



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 12:37 PM EDT

PDB ID : 1ZY7  
Title : Crystal structure of the catalytic domain of an adenosine deaminase that acts on RNA (hADAR2) bound to inositol hexakisphosphate (IHP)  
Authors : Macbeth, M.R.; Schubert, H.L.; Vandemark, A.P.; Lingam, A.T.; Hill, C.P.; Bass, B.L.  
Deposited on : 2005-06-09  
Resolution : 1.70 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.

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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

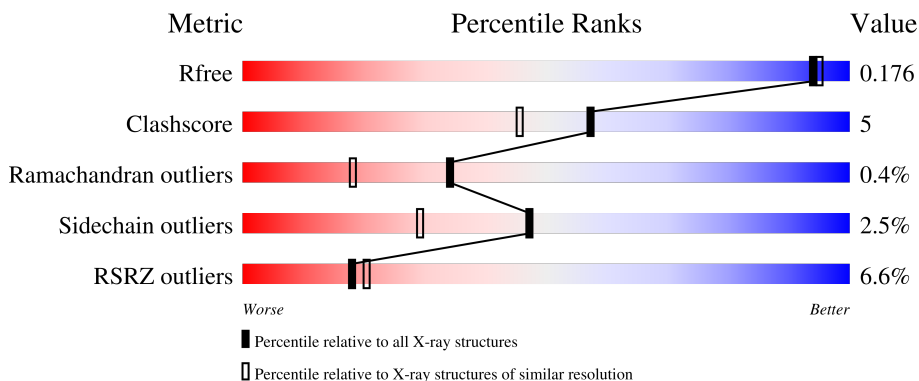
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	403	
1	B	403	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6551 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.

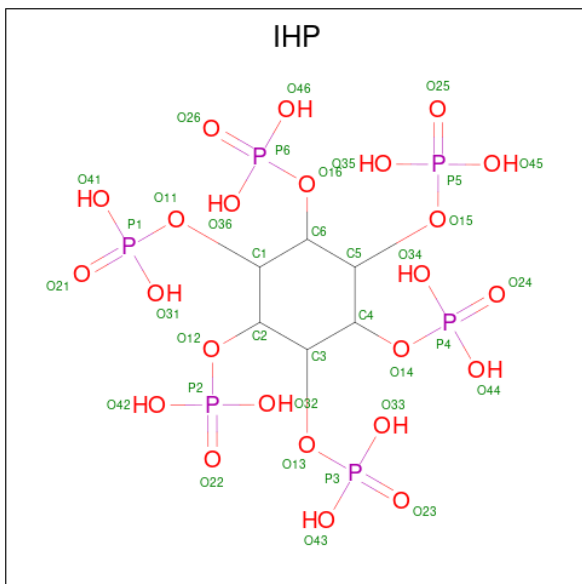
- Molecule 1 is a protein called RNA-specific adenosine deaminase B1, isoform DRADA2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	Total 2962	C 1869	N 536	O 545	S 12	0	1	0
1	B	362	Total 2841	C 1796	N 514	O 519	S 12	0	1	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

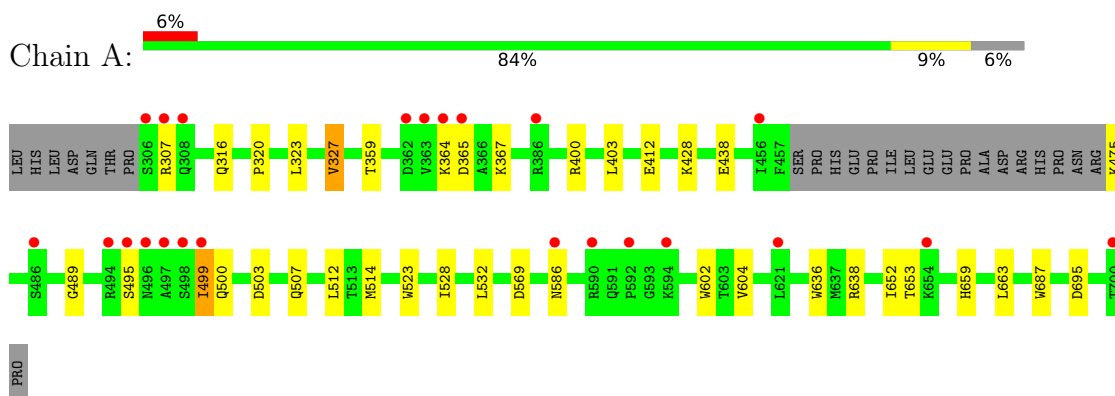
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	383	Total	O	0	0
			383	383		
5	B	286	Total	O	0	0
			286	286		

