



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2025 – 03:53 pm GMT

PDB ID : 9TFX / pdb\_00009tfx  
Title : Arabidopsis thaliana Casein Kinase 2 (CK2) alpha isoform 1 in complex with inositol hexakisphosphate (InsP6)  
Authors : Sturm, K.; Hothorn, M.  
Deposited on : 2025-11-27  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

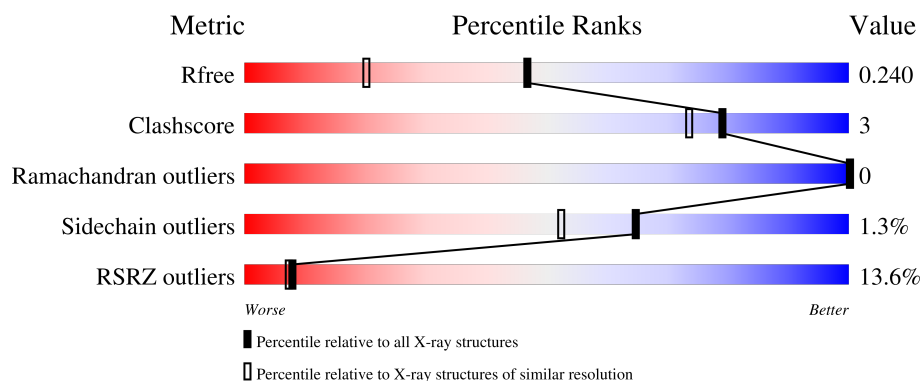
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAAA	344	<div> <div>13%</div> <div>97%</div> <div>..</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5913 atoms, of which 2840 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.

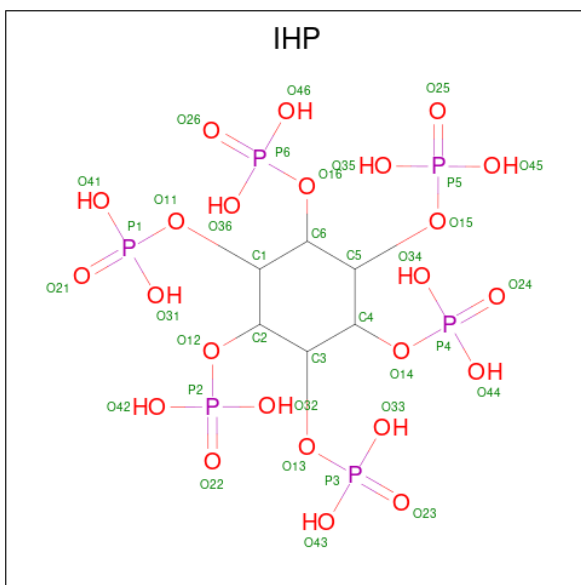
- Molecule 1 is a protein called Casein kinase II subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAAA	337	Total	C	H	N	O	S	0	3	0
			5624	1809	2811	487	506	11			

There are 11 discrepancies between the modelled and reference sequences:

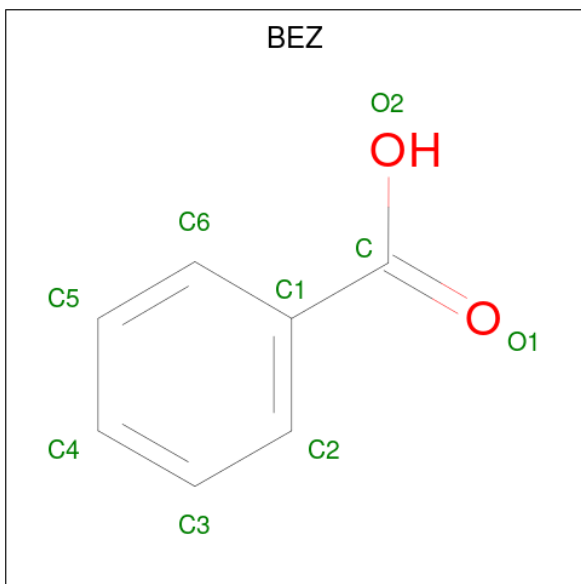
Chain	Residue	Modelled	Actual	Comment	Reference
AAAA	410	ALA	-	expression tag	UNP Q08467
AAAA	411	ALA	-	expression tag	UNP Q08467
AAAA	412	ALA	-	expression tag	UNP Q08467
AAAA	413	LEU	-	expression tag	UNP Q08467
AAAA	414	GLU	-	expression tag	UNP Q08467
AAAA	415	HIS	-	expression tag	UNP Q08467
AAAA	416	HIS	-	expression tag	UNP Q08467
AAAA	417	HIS	-	expression tag	UNP Q08467
AAAA	418	HIS	-	expression tag	UNP Q08467
AAAA	419	HIS	-	expression tag	UNP Q08467
AAAA	420	HIS	-	expression tag	UNP Q08467

