IHP	K	301	-	36,36,36	1.13	3 (8%)	54,60,60	0.87	2 (3%)
2	IHP	D	301	-	36,36,36	1.16	4 (11%)	54,60,60	0.87	2 (3%)
2	IHP	K	302[A]	-	36,36,36	1.15	4 (11%)	54,60,60	0.88	3 (5%)
2	IHP	K	302[B]	-	36,36,36	1.15	4 (11%)	54,60,60	0.87	3 (5%)
2	IHP	C	301	-	36,36,36	1.16	4 (11%)	54,60,60	0.87	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	K	301	-	-	3/30/54/54	0/1/1/1
2	IHP	D	301	-	-	3/30/54/54	0/1/1/1
2	IHP	K	302[A]	-	-	3/30/54/54	0/1/1/1
2	IHP	K	302[B]	-	-	3/30/54/54	0/1/1/1
2	IHP	C	301	-	-	3/30/54/54	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	302[A]	IHP	P6-O16	3.00	1.65	1.59
2	K	302[B]	IHP	P6-O16	2.98	1.64	1.59
2	D	301	IHP	P6-O16	2.98	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	IHP	P6-O16	2.96	1.64	1.59
2	C	301	IHP	P6-O16	2.94	1.64	1.59

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	301	IHP	O43-P3-O23	2.25	119.48	110.68
2	K	302[B]	IHP	O43-P3-O23	2.24	119.45	110.68
2	C	301	IHP	O43-P3-O23	2.23	119.43	110.68
2	D	301	IHP	O43-P3-O23	2.23	119.41	110.68
2	K	302[A]	IHP	O43-P3-O23	2.21	119.35	110.68

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	IHP	C2-O12-P2-O42
2	K	301	IHP	C2-O12-P2-O42
2	K	302[A]	IHP	C2-O12-P2-O42
2	K	302[B]	IHP	C2-O12-P2-O42
2	C	301	IHP	C2-O12-P2-O42

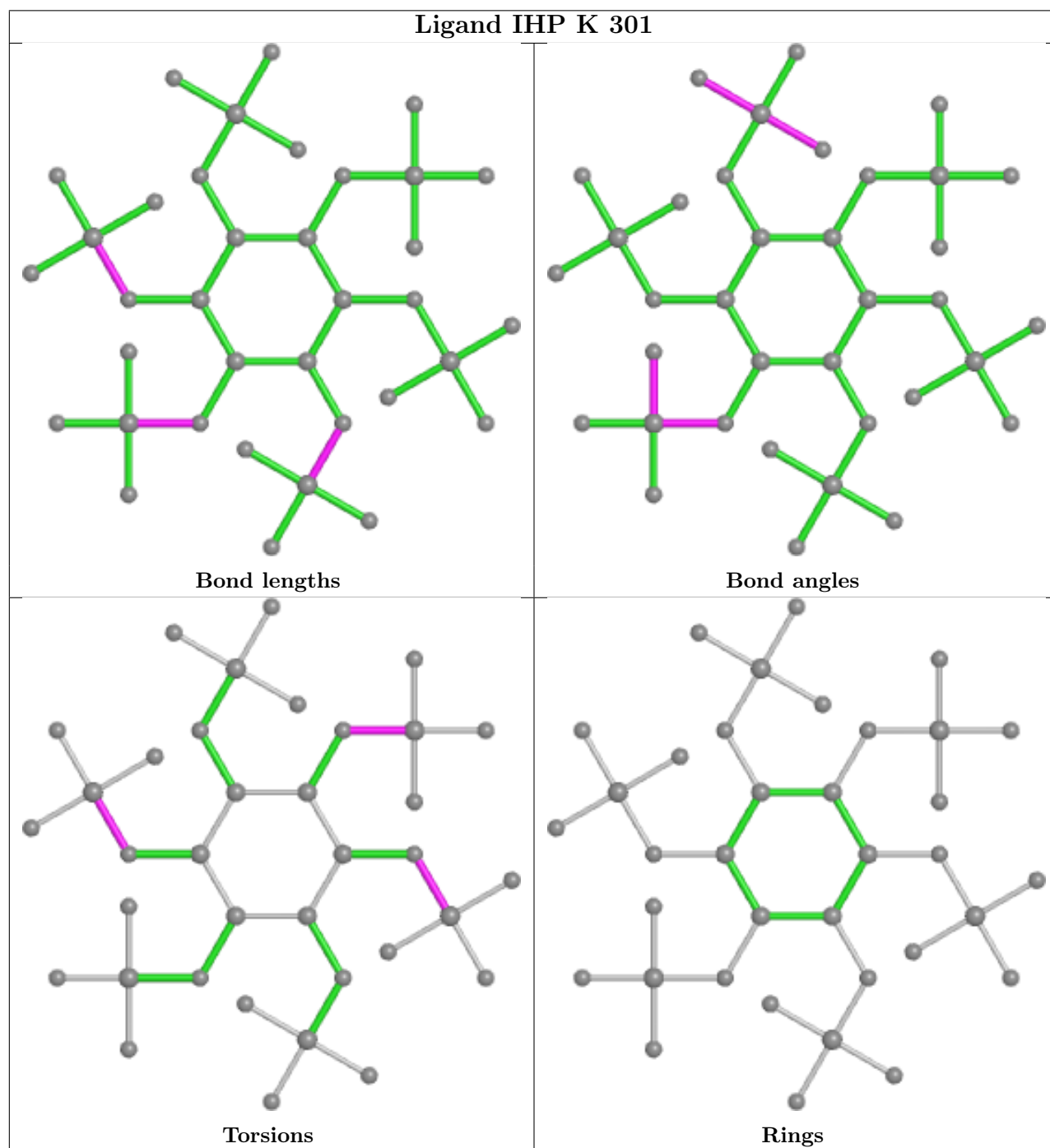
There are no ring outliers.