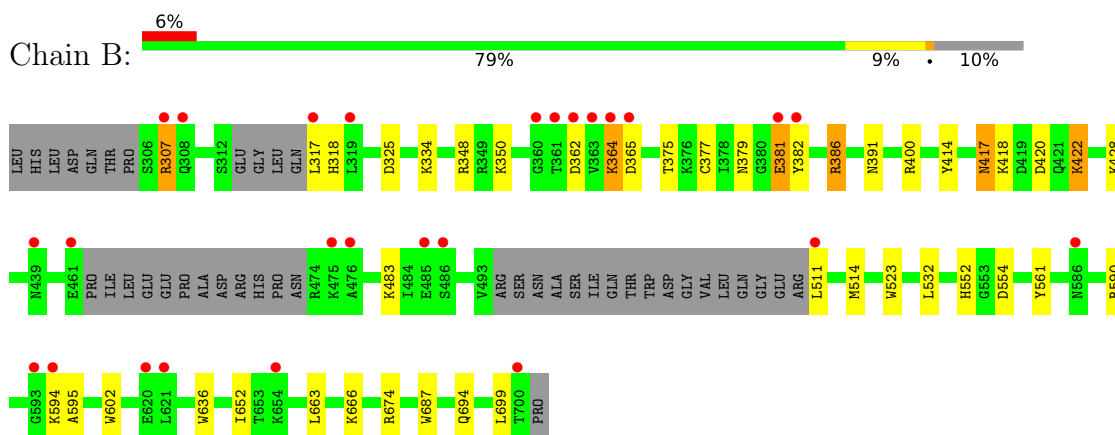
### 3 Residue-property plots

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: RNA-specific adenosine deaminase B1, isoform DRADA2a



- Molecule 1: RNA-specific adenosine deaminase B1, isoform DRADA2a



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.20Å 121.19Å 127.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.3 (20.00-1.70) 92.3 (19.95-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.173 , 0.206 0.172 , 0.176	Depositor DCC
$R_{free}$ test set	4152 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtrriage
Anisotropy	0.226	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6551	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: ZN, IHP, SO4

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	0.69	0/3024	0.76	3/4083 (0.1%)
1	B	0.68	0/2901	0.80	5/3914 (0.1%)
All	All	0.68	0/5925	0.78	8/7997 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	590	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	B	590	ARG	NE-CZ-NH1	11.71	126.15	120.30
1	B	325	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	381	GLU	CB-CA-C	5.30	120.99	110.40
1	A	569	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	365	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	503	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	695	ASP	CB-CG-OD2	5.11	122.90	118.30

