



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2019 – 01:30 PM EST

PDB ID : 6D06  
Title : Human ADAR2d E488Y mutant complexed with dsRNA containing an abasic site opposite the edited base  
Authors : Matthews, M.M.; Fisher, A.J.; Beal, P.A.  
Deposited on : 2018-04-10  
Resolution : 2.55 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

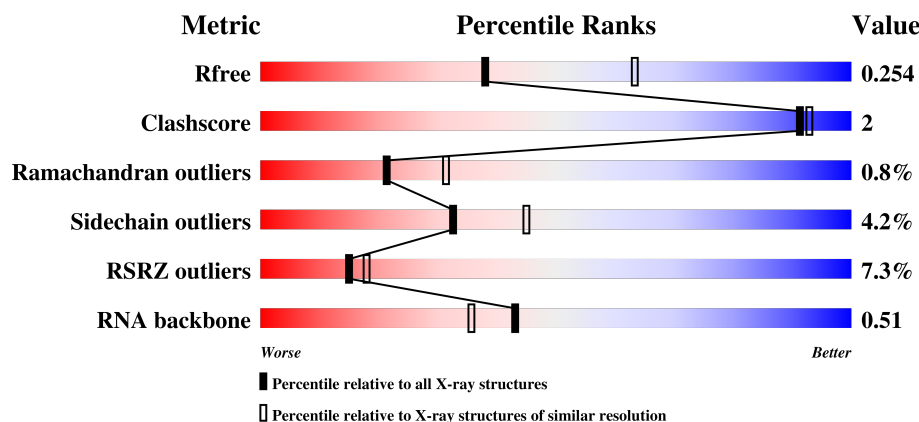
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	111664	1053 (2.56-2.52)
Clashscore	122126	1098 (2.56-2.52)
Ramachandran outliers	120053	1088 (2.56-2.52)
Sidechain outliers	120020	1088 (2.56-2.52)
RSRZ outliers	108989	1043 (2.56-2.52)
RNA backbone	2636	1015 (2.90-2.18)

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. 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	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	D	403	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>13%</div> </div> </div>
2	B	23	<div> <div></div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
3	C	23	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6877 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 Double-stranded RNA-specific editase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	4	0
			3034	1916	549	558	11			
1	D	352	Total	C	N	O	S	0	0	0
			2754	1746	494	503	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	TYR	GLU	engineered mutation	UNP P78563
D	488	TYR	GLU	engineered mutation	UNP P78563

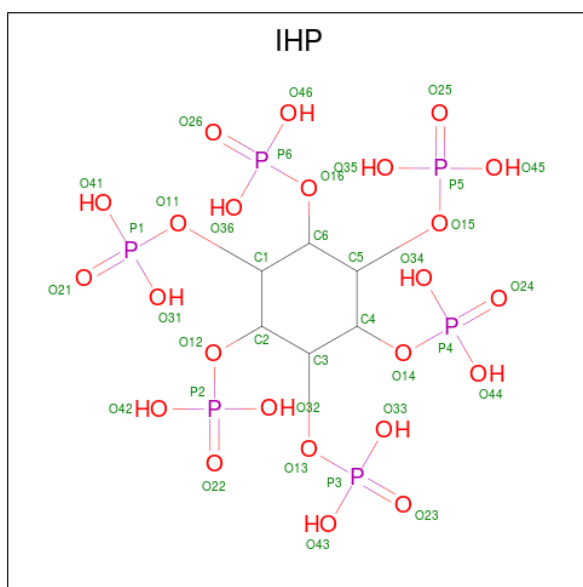
- Molecule 2 is a RNA chain called RNA (5'-R(\*GP\*CP\*UP\*CP\*GP\*CP\*GP\*AP\*UP\*GP\*CP\*UP\*(8AZ)P\*GP\*AP\*GP\*GP\*GP\*CP\*UP\*CP\*UP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	P	0	0	0
			490	218	88	162	22			

- Molecule 3 is a RNA chain called RNA (5'-R(\*CP\*AP\*GP\*AP\*GP\*CP\*CP\*CP\*CP\*NP\*AP\*GP\*CP\*AP\*UP\*CP\*GP\*CP\*GP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	23	Total	C	N	O	P	0	0	0
			477	214	87	154	22			