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAAA	1	Total	C	H	O	P	0	0
			42	6	6	24	6		

- Molecule 3 is BENZOIC ACID (CCD ID: BEZ) (formula:  $C_7H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAAA	1	Total	C	H	O	0	0
			14	7	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAAA	1	Total	C	H	O	0	0
			10	2	6	2		
4	AAAA	1	Total	C	H	O	0	0
			10	2	6	2		
4	AAAA	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAAA	2	Total	Cl	0	0
			2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAAA	4	Total	Na	0	0
			4	4		

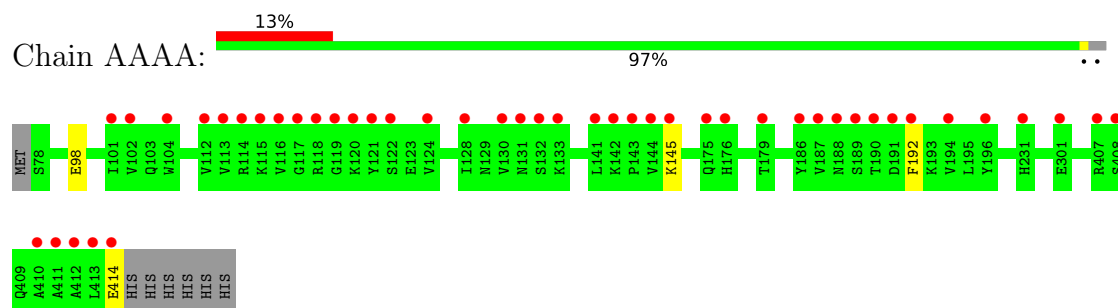
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAAA	197	Total	O	0	0
			197	197		

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

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

- Molecule 1: Casein kinase II subunit alpha-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.90Å 63.90Å 97.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.69 – 1.70 38.69 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.69-1.70) 90.0 (38.69-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.54 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.208 , 0.240 0.208 , 0.240	Depositor DCC
$R_{free}$ test set	2276 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: EDO, NA, IHP, CL, BEZ

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	AAAA	0.21	0/2888	0.41	0/3898

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	AAAA	2813	2811	0	0	0
2	AAAA	36	6	0	0	0
3	AAAA	9	5	0	0	0
4	AAAA	12	18	0	0	0
5	AAAA	2	0	0	0	0
6	AAAA	4	0	0	0	0
7	AAAA	197	0	0	0	0
All	All	3073	2840	0	0	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.

There are no clashes within the asymmetric unit.