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	2962	0	3004	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2841	0	2885	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	36	0	6	1	0
3	B	36	0	6	1	0
4	B	5	0	0	1	0
5	A	383	0	0	8	0
5	B	286	0	0	8	0
All	All	6551	0	5901	58	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 5.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:OE2	1:A:638:ARG:HD2	1.73	0.88
1:A:586:ASN:HB2	5:A:1273:HOH:O	1.74	0.85
1:A:500:GLN:HE22	1:A:512:LEU:H	1.23	0.85
1:A:653:THR:HG22	5:A:1194:HOH:O	1.88	0.72
1:B:318:HIS:HD2	5:B:1188:HOH:O	1.77	0.68
1:A:438:GLU:CD	1:A:438:GLU:H	1.98	0.66
1:B:417:ASN:ND2	1:B:420:ASP:H	1.94	0.65
1:A:507:GLN:HG3	5:A:1225:HOH:O	1.97	0.64
1:B:595:ALA:HB1	5:B:1167:HOH:O	2.01	0.60
1:B:552:HIS:HD2	1:B:554:ASP:H	1.49	0.60
1:B:362:ASP:OD1	1:B:364:LYS:HG3	2.02	0.59
1:B:674:ARG:NH2	5:B:1003:HOH:O	2.34	0.59
3:B:902:IHP:O33	3:B:902:IHP:O34	2.21	0.58
1:A:403:LEU:HD21	1:A:528:ILE:HD12	1.86	0.58
1:B:377[B]:CYS:SG	1:B:483:LYS:HD3	2.44	0.58
1:B:350:LYS:HD2	1:B:595:ALA:HB2	1.85	0.57
1:A:500:GLN:NE2	1:A:512:LEU:H	2.00	0.57
1:B:307:ARG:H	1:B:307:ARG:NE	2.03	0.55
1:A:514:MET:HG3	1:A:687:TRP:CE2	2.42	0.55
1:A:403:LEU:CD2	1:A:528:ILE:HD12	2.36	0.54
1:A:475:LYS:N	5:A:1184:HOH:O	2.41	0.53
1:B:391:ASN:HD21	1:B:694:GLN:NE2	2.06	0.53
1:A:367:LYS:HE3	1:A:604:VAL:HG21	1.90	0.52
1:A:400:ARG:HD3	1:A:523:TRP:CE2	2.45	0.50
1:B:400:ARG:HD3	1:B:523:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:IHP:O33	3:A:901:IHP:O34	2.29	0.50
1:B:375:THR:HG22	5:B:1167:HOH:O	2.12	0.50
1:B:379:ASN:HB3	1:B:382:TYR:HD2	1.76	0.50
1:B:552:HIS:CD2	1:B:554:ASP:H	2.27	0.49
1:A:532:LEU:HB3	1:A:636:TRP:CD1	2.47	0.49
1:A:323:LEU:O	1:A:327:VAL:HG13	2.13	0.48
1:B:552:HIS:HD2	1:B:554:ASP:N	2.12	0.47
1:B:422:LYS:HE2	1:B:422:LYS:HA	1.96	0.47
1:A:489:GLY:HA2	5:A:1074:HOH:O	2.15	0.46
1:B:532:LEU:HB3	1:B:636:TRP:CD1	2.50	0.46
1:B:418:LYS:HE3	1:B:418:LYS:HB3	1.75	0.46
1:B:414:TYR:OH	1:B:428:LYS:HG3	2.16	0.46
1:B:674:ARG:HD3	5:B:998:HOH:O	2.16	0.46
1:B:511:LEU:N	5:B:1139:HOH:O	2.48	0.45
1:B:386:ARG:HG2	4:B:903:SO4:O2	2.16	0.45
1:B:514:MET:HG3	1:B:687:TRP:CE2	2.52	0.45
1:A:316:GLN:NE2	1:A:320:PRO:HG3	2.31	0.45
1:B:391:ASN:HD21	1:B:694:GLN:HE22	1.65	0.45
1:B:663:LEU:O	1:B:666:LYS:HD3	2.17	0.45
1:B:417:ASN:C	1:B:417:ASN:HD22	2.21	0.44
1:B:674:ARG:CZ	5:B:1003:HOH:O	2.66	0.44
1:A:499:ILE:O	1:A:499:ILE:HG23	2.18	0.44
1:A:359:THR:HG23	5:A:1151:HOH:O	2.19	0.43
1:A:507:GLN:HB2	5:A:1098:HOH:O	2.19	0.43
1:A:659:HIS:CE1	1:A:663:LEU:HD11	2.54	0.43
1:B:334:LYS:HE2	1:B:602:TRP:CZ2	2.54	0.43
1:A:499:ILE:C	1:A:499:ILE:HD13	2.39	0.42
1:A:507:GLN:O	1:A:507:GLN:CG	2.68	0.42
1:B:317:LEU:HD13	5:B:1149:HOH:O	2.20	0.41
1:A:507:GLN:HB3	5:A:1213:HOH:O	2.20	0.41
1:B:307:ARG:HE	1:B:307:ARG:H	1.66	0.41
1:A:499:ILE:HD13	1:A:500:GLN:O	2.22	0.40
1:A:602:TRP:CZ2	1:A:604:VAL:HA	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	375/403 (93%)	369 (98%)	5 (1%)	1 (0%)	41	24
1	B	355/403 (88%)	345 (97%)	8 (2%)	2 (1%)	25	11
All	All	730/806 (91%)	714 (98%)	13 (2%)	3 (0%)	34	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	561	TYR
1	B	652	ILE
1	A	652	ILE