5 monomers are involved in 19 short contacts:

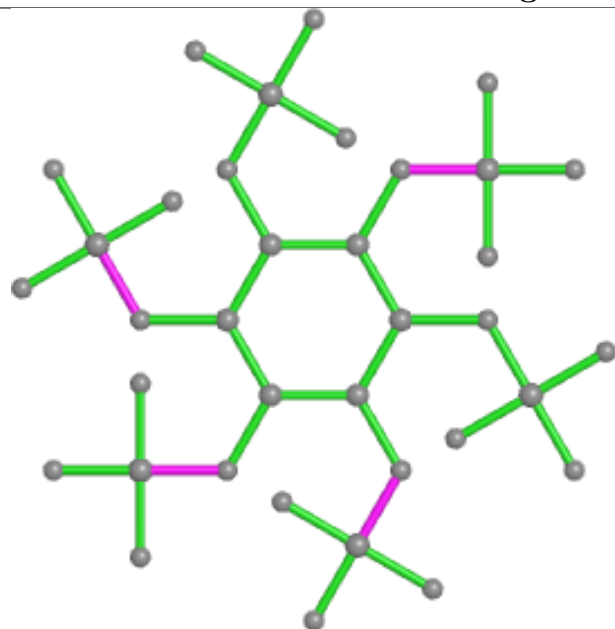
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	301	IHP	7	0
2	D	301	IHP	4	0
2	K	302[A]	IHP	1	0
2	K	302[B]	IHP	4	0
2	C	301	IHP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

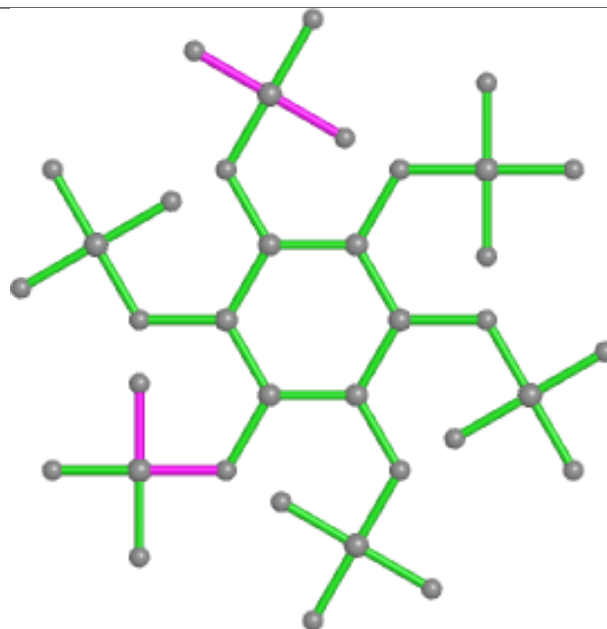
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



