WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2020 – 12:57 PM EDT

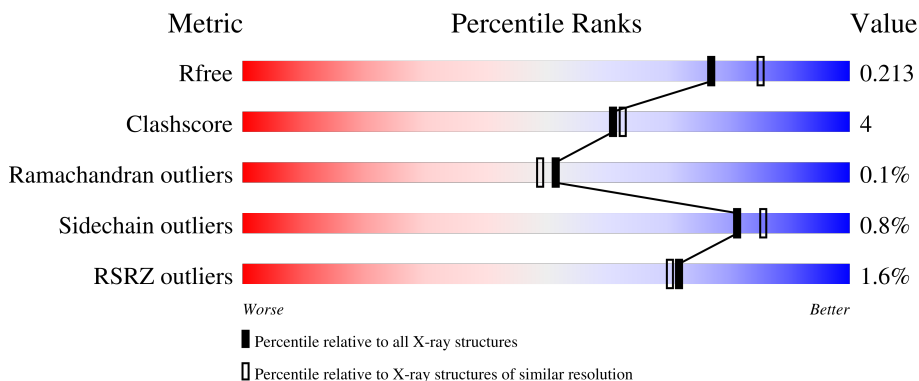|		
PDB ID	:	5KLP
Title	:	Crystal structure of HopZ1a in complex with IP6
Authors	:	Zhang, Z.-M.; Song, J.
Deposited on	:	2016-06-24
Resolution	:	2.00 Å(reported)

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 2.00 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	Percentile Ranks	Value
Rfree		0.213
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		0.8%
RSRZ outliers		1.6%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	342	% 80% 10% 10%
1	B	342	% 82% 8% · 9%
1	C	342	2% 86% 6% 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7880 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 Orf34.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	Se	0	0	0
			2356	1469	430	448	2	7			
1	B	310	Total	C	N	O	S	Se	0	0	0
			2379	1481	441	448	2	7			
1	C	315	Total	C	N	O	S	Se	0	0	0
			2424	1510	454	451	2	7			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	SER	-	expression tag	UNP Q6VE93
A	82	ALA	LYS	engineered mutation	UNP Q6VE93
A	83	ALA	LYS	engineered mutation	UNP Q6VE93
A	119	TYR	LYS	engineered mutation	UNP Q6VE93
A	120	TYR	GLU	engineered mutation	UNP Q6VE93
A	210	ALA	GLN	engineered mutation	UNP Q6VE93
A	211	ALA	LYS	engineered mutation	UNP Q6VE93
A	298	TYR	LYS	engineered mutation	UNP Q6VE93
A	299	TYR	GLN	engineered mutation	UNP Q6VE93
A	366	ALA	GLU	engineered mutation	UNP Q6VE93
A	367	ALA	GLU	engineered mutation	UNP Q6VE93
B	28	SER	-	expression tag	UNP Q6VE93
B	82	ALA	LYS	engineered mutation	UNP Q6VE93
B	83	ALA	LYS	engineered mutation	UNP Q6VE93
B	119	TYR	LYS	engineered mutation	UNP Q6VE93
B	120	TYR	GLU	engineered mutation	UNP Q6VE93
B	210	ALA	GLN	engineered mutation	UNP Q6VE93
B	211	ALA	LYS	engineered mutation	UNP Q6VE93
B	298	TYR	LYS	engineered mutation	UNP Q6VE93
B	299	TYR	GLN	engineered mutation	UNP Q6VE93
B	366	ALA	GLU	engineered mutation	UNP Q6VE93
B	367	ALA	GLU	engineered mutation	UNP Q6VE93
C	28	SER	-	expression tag	UNP Q6VE93

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Chain	Residue	Modelled	Actual	Comment	Reference
C	82	ALA	LYS	engineered mutation	UNP Q6VE93
C	83	ALA	LYS	engineered mutation	UNP Q6VE93
C	119	TYR	LYS	engineered mutation	UNP Q6VE93
C	120	TYR	GLU	engineered mutation	UNP Q6VE93
C	210	ALA	GLN	engineered mutation	UNP Q6VE93
C	211	ALA	LYS	engineered mutation	UNP Q6VE93
C	298	TYR	LYS	engineered mutation	UNP Q6VE93
C	299	TYR	GLN	engineered mutation	UNP Q6VE93
C	366	ALA	GLU	engineered mutation	UNP Q6VE93
C	367	ALA	GLU	engineered mutation	UNP Q6VE93