### 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	324/347 (93%)	317 (98%)	7 (2%)	52	34
1	B	312/347 (90%)	303 (97%)	9 (3%)	42	23
All	All	636/694 (92%)	620 (98%)	16 (2%)	47	29

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	ARG
1	A	327	VAL
1	A	364	LYS

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Mol	Chain	Res	Type
1	A	365	ASP
1	A	428	LYS
1	A	495	SER
1	A	499	ILE
1	B	307	ARG
1	B	348	ARG
1	B	364	LYS
1	B	381	GLU
1	B	386	ARG
1	B	417	ASN
1	B	422	LYS
1	B	594	LYS
1	B	699	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	479	GLN
1	A	500	GLN
1	A	507	GLN
1	A	659	HIS
1	A	696	GLN
1	B	308	GLN
1	B	318	HIS
1	B	321	GLN
1	B	341	ASN
1	B	417	ASN
1	B	421	GLN
1	B	552	HIS
1	B	597	ASN
1	B	694	GLN

### 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 [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
4	SO4	B	903	-	4,4,4	0.17	0	6,6,6	0.30	0
3	IHP	B	902	-	36,36,36	1.15	4 (11%)	54,60,60	0.88	3 (5%)
3	IHP	A	901	-	36,36,36	0.99	2 (5%)	54,60,60	1.03	2 (3%)

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	IHP	B	902	-	-	3/30/54/54	0/1/1/1
3	IHP	A	901	-	-	3/30/54/54	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	IHP	P6-O16	2.92	1.64	1.59
3	A	901	IHP	P5-O15	2.40	1.63	1.59
3	A	901	IHP	P1-O11	2.35	1.63	1.59
3	B	902	IHP	P2-O12	2.20	1.63	1.59
3	B	902	IHP	P4-O14	2.13	1.63	1.59
3	B	902	IHP	P1-O11	2.08	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	IHP	O41-P1-O31	3.18	119.77	107.64
3	A	901	IHP	O11-P1-O21	-2.57	99.47	109.39
3	B	902	IHP	O43-P3-O23	2.22	119.38	110.68
3	B	902	IHP	O11-P1-O21	-2.15	101.11	109.39
3	B	902	IHP	O41-P1-O31	2.03	115.41	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