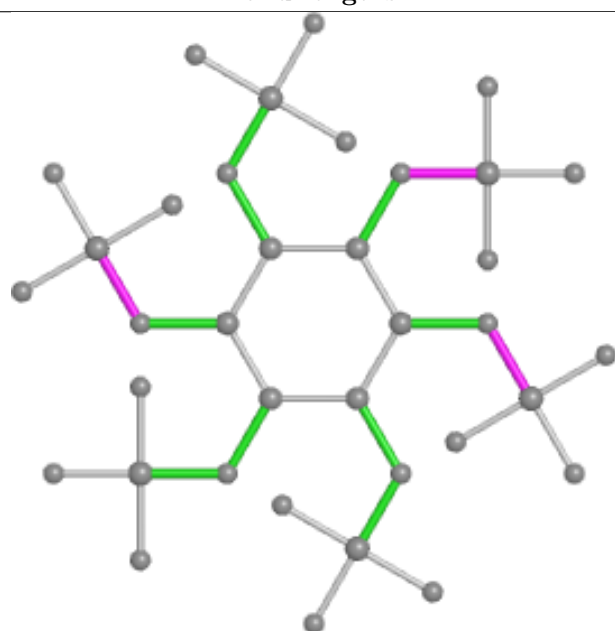
## Ligand IHP D 301



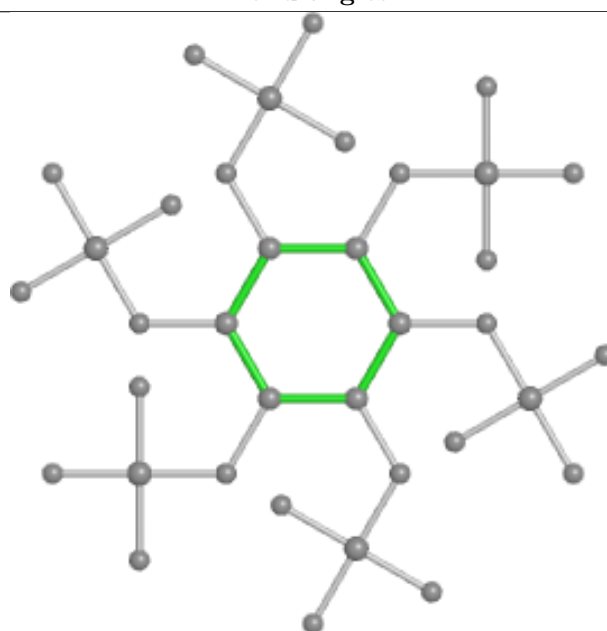
Bond lengths



Bond angles

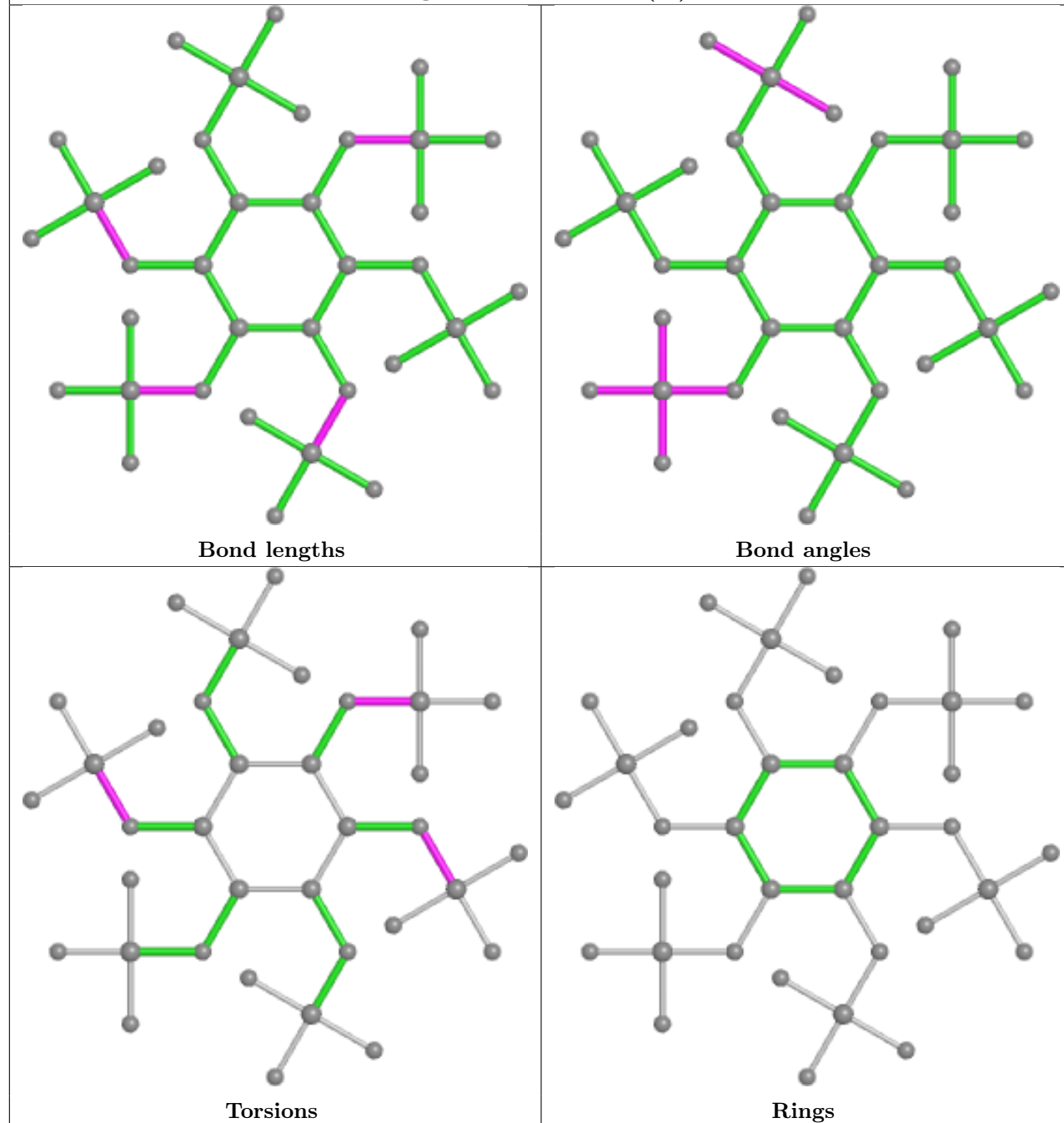


Torsions

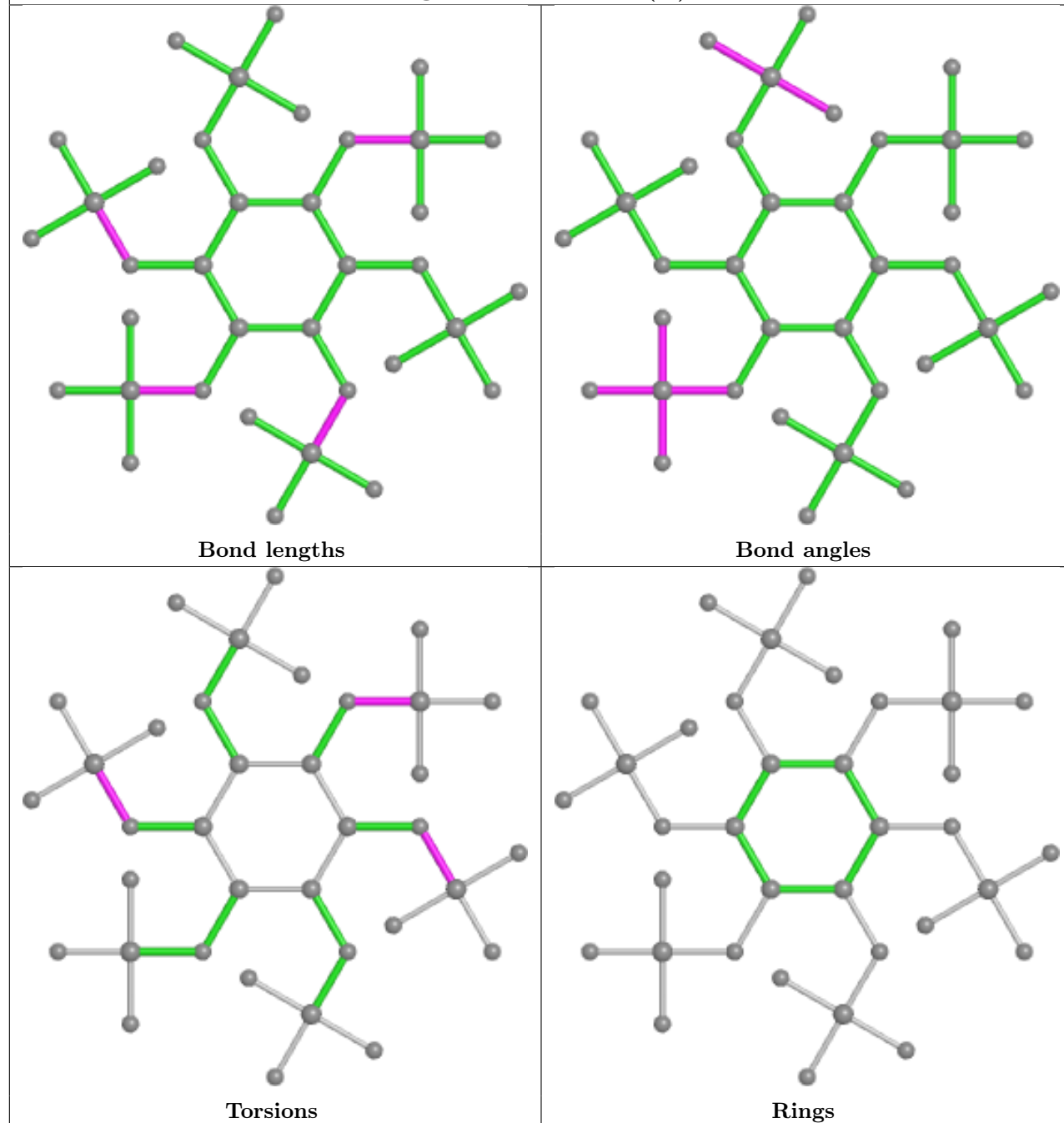


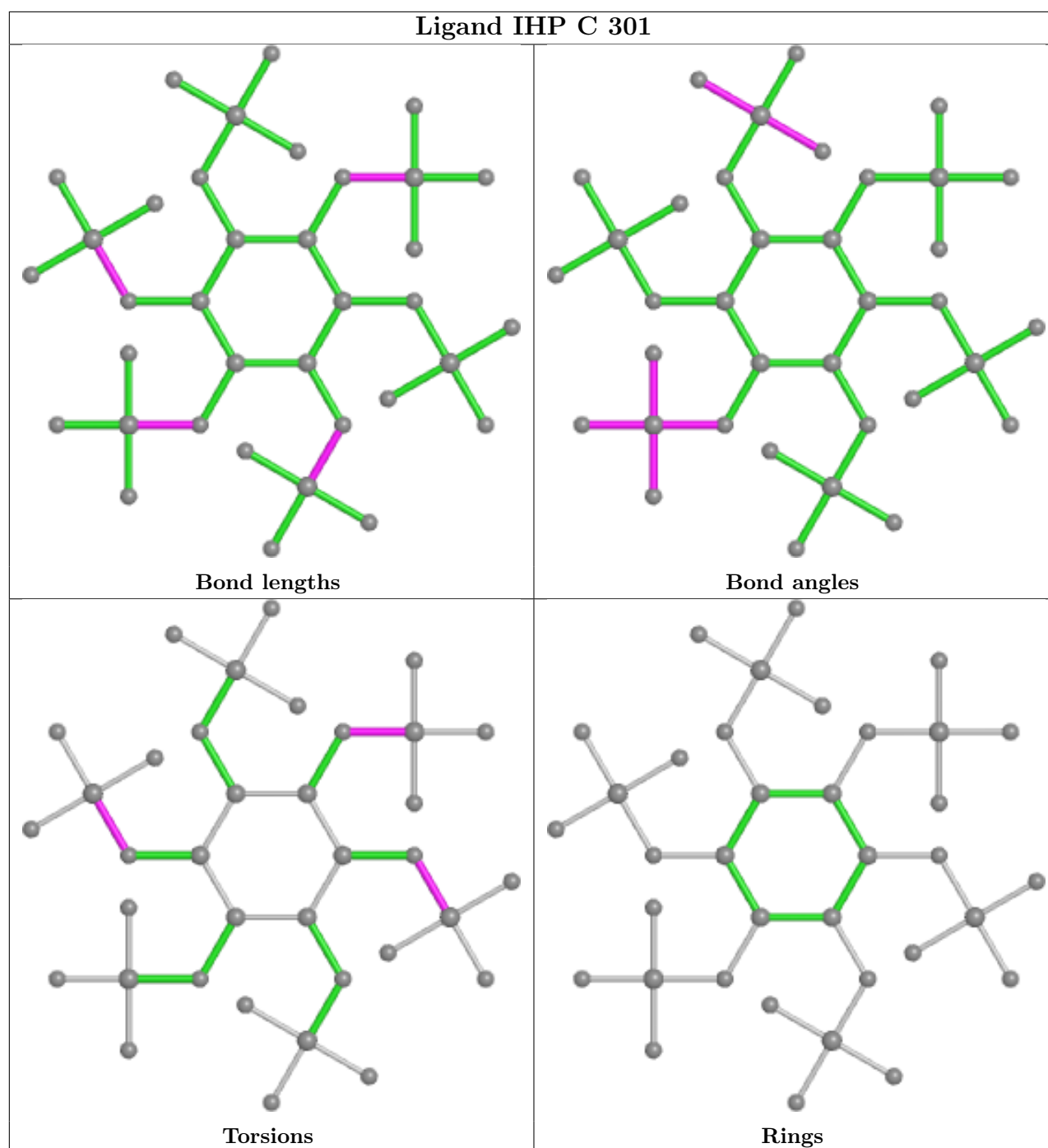
Rings

## Ligand IHP K 302 (A)



## Ligand IHP K 302 (B)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	219/231 (94%)	0.09	6 (2%) 54 54	8, 35, 93, 117	0
1	B	209/231 (90%)	0.18	6 (2%) 51 51	18, 43, 88, 106	0