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).
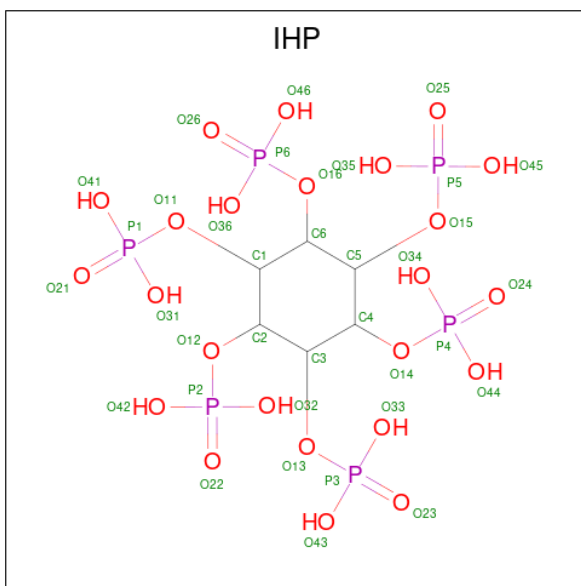
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 36	C 6	O 24	P 6	0	0
2	B	1	Total 36	C 6	O 24	P 6	0	0
2	C	1	Total 36	C 6	O 24	P 6	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0
3	A	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0
3	B	1	Total 13	C 6	O 7	0	0
3	C	1	Total 13	C 6	O 7	0	0
3	C	1	Total 13	C 6	O 7	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total 189	O 189	0	0
4	B	190	Total 190	O 190	0	0
4	C	156	Total 156	O 156	0	0

3 Residue-property plots ⓘ

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.
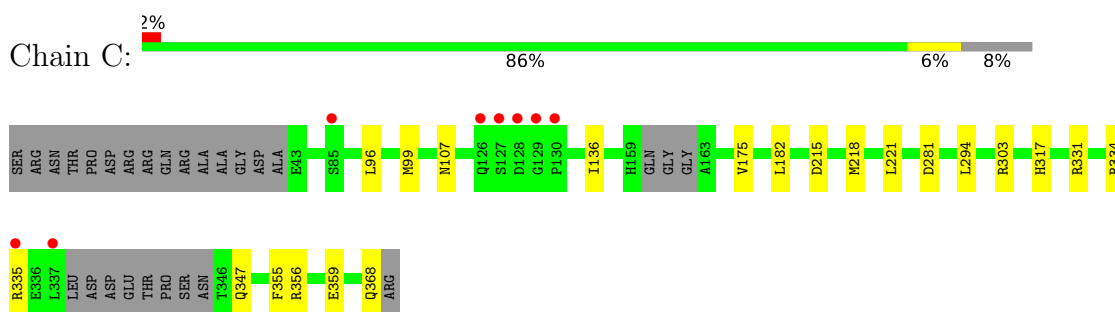
- Molecule 1: Orf34

Chain A:

- Molecule 1: Orf34

Chain B:

- Molecule 1: Orf34

Chain C:
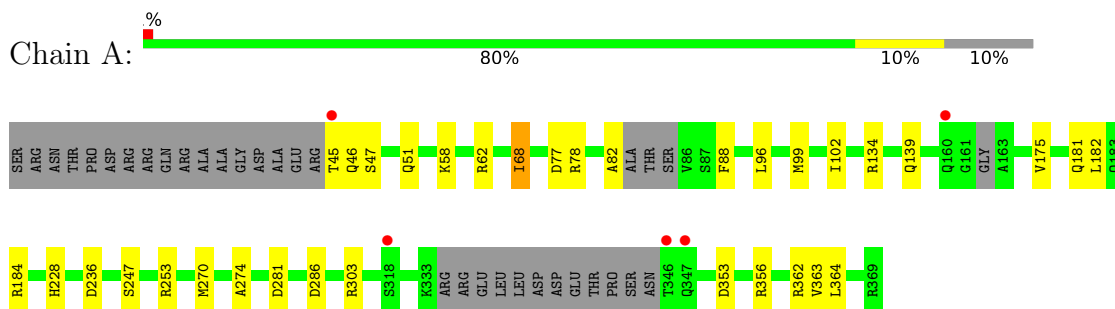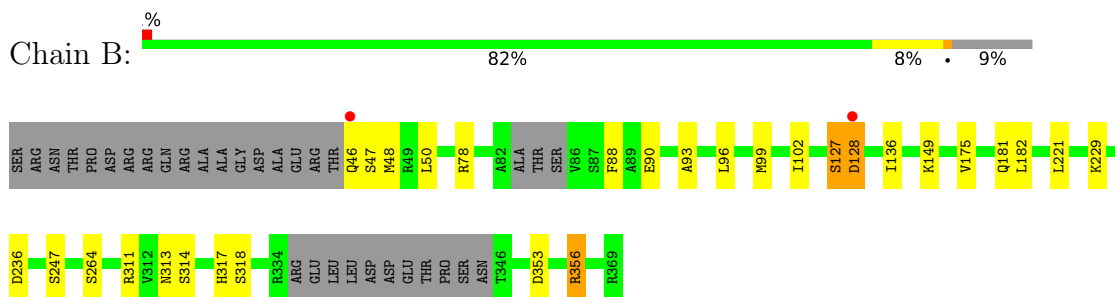
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.15Å 99.78Å 71.92Å 90.00° 103.44° 90.00°	Depositor
Resolution (Å)	49.89 – 2.00 49.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.89-2.00) 93.8 (49.89-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.168 , 0.214 0.170 , 0.213	Depositor DCC
R_{free} test set	2001 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7880	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CIT