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

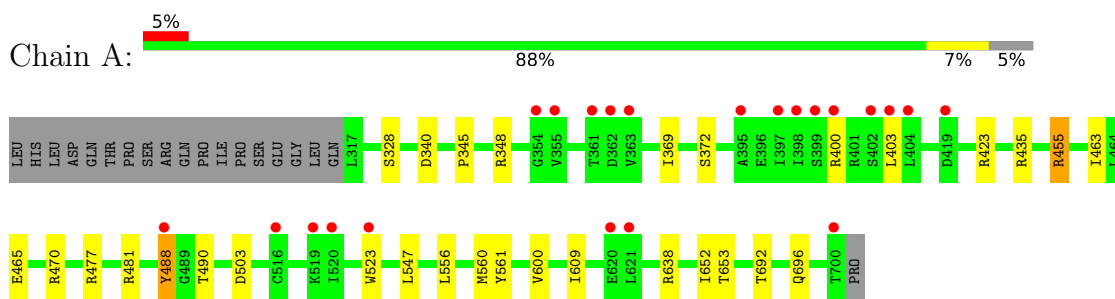
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	12	Total	O	0	0
			12	12		
6	C	4	Total	O	0	0
			4	4		
6	D	3	Total	O	0	0
			3	3		

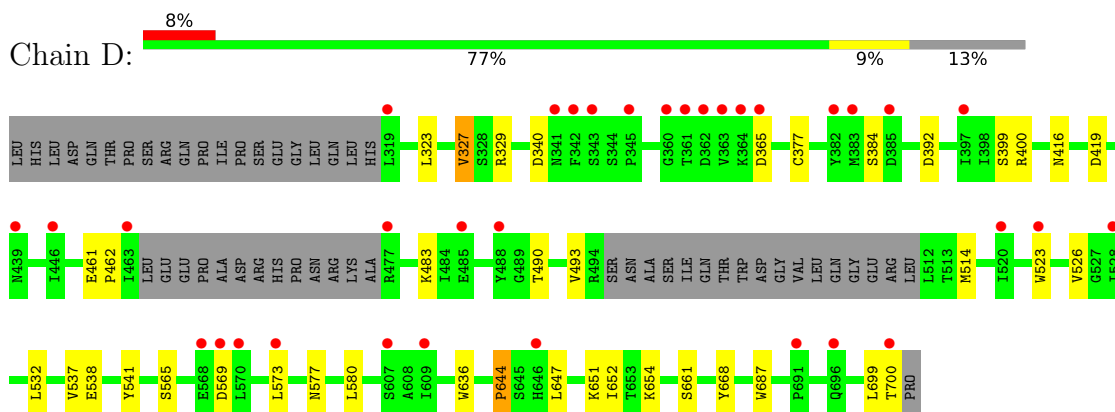
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

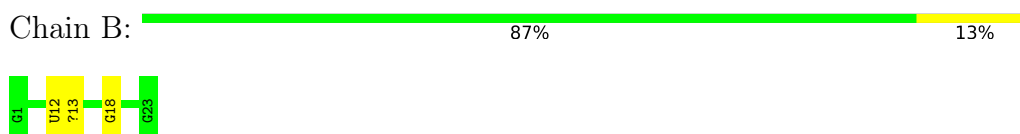
#### • Molecule 1: Double-stranded RNA-specific editase 1



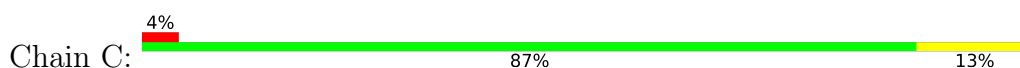
#### • Molecule 1: Double-stranded RNA-specific editase 1



#### • Molecule 2: RNA (5'-R(\*GP\*CP\*UP\*CP\*GP\*CP\*GP\*AP\*UP\*GP\*CP\*UP\*(8AZ)P\*GP\*AP\*GP\*GP\*GP\*CP\*UP\*CP\*UP\*G)-3')