1	C	219/231 (94%)	0.09	9 (4%) 37 35	17, 39, 99, 132	0
1	D	209/231 (90%)	0.04	4 (1%) 66 67	16, 44, 90, 120	0
1	E	211/231 (91%)	0.07	5 (2%) 59 59	16, 40, 84, 98	0
1	F	221/231 (95%)	-0.01	5 (2%) 60 60	14, 39, 77, 109	0
1	G	216/231 (93%)	0.53	24 (11%) 5 4	37, 65, 117, 141	0
1	H	221/231 (95%)	0.21	13 (5%) 22 20	34, 59, 101, 140	0
1	I	216/231 (93%)	0.26	11 (5%) 28 26	23, 48, 101, 138	0
1	J	207/231 (89%)	0.13	7 (3%) 45 44	21, 42, 94, 115	0
1	K	201/231 (87%)	0.38	13 (6%) 18 16	31, 56, 107, 140	0
1	L	202/231 (87%)	0.52	21 (10%) 6 4	42, 65, 111, 125	0
All	All	2551/2772 (92%)	0.21	124 (4%) 29 27	8, 49, 102, 141	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	151	LEU	6.1
1	G	189	LEU	5.6
1	G	190	LEU	5.6
1	E	6	LEU	5.6
1	K	207	PRO	4.7

### 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

There are no monosaccharides in this entry.

### 6.4 Ligands

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.