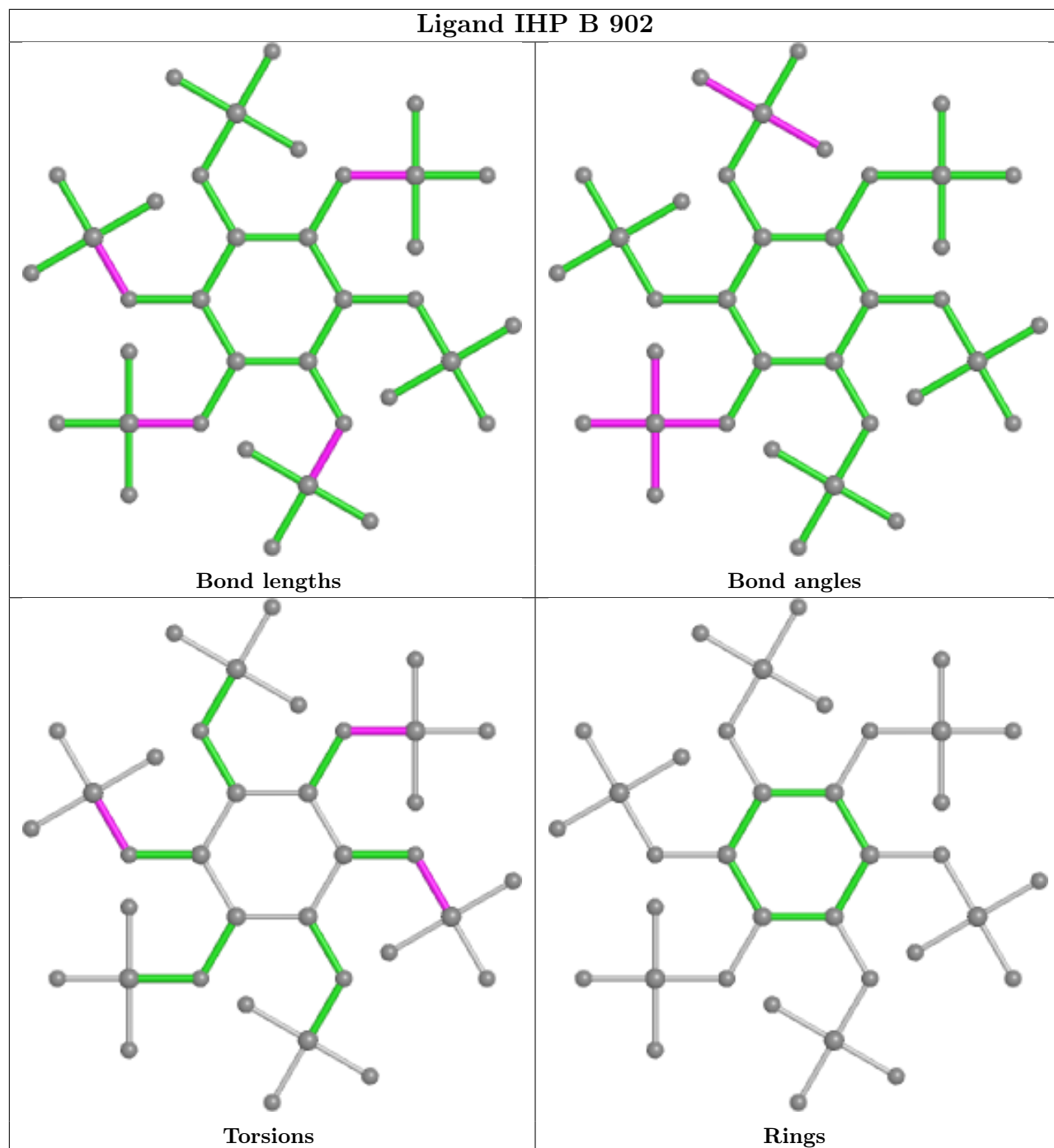
Mol	Chain	Res	Type	Atoms
3	B	902	IHP	C2-O12-P2-O42
3	A	901	IHP	C3-O13-P3-O23
3	B	902	IHP	C4-O14-P4-O44
3	B	902	IHP	C5-O15-P5-O35
3	A	901	IHP	C4-O14-P4-O44
3	A	901	IHP	C5-O15-P5-O35