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	0.36	0/2394	0.51	0/3231
1	B	0.36	0/2418	0.52	1/3260 (0.0%)
1	C	0.35	0/2463	0.52	0/3321
All	All	0.36	0/7275	0.52	1/9812 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	ARG	NE-CZ-NH2	-5.71	117.44	120.30

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	2356	0	2261	22	0
1	B	2379	0	2302	23	0
1	C	2424	0	2359	17	0
2	A	36	0	6	2	0
2	B	36	0	6	2	0
2	C	36	0	6	2	0
3	A	26	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	10	1	0
3	C	26	0	10	1	0
4	A	189	0	0	2	1
4	B	190	0	0	6	1
4	C	156	0	0	3	2
All	All	7880	0	6970	64	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 4.

The worst 5 of 64 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:218:MSE:HE2	1:C:356:ARG:HA	1.36	1.01
1:C:218:MSE:HE3	1:C:355:PHE:CD2	2.08	0.87
1:C:317:HIS:NE2	2:C:401:IHP:O33	2.06	0.87
1:B:317:HIS:NE2	2:B:401:IHP:O44	2.06	0.87
1:C:368:GLN:NE2	4:C:501:HOH:O	2.10	0.78

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)
4:A:669:HOH:O	4:C:640:HOH:O[2_444]	2.00	0.20
4:B:519:HOH:O	4:C:621:HOH:O[1_556]	2.02	0.18

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	301/342 (88%)	296 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	304/342 (89%)	298 (98%)	5 (2%)	1 (0%)	41	37
1	C	309/342 (90%)	304 (98%)	5 (2%)	0	100	100
All	All	914/1026 (89%)	898 (98%)	15 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	128	ASP

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	239/270 (88%)	237 (99%)	2 (1%)	81	86
1	B	242/270 (90%)	240 (99%)	2 (1%)	81	86
1	C	246/270 (91%)	244 (99%)	2 (1%)	81	86
All	All	727/810 (90%)	721 (99%)	6 (1%)	81	86

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	SER
1	C	335	ARG
1	B	264	SER
1	A	286	ASP
1	C	107	ASN

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\#|Z| > 2$
3	CIT	C	403	-	3,12,12	1.15	0	3,17,17	3.96	2 (66%)
3	CIT	B	403	-	3,12,12	1.24	0	3,17,17	1.94	1 (33%)
3	CIT	A	403	-	3,12,12	1.20	0	3,17,17	2.19	2 (66%)
3	CIT	B	402	-	3,12,12	1.45	0	3,17,17	0.84	0
2	IHP	C	401	-	36,36,36	2.72	13 (36%)	54,60,60	1.74	14 (25%)
2	IHP	B	401	-	36,36,36	2.85	15 (41%)	54,60,60	2.35	17 (31%)
2	IHP	A	401	-	36,36,36	2.58	14 (38%)	54,60,60	1.64	9 (16%)
3	CIT	C	402	-	3,12,12	1.17	0	3,17,17	0.45	0
3	CIT	A	402	-	3,12,12	1.26	0	3,17,17	2.13	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	C	403	-	-	4/6/16/16	-
3	CIT	B	403	-	-	6/6/16/16	-
3	CIT	A	403	-	-	5/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	B	402	-	-	3/6/16/16	-
2	IHP	C	401	-	-	4/30/54/54	0/1/1/1
2	IHP	B	401	-	-	4/30/54/54	0/1/1/1
2	IHP	A	401	-	-	6/30/54/54	0/1/1/1
3	CIT	C	402	-	-	0/6/16/16	-
3	CIT	A	402	-	-	3/6/16/16	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	IHP	P3-O13	8.28	1.74	1.59
2	C	401	IHP	P2-O12	7.96	1.74	1.59
2	C	401	IHP	P4-O14	7.26	1.73	1.59
2	A	401	IHP	P5-O15	6.20	1.71	1.59
2	B	401	IHP	P5-O15	6.11	1.70	1.59