#### • Molecule 3: RNA (5'-R(\*CP\*AP\*GP\*AP\*GP\*CP\*CP\*CP\*CP\*NP\*AP\*GP\*CP\*AP\*UP\*CP\*GP\*CP\*GP\*AP\*GP\*C)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.68Å 63.44Å 132.06Å 90.00° 126.64° 90.00°	Depositor
Resolution (Å)	105.96 – 2.55 39.17 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.7 (105.96-2.55) 97.7 (39.17-2.55)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.190 , 0.255 0.196 , 0.254	Depositor DCC
$R_{free}$ test set	1862 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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, 8AZ

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	0.68	0/3100	0.93	8/4191 (0.2%)
1	D	0.60	0/2809	0.82	1/3794 (0.0%)
2	B	0.47	0/521	0.89	1/809 (0.1%)
3	C	0.59	1/518 (0.2%)	0.81	0/803
All	All	0.63	1/6948 (0.0%)	0.87	10/9597 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	G	O3'-P	-6.59	1.53	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ARG	NE-CZ-NH2	-16.27	112.16	120.30
1	A	481	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	A	455	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	B	12	U	O5'-P-OP2	-6.89	99.50	105.70
1	A	423	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	329	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	638	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	477	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	477	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	435	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.



## 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	3034	0	3053	11	0
1	D	2754	0	2788	12	0
2	B	490	0	239	1	0
3	C	477	0	251	0	0
4	A	36	0	6	1	0
4	D	36	0	6	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	29	0	0	0	0
6	B	12	0	0	0	0
6	C	4	0	0	0	0
6	D	3	0	0	0	0
All	All	6877	0	6343	23	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 2.

All (23) 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)
4:A:801:IHP:O26	4:A:801:IHP:O21	2.19	0.60
1:D:377:CYS:SG	1:D:483:LYS:HD3	2.43	0.58
1:D:526:VAL:HB	1:D:668:TYR:CE1	2.39	0.57
1:A:400:ARG:HD3	1:A:523:TRP:CE2	2.41	0.55
1:D:541:TYR:HB3	1:D:577:ASN:ND2	2.27	0.50
1:D:532:LEU:HB3	1:D:636:TRP:CD1	2.48	0.48
1:A:488[A]:TYR:N	1:A:488[A]:TYR:CD1	2.83	0.47
1:D:400:ARG:HD3	1:D:523:TRP:CZ2	2.50	0.46
1:D:400:ARG:HD3	1:D:523:TRP:CE2	2.50	0.46
1:A:547:LEU:HD11	1:A:556:LEU:HD22	1.99	0.45
1:A:369:ILE:HG21	1:A:403:LEU:HD12	1.98	0.44
1:D:644:PRO:HD2	1:D:647:LEU:HD12	2.00	0.43
1:D:323:LEU:O	1:D:327:VAL:HG13	2.18	0.43
1:A:463:ILE:HD12	1:A:463:ILE:O	2.19	0.43
1:D:514:MET:HG3	1:D:687:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASP:OD2	1:D:483:LYS:NZ	2.48	0.43
1:A:372:SER:HA	1:A:600:VAL:O	2.20	0.42
1:A:503:ASP:OD2	1:D:490:THR:OG1	2.24	0.42
1:A:600:VAL:HG13	1:A:609:ILE:HB	2.01	0.42
1:A:455:ARG:HD3	2:B:13:8AZ:OP1	2.20	0.41
1:D:537:VAL:HG23	1:D:538:GLU:O	2.20	0.41
1:A:692:THR:HG22	1:A:696:GLN:HE21	1.84	0.41
1:A:556:LEU:O	1:A:560:MET:HG2	2.21	0.40

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	386/403 (96%)	368 (95%)	16 (4%)	2 (0%)	31	44
1	D	346/403 (86%)	319 (92%)	23 (7%)	4 (1%)	14	20
All	All	732/806 (91%)	687 (94%)	39 (5%)	6 (1%)	21	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	699	LEU
1	A	465	GLU
1	D	462	PRO
1	D	573	LEU
1	A	561	TYR
1	D	652	ILE