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	AAAA	338/344 (98%)	326 (96%)	12 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAAA	305/309 (99%)	301 (99%)	4 (1%)	65	52

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAAA	98	GLU
1	AAAA	145	LYS
1	AAAA	192	PHE
1	AAAA	414	GLU

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	EDO	AAAA	505	-	3,3,3	0.35	0	2,2,2	0.56	0
4	EDO	AAAA	503	-	3,3,3	0.30	0	2,2,2	0.06	0
2	IHP	AAAA	501	-	36,36,36	1.86	6 (16%)	54,60,60	1.11	3 (5%)
4	EDO	AAAA	504	-	3,3,3	0.27	0	2,2,2	0.24	0
3	BEZ	AAAA	502	-	9,9,9	0.93	0	11,11,11	0.77	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
4	EDO	AAAA	505	-	-	0/1/1/1	-
4	EDO	AAAA	503	-	-	1/1/1/1	-
2	IHP	AAAA	501	-	-	8/30/54/54	0/1/1/1
4	EDO	AAAA	504	-	-	1/1/1/1	-
3	BEZ	AAAA	502	-	-	0/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAAA	501	IHP	P5-O15	4.76	1.68	1.59
2	AAAA	501	IHP	P4-O14	4.37	1.67	1.59
2	AAAA	501	IHP	P6-O16	4.35	1.67	1.59
2	AAAA	501	IHP	P2-O12	4.13	1.67	1.59
2	AAAA	501	IHP	P3-O13	3.90	1.66	1.59
2	AAAA	501	IHP	P1-O11	3.86	1.66	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAAA	501	IHP	C4-C3-C2	3.02	117.03	110.41
2	AAAA	501	IHP	O32-P2-O12	-2.25	95.92	105.99
2	AAAA	501	IHP	O15-C5-C4	2.15	113.75	108.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