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	403	CIT	C3-C4-C5	-5.65	105.93	114.98
2	A	401	IHP	C3-C2-C1	5.64	122.77	110.41
2	C	401	IHP	C5-C6-C1	5.44	122.32	110.41
2	B	401	IHP	O13-C3-C2	5.42	121.46	108.69
2	B	401	IHP	O16-C6-C1	5.15	120.82	108.69

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	CIT	C1-C2-C3-O7
3	C	403	CIT	C1-C2-C3-C4
3	C	403	CIT	C1-C2-C3-C6
3	B	403	CIT	C1-C2-C3-O7
3	B	403	CIT	C1-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 9 short contacts:

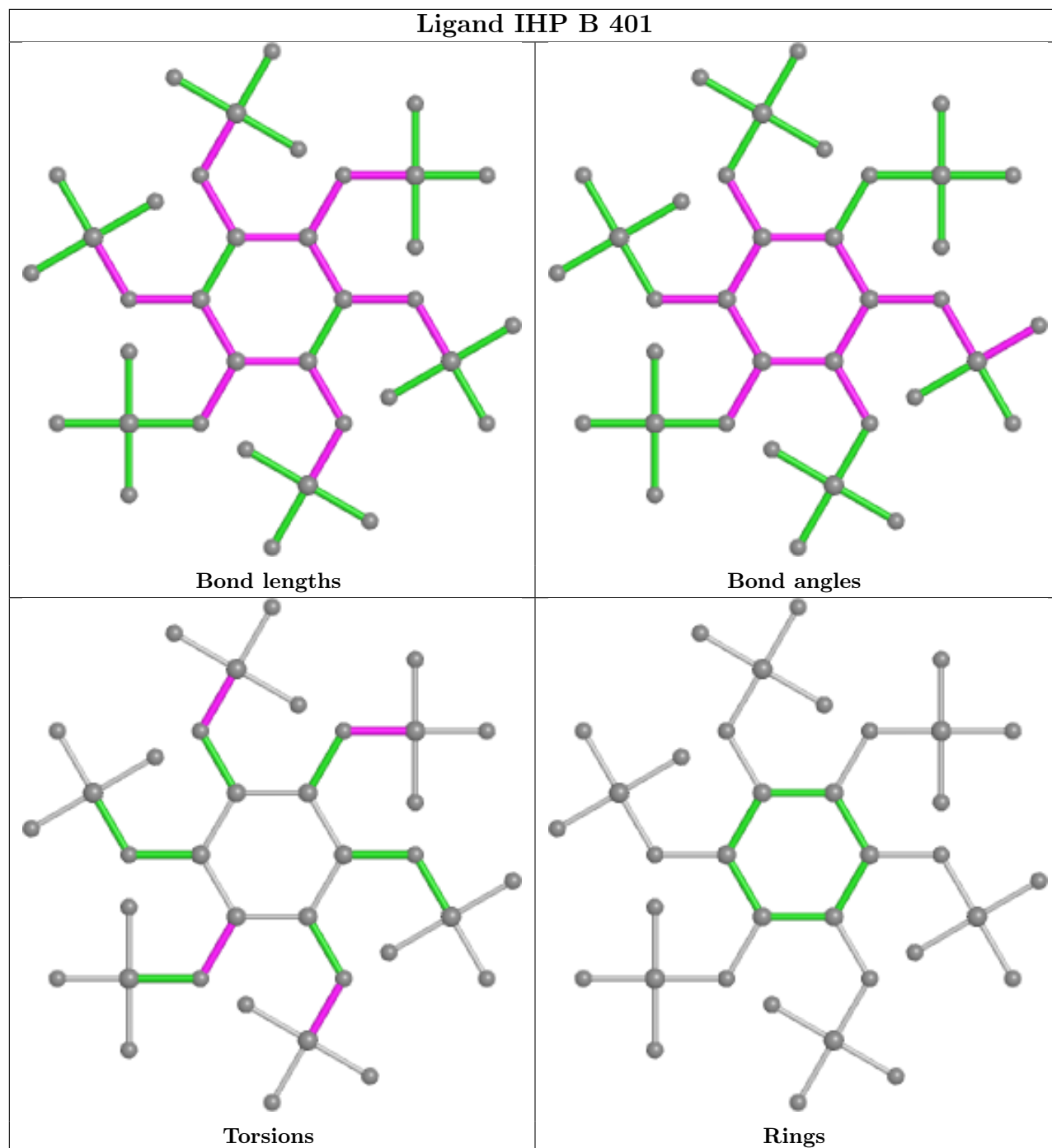| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	CIT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	CIT	1	0
2	C	401	IHP	2	0
2	B	401	IHP	2	0
2	A	401	IHP	2	0
3	A	402	CIT	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 then 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 C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand IHP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand IHP A 401