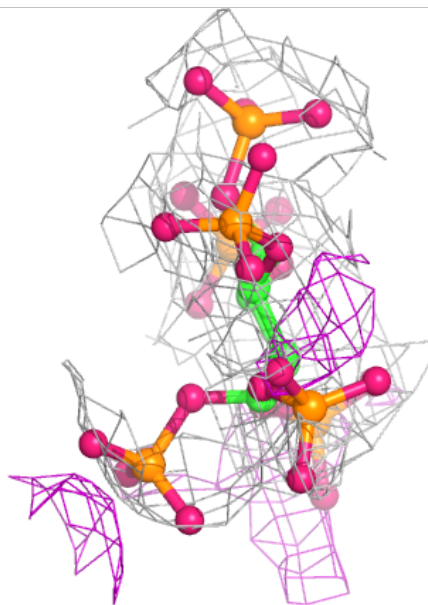
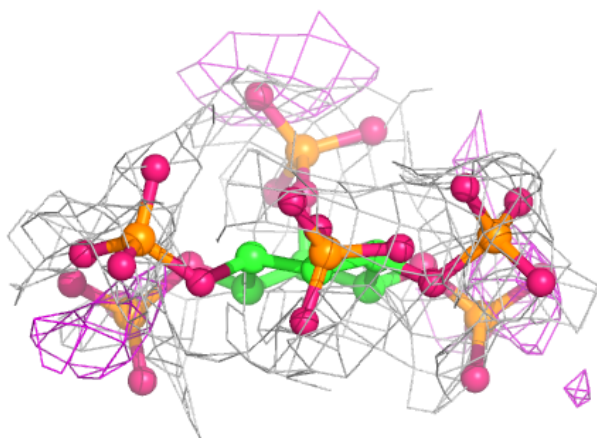
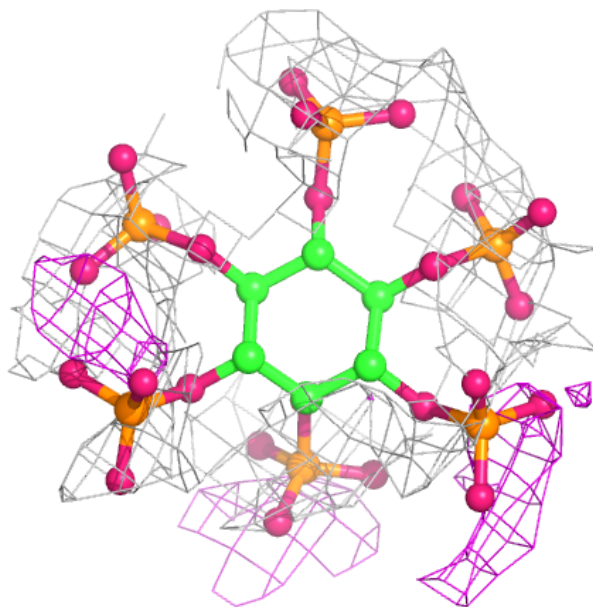
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IHP	K	301	36/36	0.58	0.28	135,152,156,157	0
2	IHP	C	301	36/36	0.61	0.27	153,166,172,174	0
2	IHP	K	302[A]	36/36	0.64	0.32	134,142,144,145	36
2	IHP	K	302[B]	36/36	0.64	0.32	128,142,144,145	36
2	IHP	D	301	36/36	0.64	0.26	162,172,180,180	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.