### 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	328/347 (94%)	318 (97%)	10 (3%)	44	60
1	D	300/347 (86%)	283 (94%)	17 (6%)	23	31
All	All	628/694 (90%)	601 (96%)	27 (4%)	32	44

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	SER
1	A	340	ASP
1	A	345	PRO
1	A	348	ARG
1	A	470	ARG
1	A	488[A]	TYR
1	A	488[B]	TYR
1	A	490	THR
1	A	652	ILE
1	A	653	THR
1	D	327	VAL
1	D	340	ASP
1	D	365	ASP
1	D	384	SER
1	D	399	SER
1	D	416	ASN
1	D	419	ASP
1	D	461	GLU
1	D	493	VAL
1	D	565	SER
1	D	569	ASP
1	D	580	LEU
1	D	644	PRO
1	D	651	LYS
1	D	654	LYS
1	D	661	SER
1	D	700	THR

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

Mol	Chain	Res	Type
1	A	427	GLN
1	A	479	GLN
1	A	630	HIS
1	A	696	GLN
1	D	416	ASN
1	D	421	GLN
1	D	427	GLN
1	D	562	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	21/23 (91%)	1 (4%)	0
3	C	21/23 (91%)	2 (9%)	0
All	All	42/46 (91%)	3 (7%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	18	G
3	C	7	C
3	C	14	C

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	8AZ	B	13	2,5	16,24,25	0.83	0	13,35,38	0.79	0

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	8AZ	B	13	2,5	-	0/3/35/36	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	13	8AZ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	IHP	A	801	-	36,36,36	0.96	1 (2%)	54,60,60	1.19	4 (7%)
4	IHP	D	801	-	36,36,36	0.87	1 (2%)	54,60,60	1.18	7 (12%)

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
4	IHP	A	801	-	-	4/30/54/54	0/1/1/1
4	IHP	D	801	-	-	2/30/54/54	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	801	IHP	P4-O14	2.34	1.63	1.59
4	A	801	IHP	P1-O11	2.33	1.63	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	IHP	O13-C3-C4	3.32	116.52	108.68
4	D	801	IHP	O46-P6-O26	2.76	121.43	110.53
4	D	801	IHP	O46-P6-O16	-2.68	93.97	105.99
4	D	801	IHP	O41-P1-O31	2.32	116.61	107.57
4	A	801	IHP	O41-P1-O21	2.28	119.51	110.53
4	D	801	IHP	O44-P4-O34	2.23	116.25	107.57
4	A	801	IHP	O11-C1-C6	2.16	113.79	108.68
4	D	801	IHP	O46-P6-O36	2.13	115.87	107.57
4	D	801	IHP	C6-C5-C4	2.11	115.05	110.40
4	A	801	IHP	O16-C6-C5	2.05	113.52	108.68
4	D	801	IHP	O42-P2-O12	-2.05	96.81	105.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	IHP	C1-O11-P1-O21
4	A	801	IHP	C2-O12-P2-O22
4	A	801	IHP	C3-O13-P3-O23
4	D	801	IHP	C4-O14-P4-O24
4	A	801	IHP	C6-O16-P6-O46
4	D	801	IHP	C2-O12-P2-O32

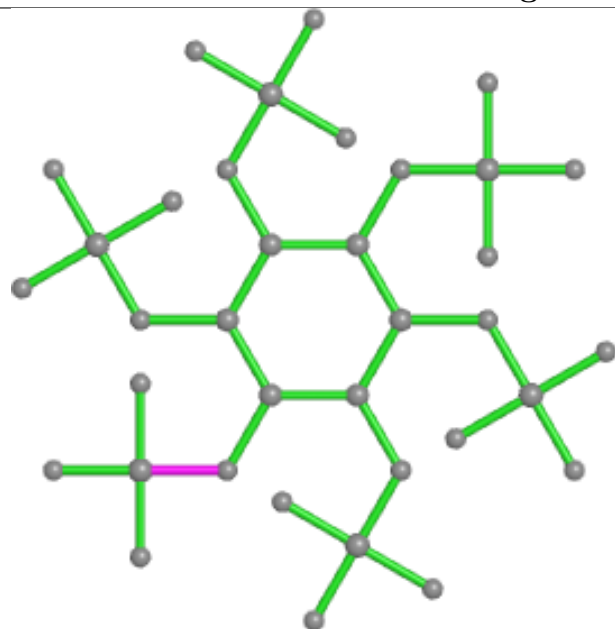
There are no ring outliers.