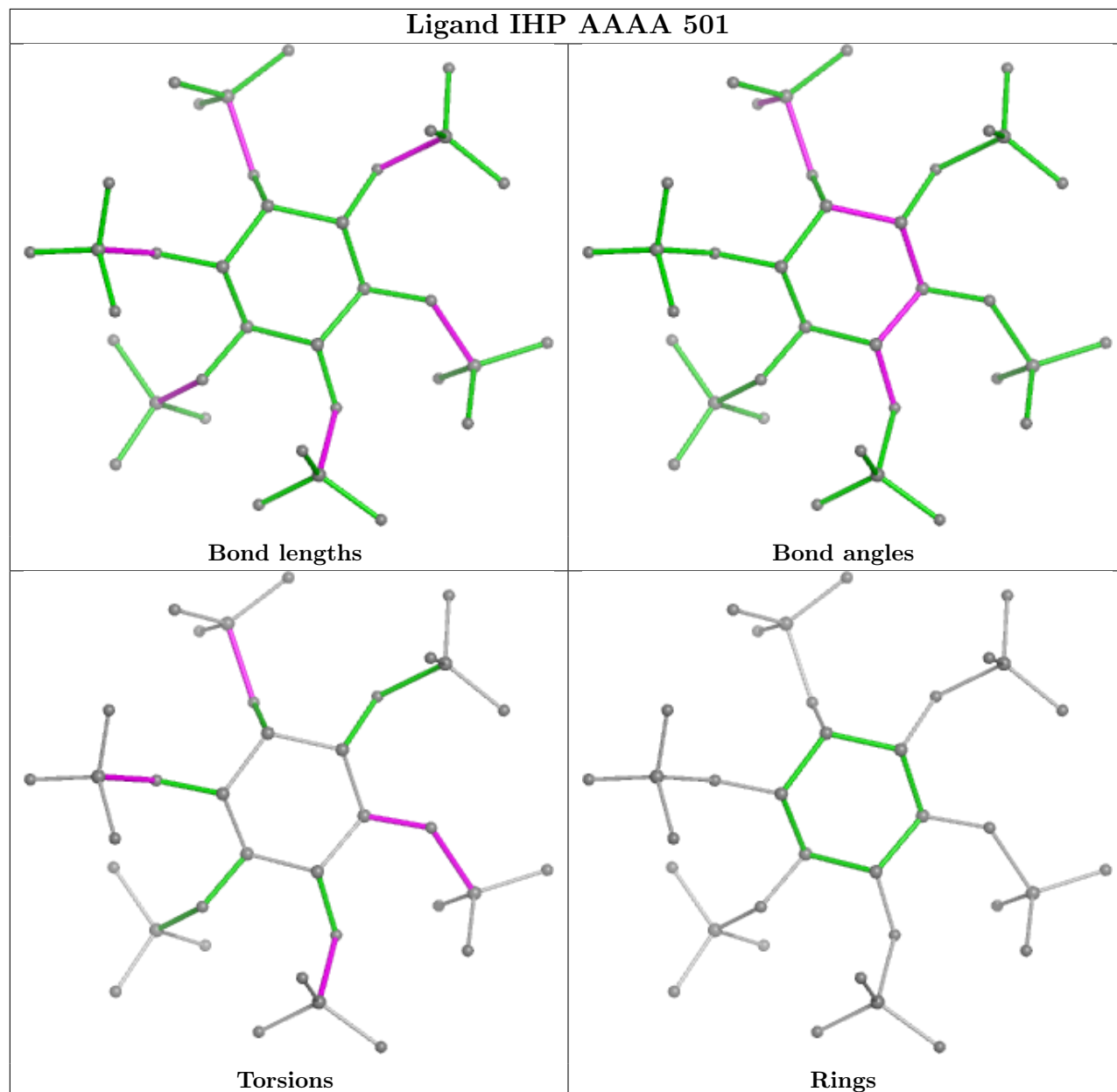
Mol	Chain	Res	Type	Atoms
2	AAAA	501	IHP	C3-C4-O14-P4
2	AAAA	501	IHP	C5-C4-O14-P4
2	AAAA	501	IHP	C2-O12-P2-O42
2	AAAA	501	IHP	C4-O14-P4-O24
2	AAAA	501	IHP	C5-O15-P5-O25
4	AAAA	504	EDO	O1-C1-C2-O2
2	AAAA	501	IHP	C1-O11-P1-O41
2	AAAA	501	IHP	C4-O14-P4-O34
2	AAAA	501	IHP	C5-O15-P5-O45
4	AAAA	503	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	AAAA	337/344 (97%)	0.54	46 (13%) 8 7	13, 38, 89, 136	4 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAAA	121	TYR	7.0
1	AAAA	116	VAL	5.4
1	AAAA	187	VAL	4.9
1	AAAA	413	LEU	4.7
1	AAAA	412	ALA	4.5
1	AAAA	192	PHE	4.3
1	AAAA	410	ALA	4.3
1	AAAA	414	GLU	4.1
1	AAAA	411	ALA	3.7
1	AAAA	117	GLY	3.6
1	AAAA	130	VAL	3.6
1	AAAA	119	GLY	3.5
1	AAAA	194	VAL	3.4
1	AAAA	144	VAL	3.3
1	AAAA	118	ARG	3.3
1	AAAA	143	PRO	3.3
1	AAAA	191	ASP	3.1
1	AAAA	175	GLN	3.0
1	AAAA	115	LYS	3.0
1	AAAA	131	ASN	3.0
1	AAAA	120	LYS	3.0
1	AAAA	196	TYR	2.9
1	AAAA	301	GLU	2.9
1	AAAA	122	SER	2.9
1	AAAA	189	SER	2.8
1	AAAA	113	VAL	2.8
1	AAAA	231	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	AAAA	102	VAL	2.6
1	AAAA	176	HIS	2.5
1	AAAA	132	SER	2.5
1	AAAA	128	ILE	2.4
1	AAAA	104	TRP	2.4
1	AAAA	101	ILE	2.3
1	AAAA	408	SER	2.3
1	AAAA	188	ASN	2.2
1	AAAA	190	THR	2.2
1	AAAA	114	ARG	2.2
1	AAAA	124	VAL	2.2
1	AAAA	145	LYS	2.2
1	AAAA	407	ARG	2.2
1	AAAA	133	LYS	2.1
1	AAAA	112	VAL	2.1
1	AAAA	141	LEU	2.1
1	AAAA	179	THR	2.1
1	AAAA	142	LYS	2.0
1	AAAA	186	TYR	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	AAAA	504	4/4	0.72	0.24	52,63,82,82	0
2	IHP	AAAA	501	36/36	0.80	0.13	39,94,118,124	0
6	NA	AAAA	509	1/1	0.85	0.12	68,68,68,68	0
6	NA	AAAA	511	1/1	0.85	0.16	65,65,65,65	0