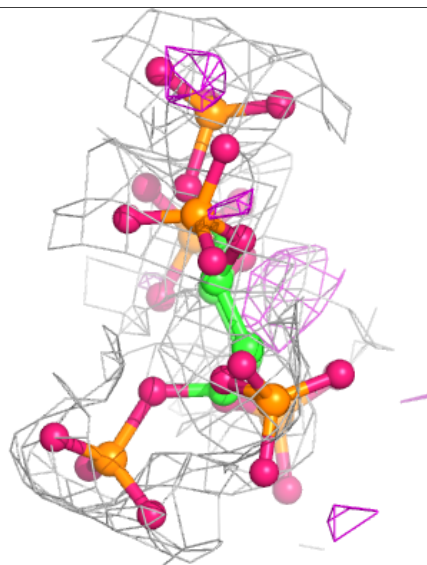
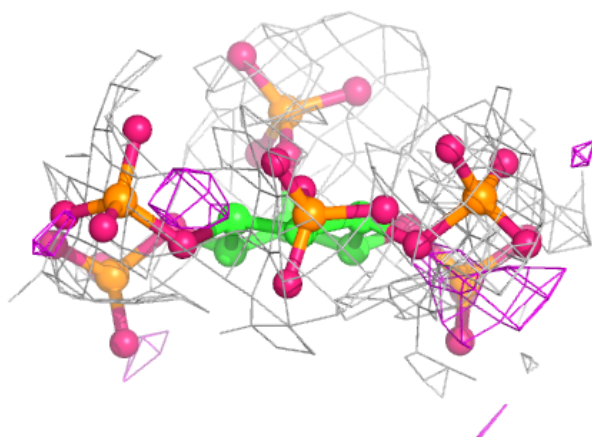
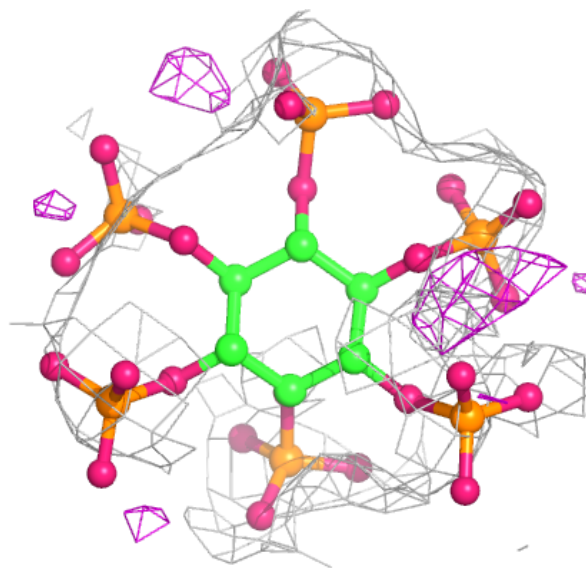
**Electron density around IHP K 301:**

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



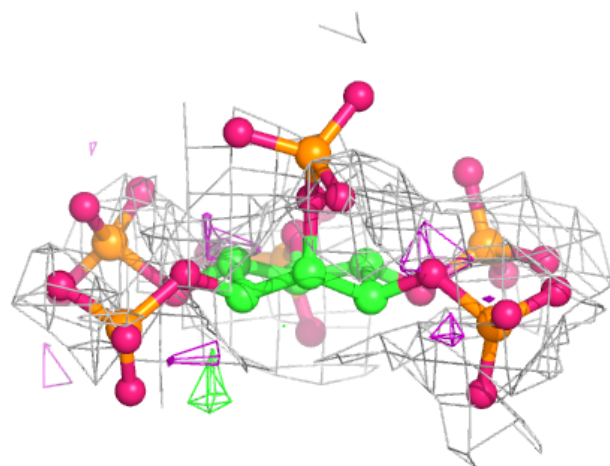
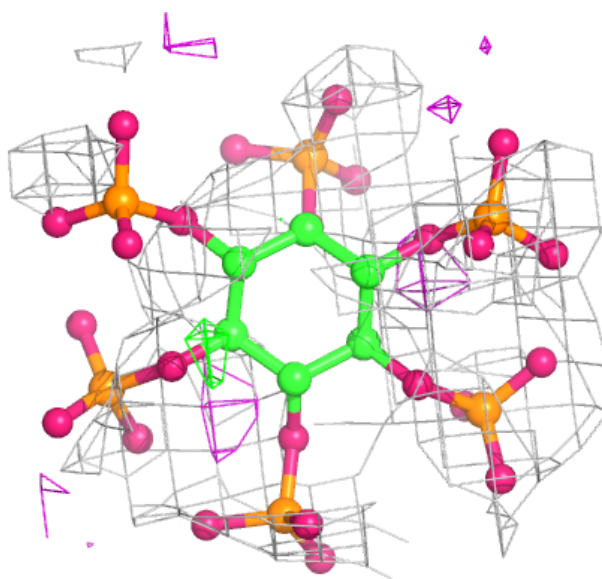
**Electron density around IHP C 301:**