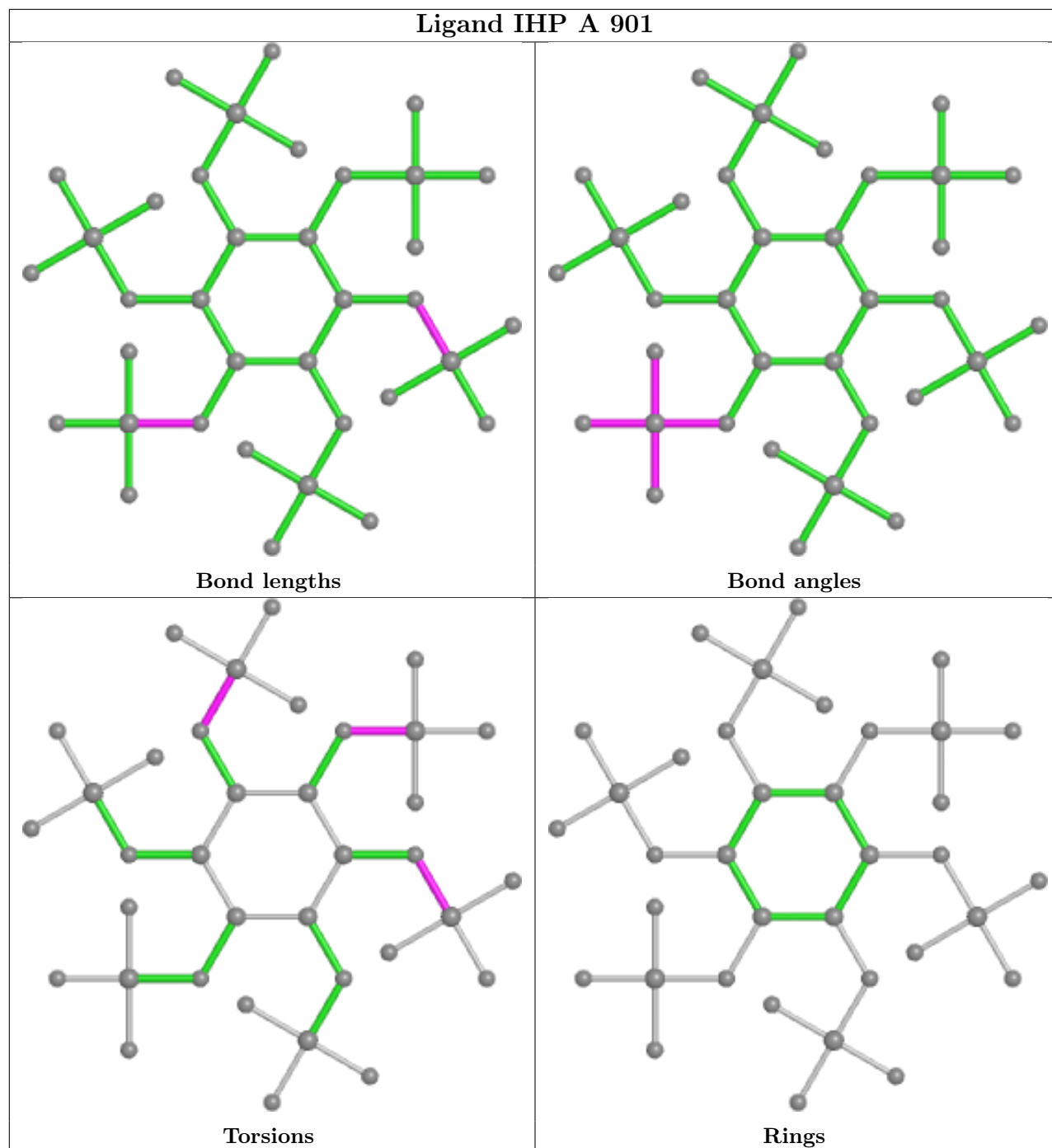
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	SO4	1	0
3	B	902	IHP	1	0
3	A	901	IHP	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	378/403 (93%)	0.08	23 (6%) 21 23	10, 16, 31, 39	0
1	B	362/403 (89%)	0.14	26 (7%) 15 17	11, 17, 32, 45	0
All	All	740/806 (91%)	0.11	49 (6%) 18 20	10, 17, 32, 45	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	700	THR	7.2
1	B	361	THR	6.9
1	B	700	THR	5.0
1	B	476	ALA	4.7
1	B	621	LEU	4.7
1	A	307	ARG	4.2
1	A	496	ASN	4.2
1	A	495	SER	4.1
1	B	360	GLY	4.1
1	B	381	GLU	4.1
1	B	461	GLU	4.0
1	B	363	VAL	3.8
1	A	497	ALA	3.7
1	B	317	LEU	3.7
1	B	364	LYS	3.6
1	A	592	PRO	3.6
1	B	486	SER	3.5
1	A	499	ILE	3.5
1	B	620	GLU	3.4
1	B	307	ARG	3.2
1	B	475	LYS	3.2
1	B	382	TYR	3.1
1	A	590	ARG	3.1
1	A	486	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	308	GLN	3.0
1	B	511	LEU	3.0
1	B	593	GLY	2.9
1	A	654	LYS	2.8
1	B	654	LYS	2.8
1	A	365	ASP	2.7
1	A	494	ARG	2.6
1	B	365	ASP	2.6
1	B	439	ASN	2.6
1	A	386	ARG	2.5
1	A	362	ASP	2.5
1	B	594	LYS	2.4
1	A	364	LYS	2.4
1	B	308	GLN	2.4
1	A	586	ASN	2.4
1	B	586	ASN	2.3
1	A	456	ILE	2.3
1	A	498	SER	2.2
1	A	594	LYS	2.2
1	A	621	LEU	2.2
1	A	306	SER	2.1
1	A	363	VAL	2.1
1	B	362	ASP	2.1
1	B	319	LEU	2.0
1	B	485	GLU	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](#)