1 monomer is involved in 1 short contact:

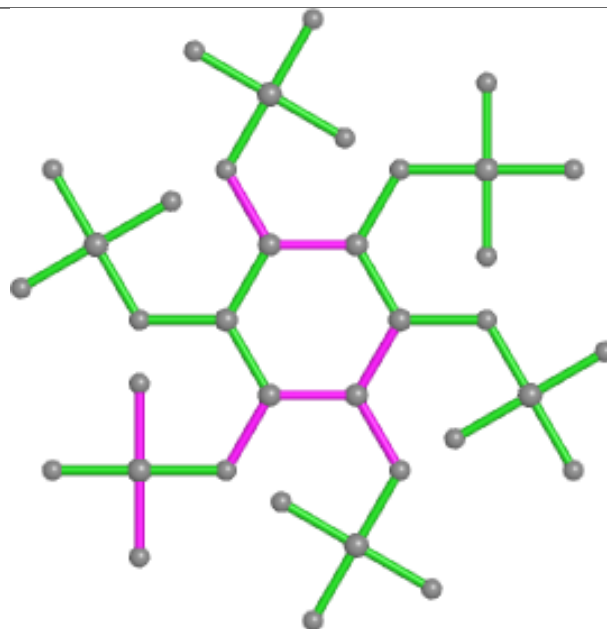
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	IHP	1	0

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.