Bond lengths

Bond angles

Torsions

Rings
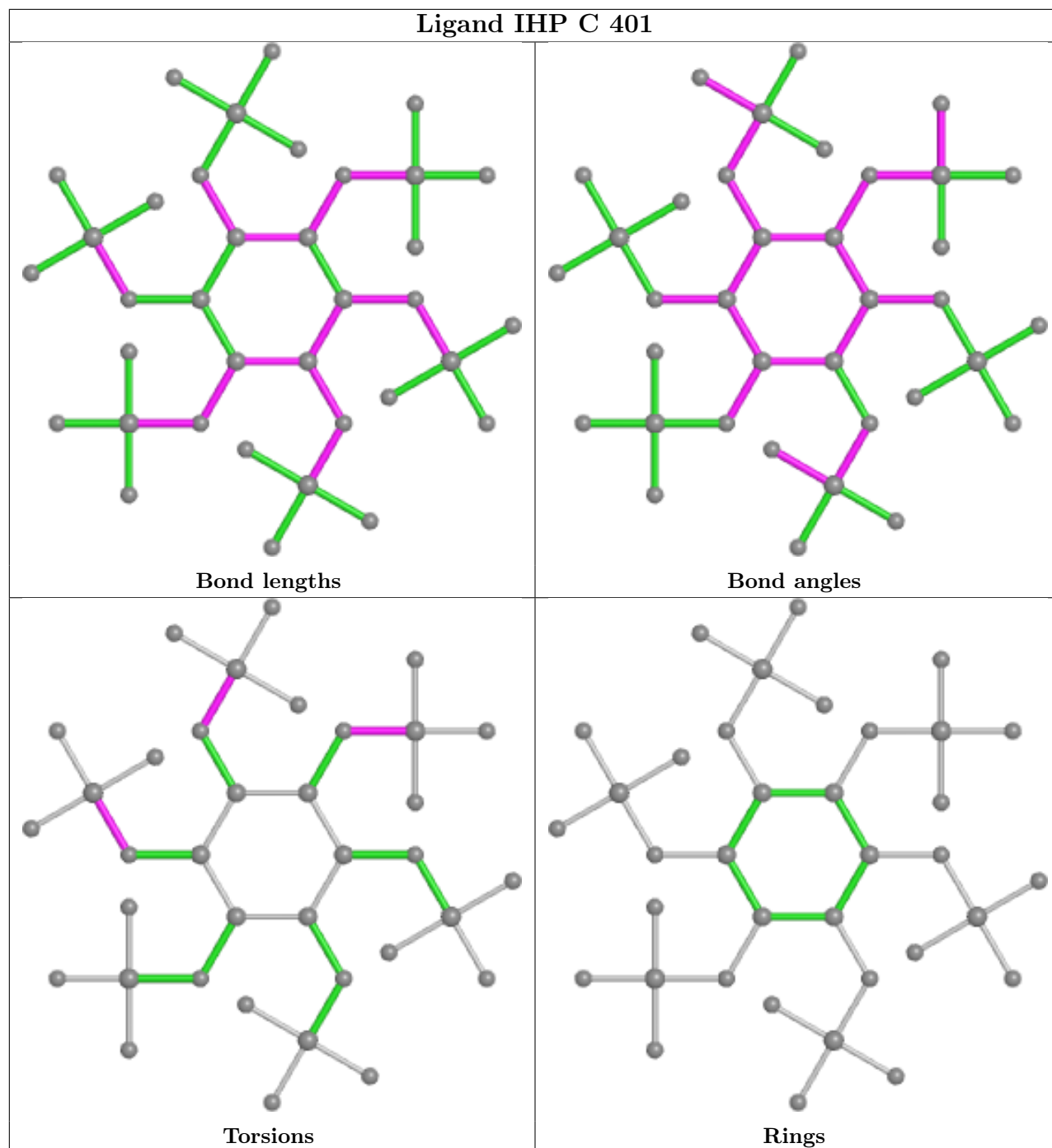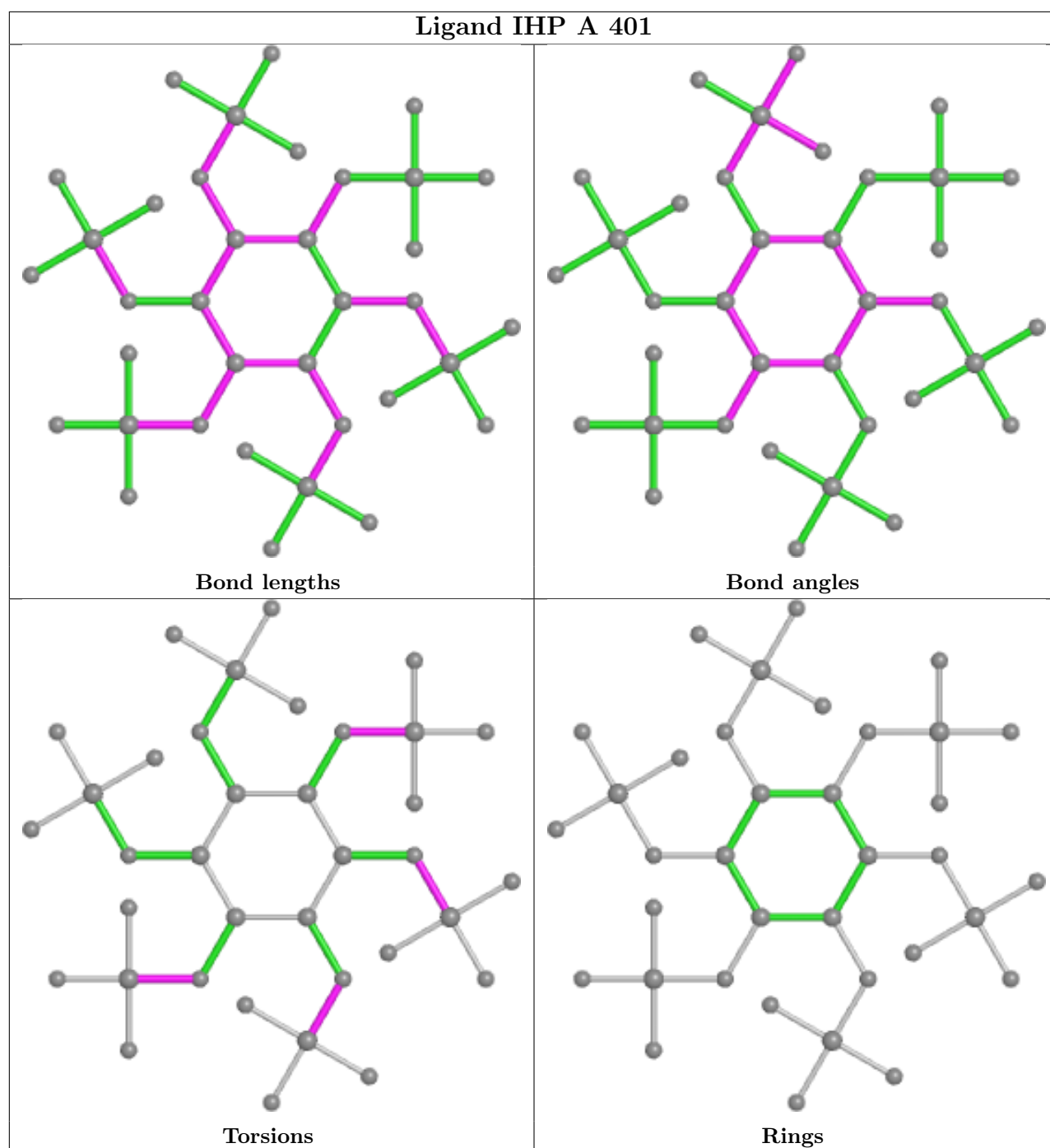
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	302/342 (88%)	-0.43	5 (1%)	70	68	15, 27, 58, 77	0
1	B	303/342 (88%)	-0.55	2 (0%)	87	87	14, 25, 53, 87	0
1	C	308/342 (90%)	-0.35	8 (2%)	56	54	17, 30, 60, 80	0
All	All	913/1026 (88%)	-0.44	15 (1%)	72	70	14, 27, 60, 87	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	THR	6.4
1	C	129	GLY	4.2
1	A	346	THR	3.6
1	C	337	LEU	3.1
1	C	128	ASP	2.9