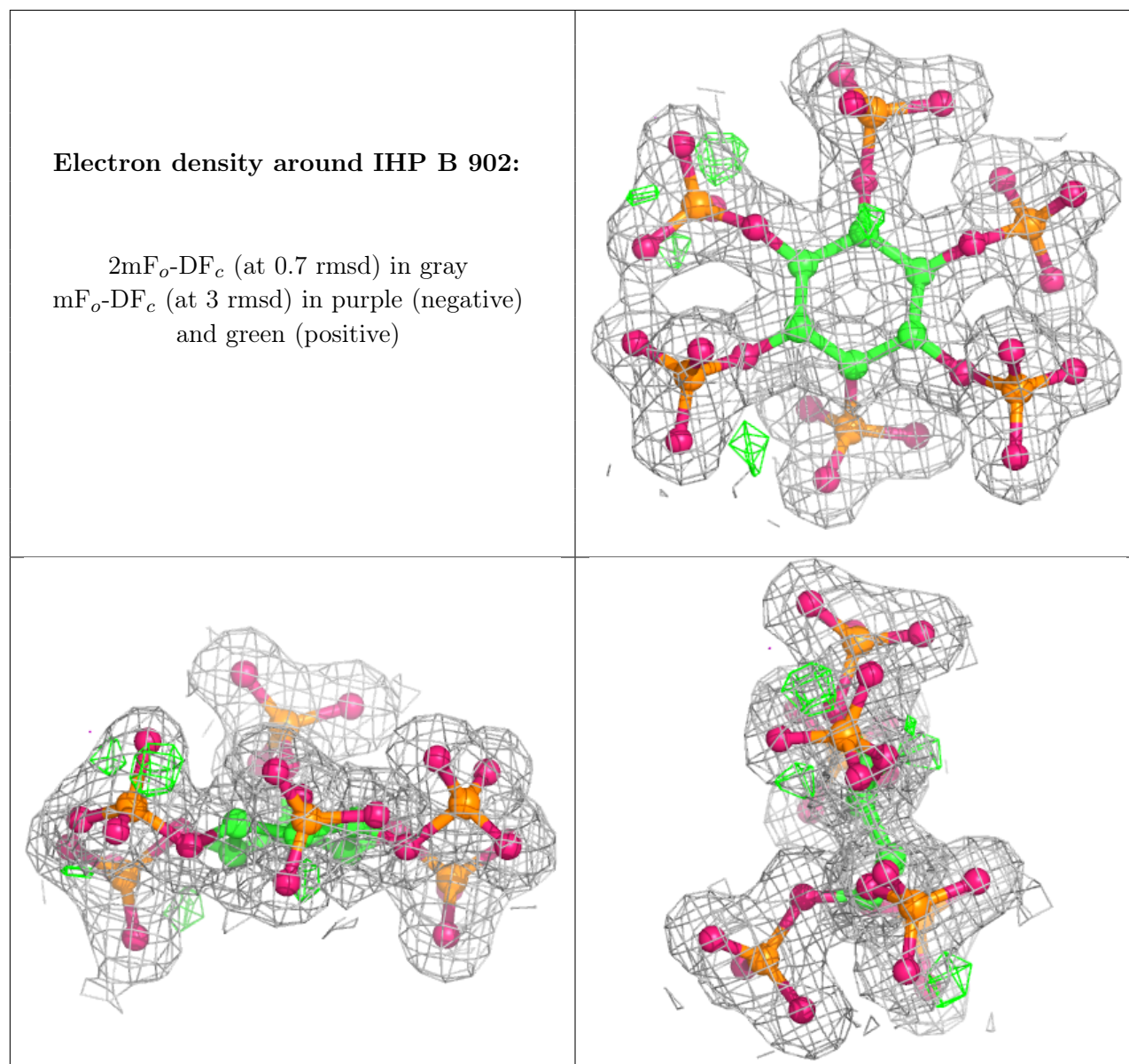
There are no monosaccharides in this entry.