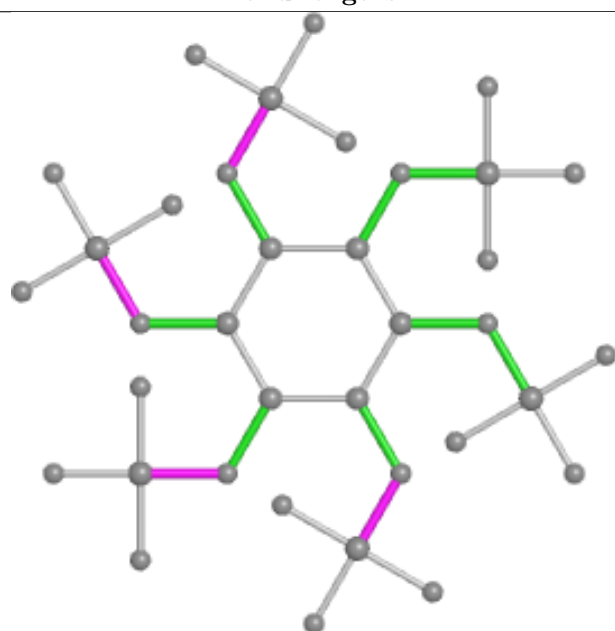
## Ligand IHP A 801



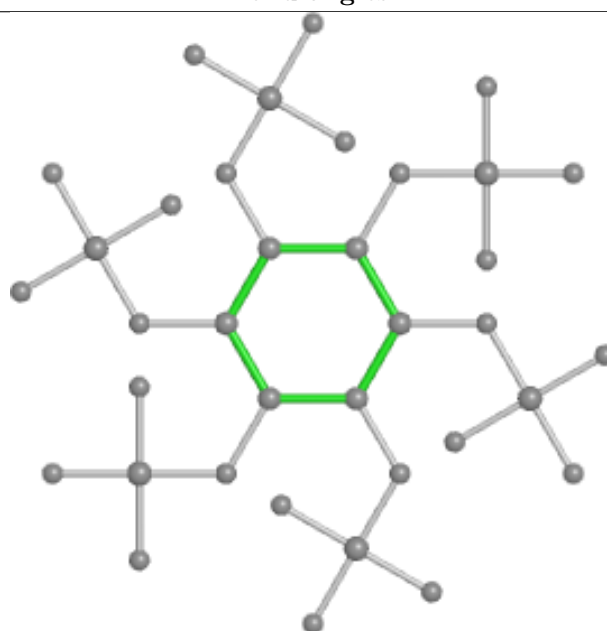
Bond lengths



Bond angles

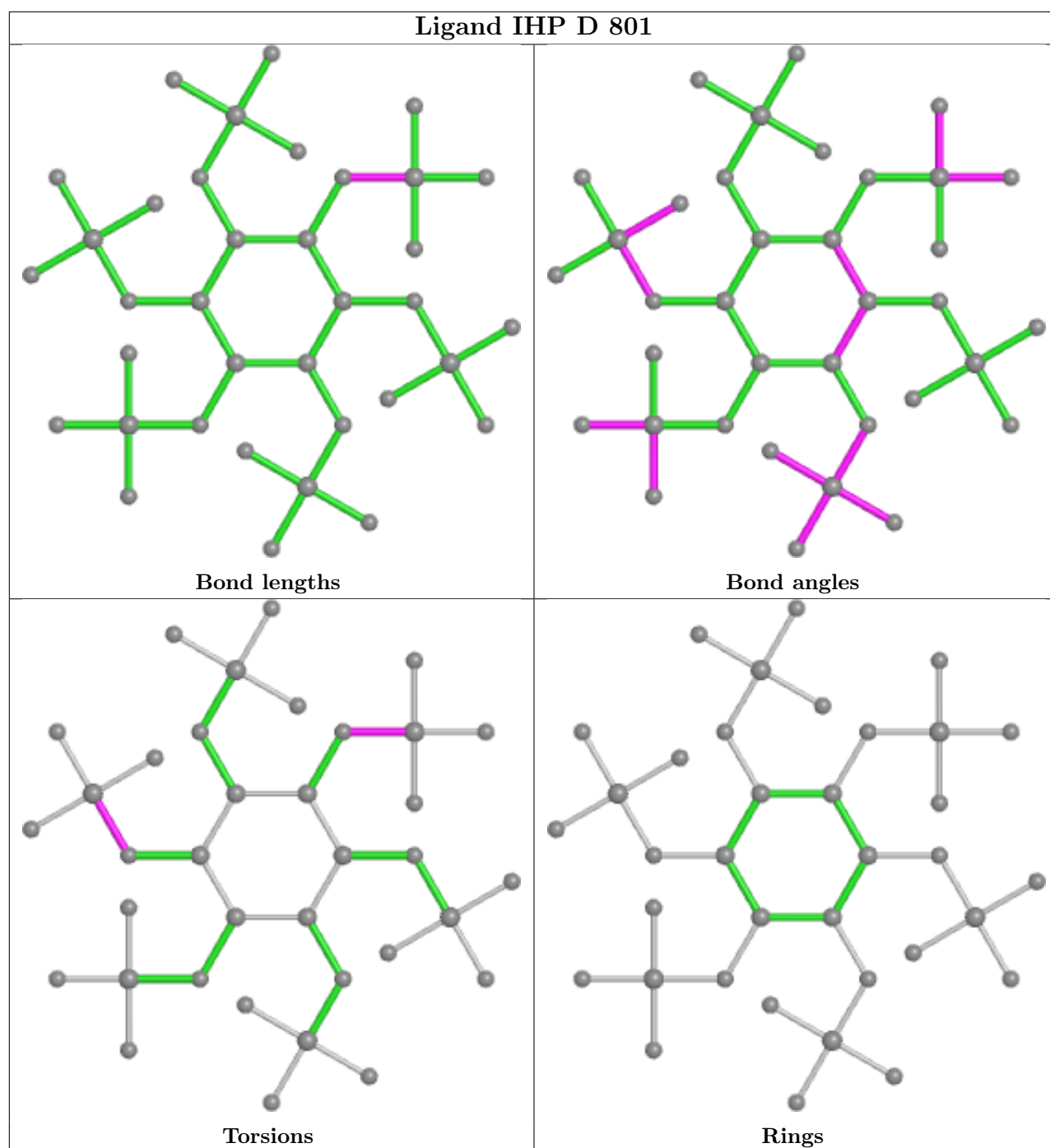


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	384/403 (95%)	0.20	22 (5%) 24 28	37, 51, 86, 126	0
1	D	352/403 (87%)	0.45	34 (9%) 8 10	50, 76, 111, 130	0
2	B	22/23 (95%)	-0.15	0 100 100	45, 60, 81, 90	0
3	C	22/23 (95%)	0.15	1 (4%) 33 40	44, 69, 83, 120	0
All	All	780/852 (91%)	0.30	57 (7%) 15 18	37, 63, 103, 130	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	VAL	6.9
3	C	1	C	6.2
1	D	361	THR	5.9
1	A	700	THR	5.8
1	D	385	ASP	4.6
1	D	383	MET	4.6
1	A	397	ILE	4.4
1	D	463	ILE	4.2
1	D	360	GLY	4.2
1	D	362	ASP	3.6
1	D	607	SER	3.4
1	D	573	LEU	3.4
1	A	363	VAL	3.3
1	D	691	PRO	3.1
1	D	319	LEU	3.1
1	A	398	ILE	3.0
1	D	382	TYR	3.0
1	D	397	ILE	2.9
1	A	400	ARG	2.9
1	A	355	VAL	2.9
1	D	439	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	365	ASP	2.7
1	A	621	LEU	2.7
1	D	488	TYR	2.7
1	D	646	HIS	2.7
1	A	516	CYS	2.6
1	A	488[A]	TYR	2.6
1	A	419	ASP	2.6
1	D	342	PHE	2.6