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



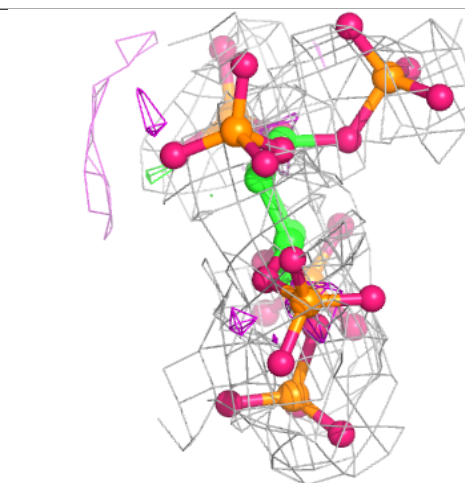
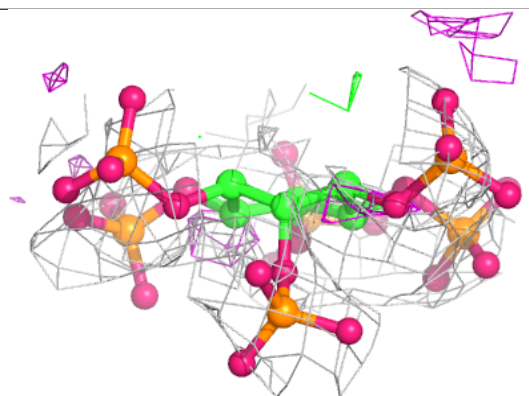
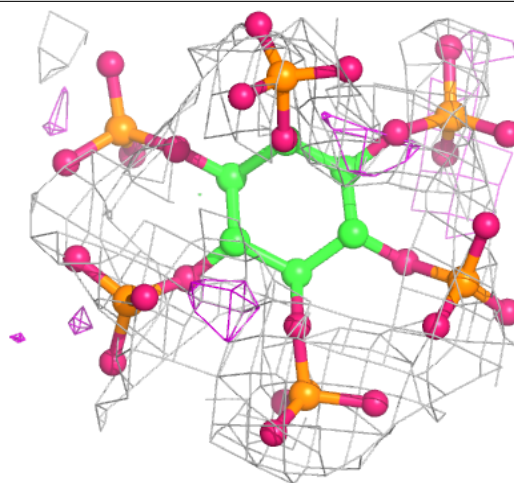
**Electron density around IHP K 302 (A):**

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)



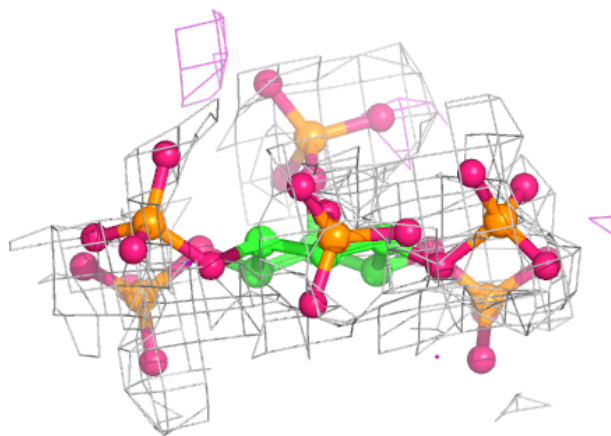
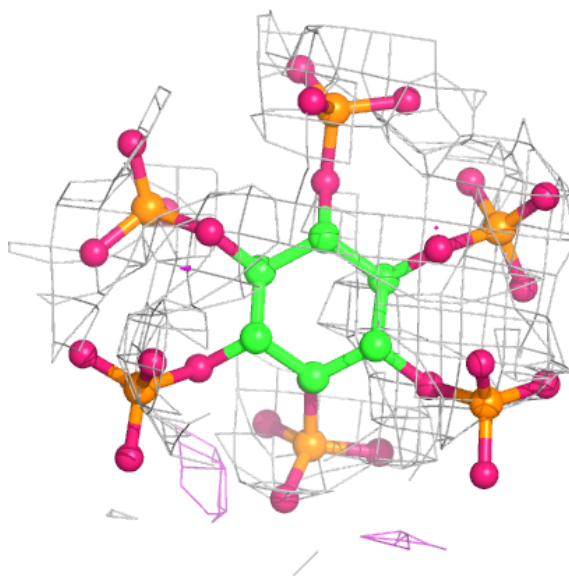
**Electron density around IHP K 302 (B):**

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



**Electron density around IHP D 301:**

$2mF_o-DF_c$  (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.