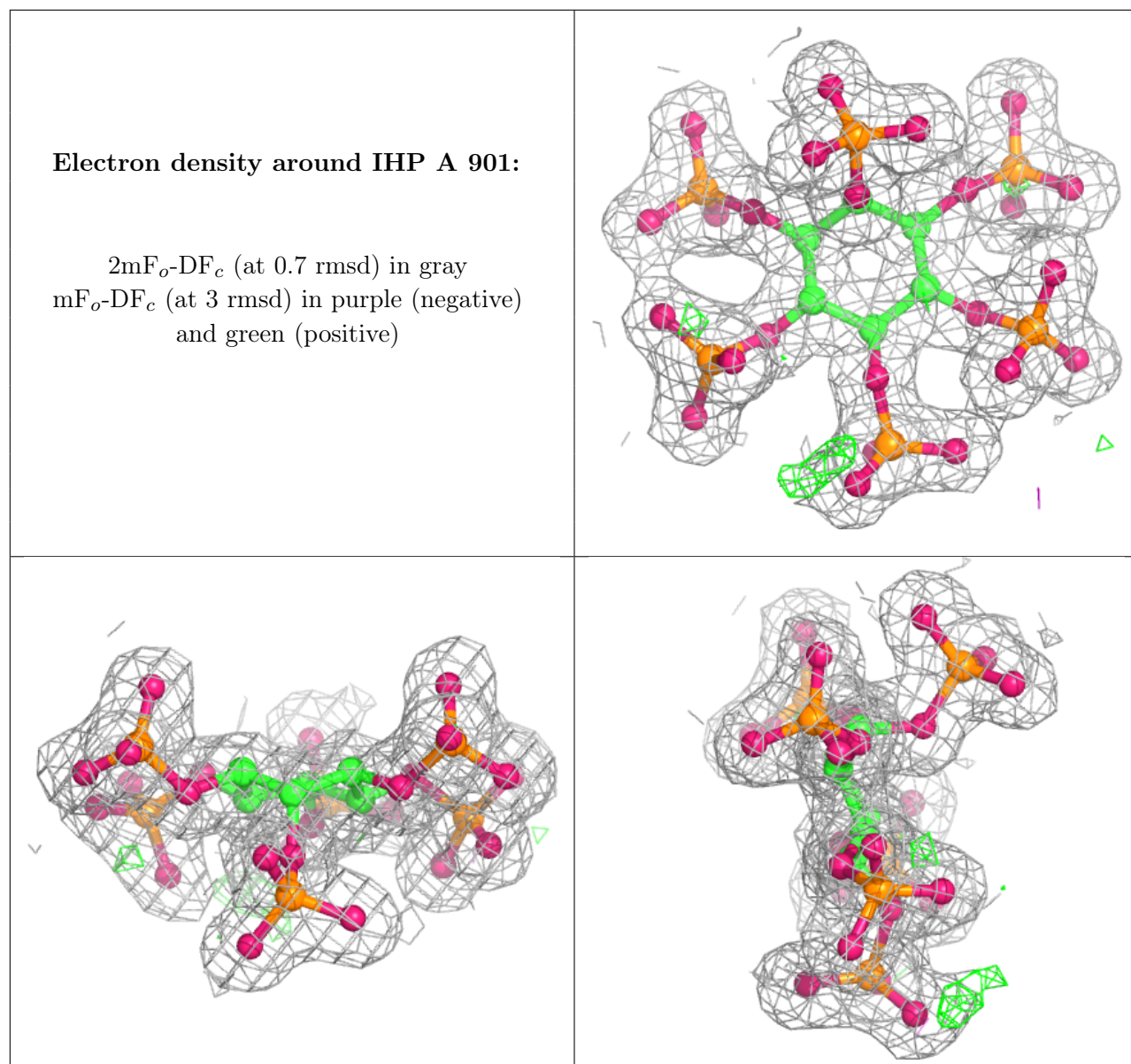
## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	903	5/5	0.98	0.24	37,38,39,42	0
3	IHP	B	902	36/36	0.98	0.07	11,14,20,24	0
3	IHP	A	901	36/36	0.99	0.06	9,13,18,23	0
2	ZN	B	802	1/1	1.00	0.04	15,15,15,15	0
2	ZN	A	801	1/1	1.00	0.05	14,14,14,14	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.