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

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

6.3 Carbohydrates ⓘ

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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CIT	C	403	13/13	0.76	0.36	46,78,90,93	0
3	CIT	B	403	13/13	0.84	0.18	36,58,79,80	0
3	CIT	A	403	13/13	0.87	0.15	25,57,68,72	0
3	CIT	C	402	13/13	0.88	0.14	39,51,55,60	0
3	CIT	B	402	13/13	0.90	0.19	23,64,77,80	0
3	CIT	A	402	13/13	0.92	0.11	28,46,49,50	0
2	IHP	C	401	36/36	0.95	0.11	18,30,54,56	0
2	IHP	B	401	36/36	0.96	0.11	16,25,49,56	0
2	IHP	A	401	36/36	0.97	0.10	18,32,48,55	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.
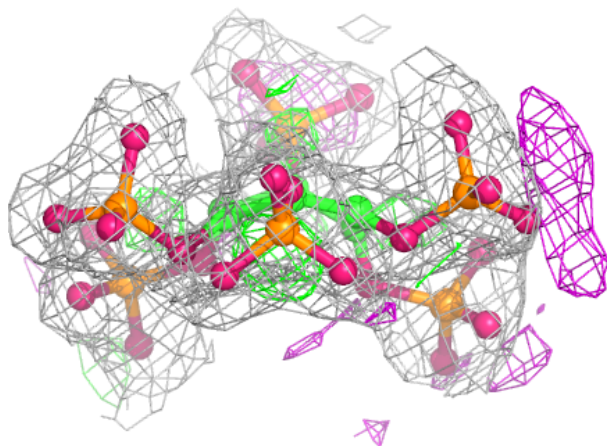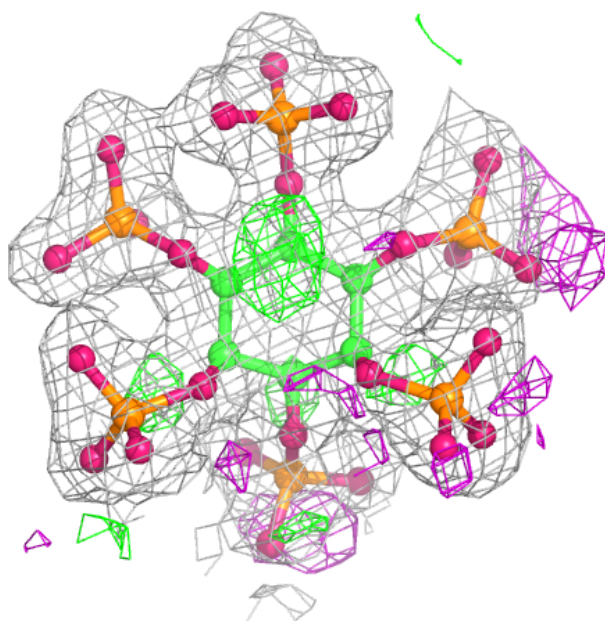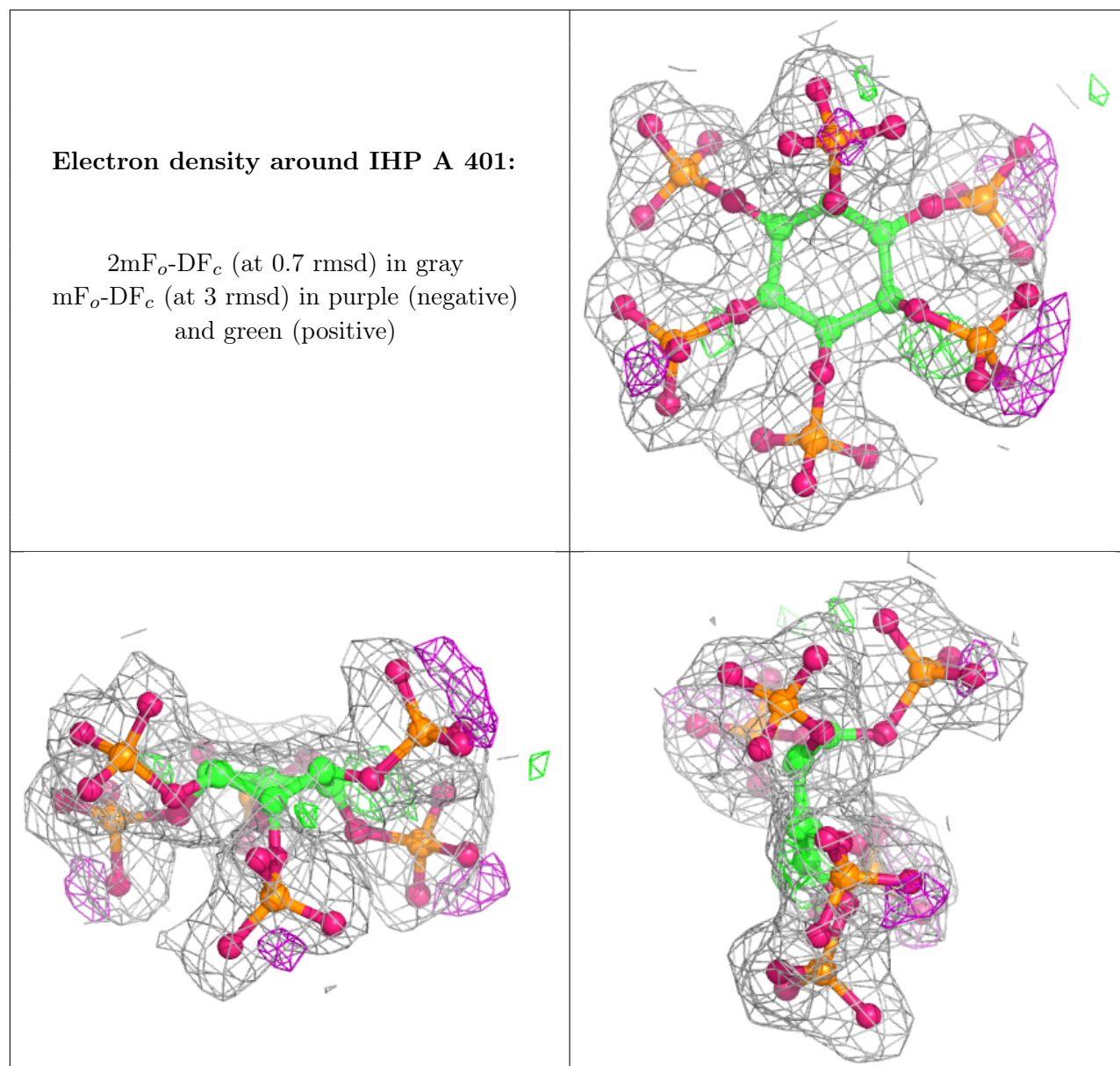
Electron density around IHP C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
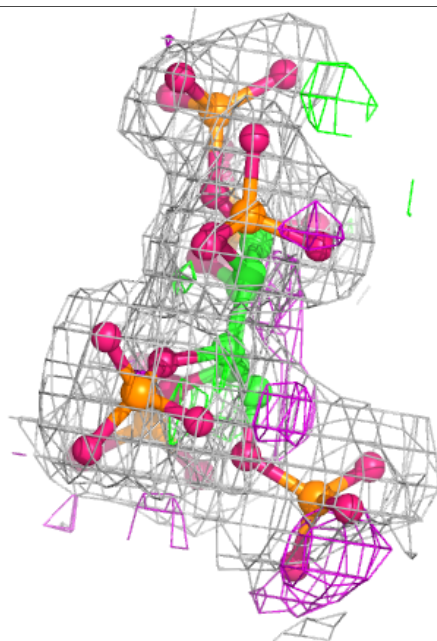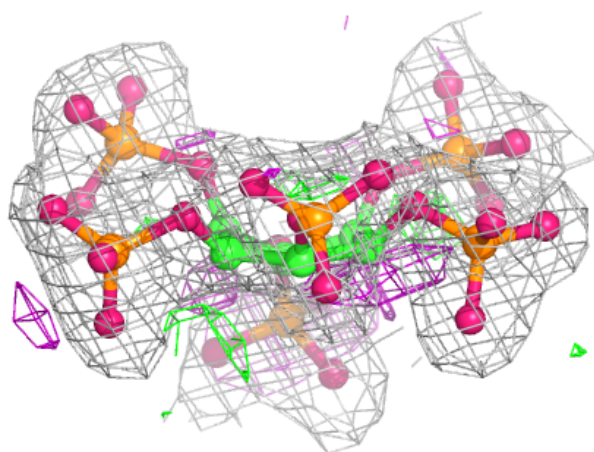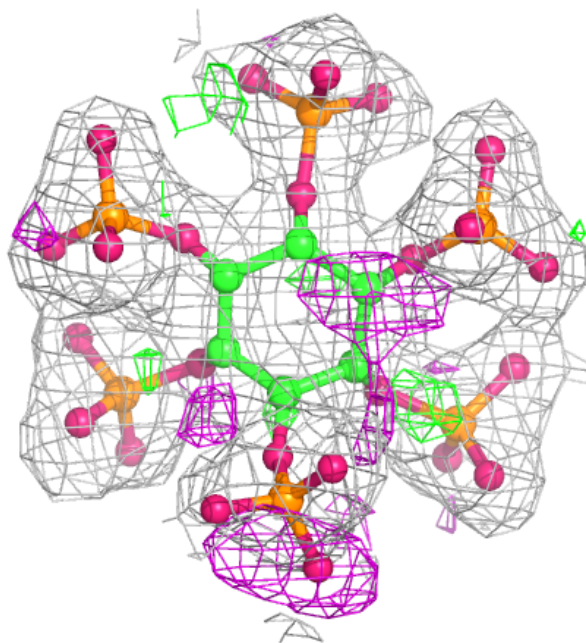
Electron density around IHP B 401:

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

Electron density around IHP A 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.