1	A	520	ILE	2.6
1	A	402	SER	2.6
1	A	403	LEU	2.5
1	A	362	ASP	2.4
1	D	568	GLU	2.4
1	D	341	ASN	2.4
1	A	404	LEU	2.4
1	D	609	ILE	2.4
1	D	364	LYS	2.4
1	D	569	ASP	2.4
1	A	399	SER	2.3
1	D	528	ILE	2.3
1	A	361	THR	2.3
1	D	570	LEU	2.3
1	D	523	TRP	2.3
1	D	446	ILE	2.3
1	A	523	TRP	2.3
1	A	354	GLY	2.2
1	D	485	GLU	2.2
1	D	696	GLN	2.2
1	D	700	THR	2.2
1	D	343	SER	2.2
1	A	519	LYS	2.1
1	D	520	ILE	2.1
1	D	345	PRO	2.1
1	D	477	ARG	2.1
1	A	395	ALA	2.1
1	A	620	GLU	2.0

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

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	8AZ	B	13	22/23	0.98	0.17	37,41,50,54	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

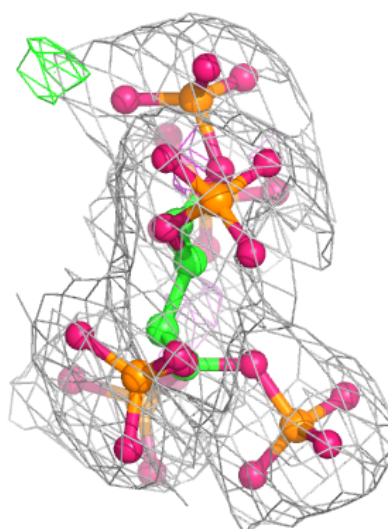
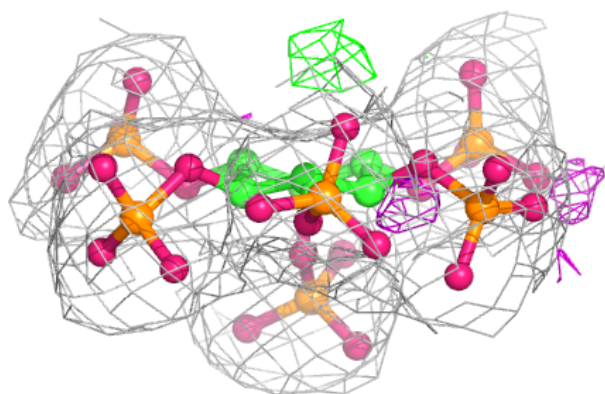
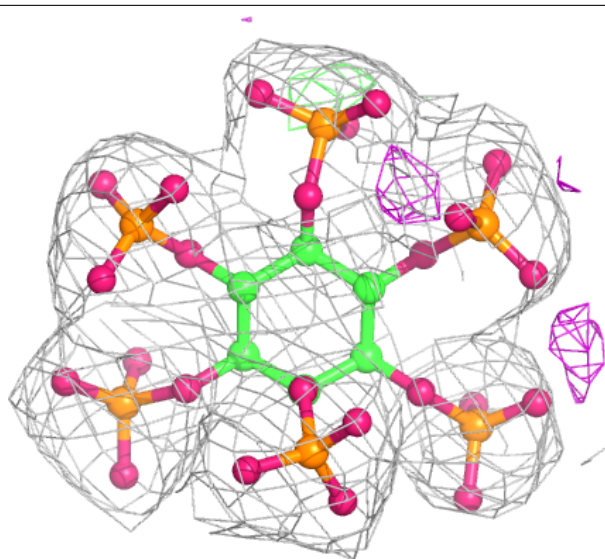
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	IHP	D	801	36/36	0.95	0.16	52,73,87,89	0
5	ZN	D	802	1/1	0.99	0.17	58,58,58,58	0
4	IHP	A	801	36/36	0.99	0.19	34,41,47,48	0
5	ZN	A	802	1/1	1.00	0.18	42,42,42,42	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.