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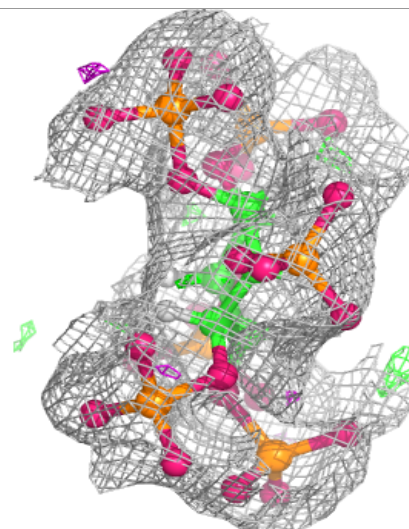
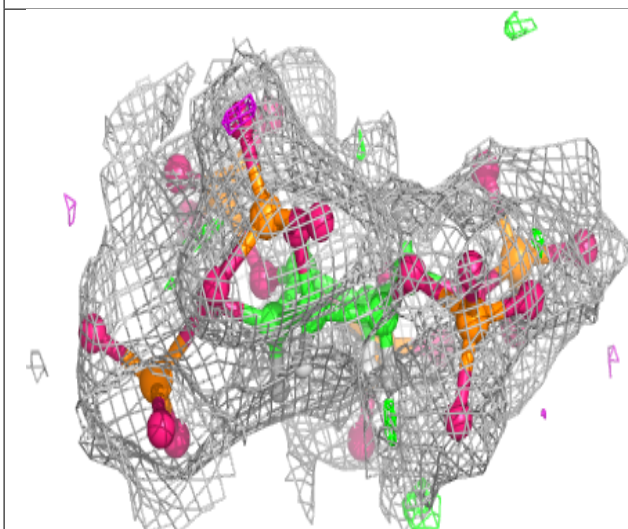
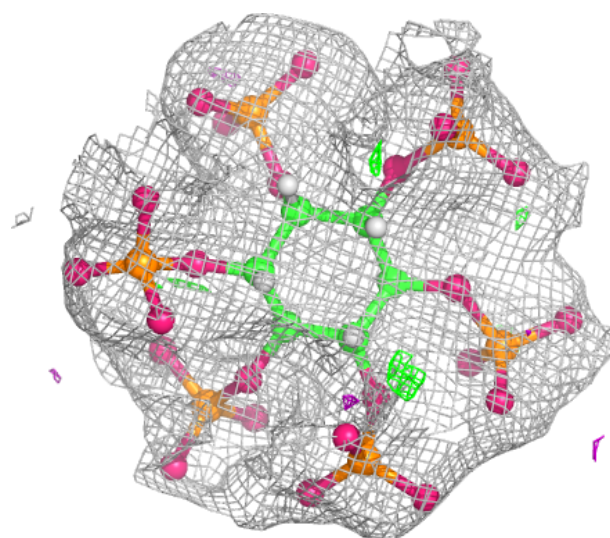
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BEZ	AAAA	502	9/9	0.87	0.13	31,40,50,56	0
6	NA	AAAA	510	1/1	0.88	0.13	48,48,48,48	0
4	EDO	AAAA	503	4/4	0.88	0.13	39,47,52,62	0
4	EDO	AAAA	505	4/4	0.93	0.28	23,33,40,40	0
6	NA	AAAA	508	1/1	0.95	0.14	35,35,35,35	0
5	CL	AAAA	507	1/1	0.97	0.19	35,35,35,35	0
5	CL	AAAA	506	1/1	0.98	0.17	33,33,33,33	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 AAAA 501:**

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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.