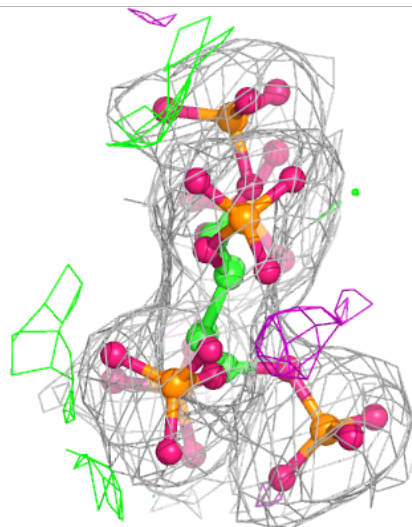
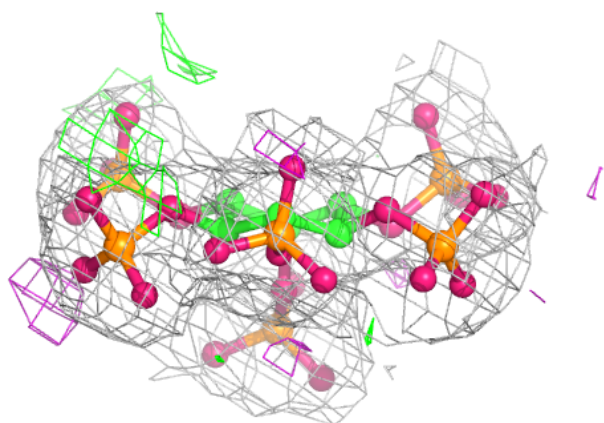
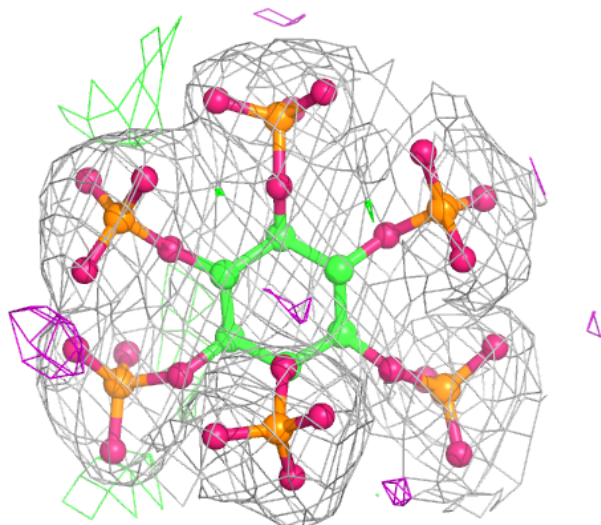
**Electron density around IHP D 801:**

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



**Electron density around IHP A 801:**

$2mF_o-DF_c$  (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.