Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2022 – 10:33 AM EST

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PDB ID	:	7MOF
Title	:	Crystal Structure of Arabidopsis thaliana Plant and Fungi Atypical Dual Specificity Phosphatase 1(AtPFA-DSP1) Cys150Ser in complex with 6-diphosphoinositol 1,2,3,4,5-pentakisphosphate 6-InsP7
Authors	:	Wang, H.; Shears, S.B.
Deposited on	:	2021-05-01
Resolution	:	1.95 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 1.95 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.
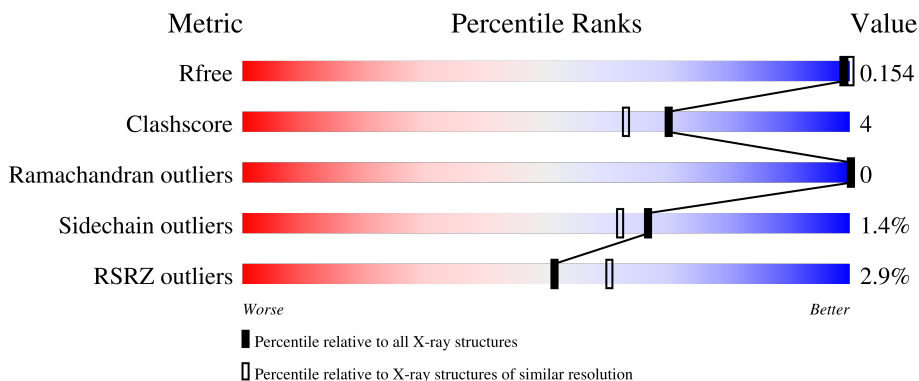
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 >=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	171	2% / 85% / 5% / 10%
1	B	171	4% / 78% / 11% / · / 11%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3019 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 Tyrosine-protein phosphatase DSP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	5	0
			1283	826	225	222	10			
1	B	153	Total	C	N	O	S	0	5	0
			1283	827	225	221	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP Q9ZVN4
A	46	SER	-	expression tag	UNP Q9ZVN4
A	47	PHE	-	expression tag	UNP Q9ZVN4
A	48	THR	-	expression tag	UNP Q9ZVN4
A	150	SER	CYS	engineered mutation	UNP Q9ZVN4
B	45	GLY	-	expression tag	UNP Q9ZVN4
B	46	SER	-	expression tag	UNP Q9ZVN4
B	47	PHE	-	expression tag	UNP Q9ZVN4
B	48	THR	-	expression tag	UNP Q9ZVN4
B	150	SER	CYS	engineered mutation	UNP Q9ZVN4

- Molecule 2 is (1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentakis(phosphonooxy)cyclohexyl trihydrogen diphosphate (three-letter code: ZKS) (formula: $C_6H_{19}O_{27}P_7$) (labeled as "Ligand of Interest" by depositor).

ZKS
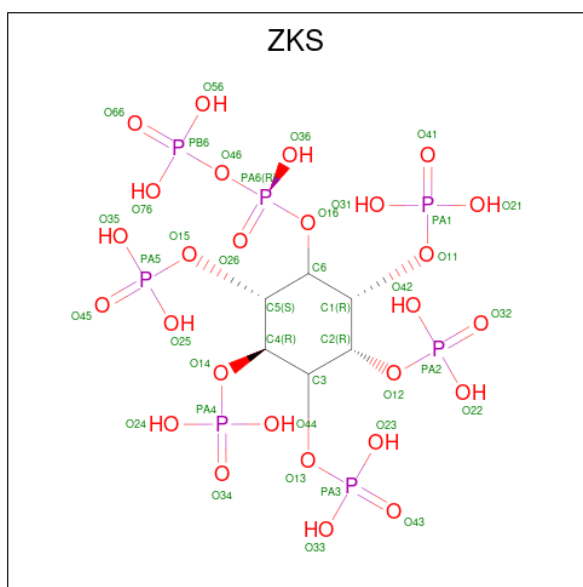
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 40	C 6	O 27	P 7	0	0
2	B	1	Total 40	C 6	O 27	P 7	0	0

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

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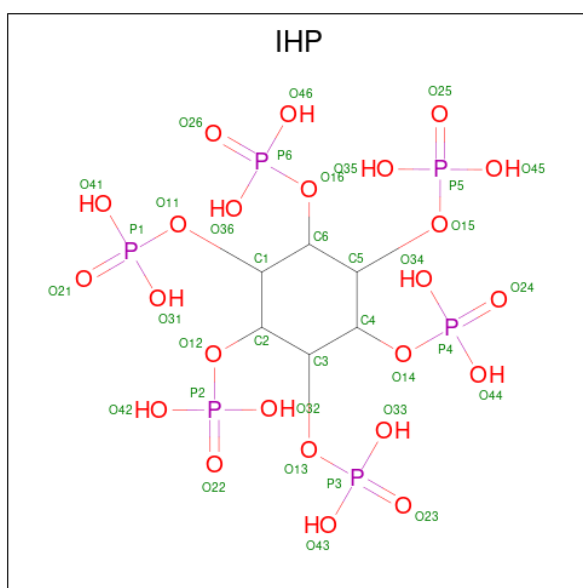
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 36	C 6	O 24	P 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	B	153	Total O 153 153	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: Tyrosine-protein phosphatase DSP1

Chain A:

• Molecule 1: Tyrosine-protein phosphatase DSP1

Chain B:
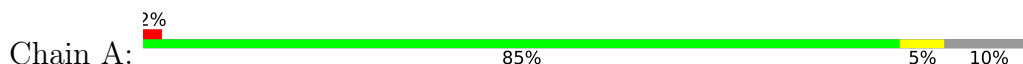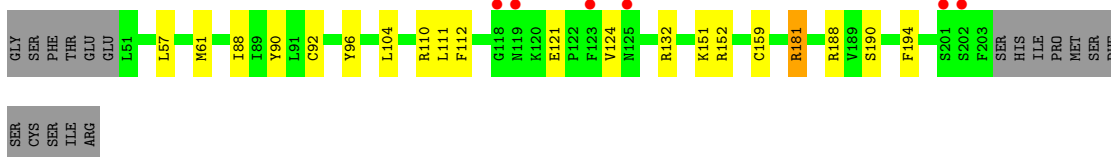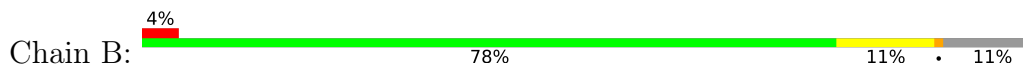
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	124.90Å 124.90Å 124.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 1.95 39.50 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.53-1.95) 99.7 (39.50-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.110 , 0.153 0.111 , 0.154	Depositor DCC
R_{free} test set	2391 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3019	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, ZKS

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	0.73	1/1315 (0.1%)	0.80	1/1770 (0.1%)
1	B	0.69	0/1315	0.81	2/1769 (0.1%)
All	All	0.71	1/2630 (0.0%)	0.80	3/3539 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLU	CD-OE1	7.30	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	181	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	B	181	ARG	NE-CZ-NH2	5.39	122.99	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	1283	0	1285	4	0
1	B	1283	0	1290	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	0	1	0
2	B	40	0	0	2	0
3	A	36	0	6	1	0
4	A	184	0	0	2	0
4	B	153	0	0	4	0
All	All	3019	0	2581	19	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 4.

All (19) 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:B:501:ZKS:O24	4:B:601:HOH:O	1.88	0.90
2:A:501:ZKS:O36	2:A:501:ZKS:O25	2.00	0.78
1:A:159[B]:CYS:SG	1:A:194:PHE:CD2	2.79	0.75
2:B:501:ZKS:O25	2:B:501:ZKS:O36	2.07	0.71
1:B:159[A]:CYS:SG	1:B:194:PHE:CD2	2.85	0.70
1:B:88:ILE:HD12	1:B:104:LEU:HD11	1.77	0.66
1:A:180[A]:GLN:NE2	4:A:602:HOH:O	2.23	0.64
1:B:124:VAL:HG21	1:B:190:SER:OG	2.02	0.60
1:A:127:PRO:HA	3:A:502:IHP:O34	2.04	0.58
1:B:188:ARG:NH2	4:B:603:HOH:O	2.26	0.51
1:B:124:VAL:HG21	1:B:190:SER:CB	2.43	0.48
1:A:181:ARG:HG2	1:B:181:ARG:HG2	1.96	0.48
1:B:188:ARG:NH1	4:B:609:HOH:O	2.43	0.48
4:A:614:HOH:O	1:B:61[A]:MET:HE3	2.15	0.47
1:B:104:LEU:HD23	1:B:111:LEU:HB2	1.96	0.47
1:B:121:GLU:OE1	4:B:602:HOH:O	2.21	0.44
1:B:110:ARG:HD2	1:B:112:PHE:CZ	2.53	0.44
1:B:57:LEU:HD23	1:B:152:ARG:HA	2.02	0.41
1:B:90:TYR:CZ	1:B:92:CYS:HB2	2.55	0.41

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	157/171 (92%)	150 (96%)	7 (4%)	0	100	100
1	B	157/171 (92%)	151 (96%)	6 (4%)	0	100	100
All	All	314/342 (92%)	301 (96%)	13 (4%)	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	144/155 (93%)	143 (99%)	1 (1%)	84	82
1	B	144/155 (93%)	141 (98%)	3 (2%)	53	46
All	All	288/310 (93%)	284 (99%)	4 (1%)	67	62

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

Mol	Chain	Res	Type
1	A	96	TYR
1	B	96	TYR
1	B	132	ARG
1	B	151	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	B	180	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	ZKS	B	501	-	38,40,40	2.01	9 (23%)	60,67,67	1.92	14 (23%)
2	ZKS	A	501	-	38,40,40	1.75	8 (21%)	60,67,67	1.63	9 (15%)
3	IHP	A	502	-	36,36,36	2.13	8 (22%)	54,60,60	1.91	13 (24%)

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	ZKS	B	501	-	-	5/36/60/60	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZKS	A	501	-	-	7/36/60/60	0/1/1/1
3	IHP	A	502	-	-	3/30/54/54	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	IHP	P6-O16	7.13	1.72	1.59
2	B	501	ZKS	PA4-O14	5.77	1.70	1.59
2	A	501	ZKS	PA1-O11	4.68	1.68	1.59
2	B	501	ZKS	PA6-O16	-4.22	1.49	1.60
2	A	501	ZKS	PA4-O14	4.01	1.66	1.59
2	B	501	ZKS	PB6-O76	-3.99	1.39	1.54
3	A	502	IHP	P6-O46	3.75	1.69	1.54
2	B	501	ZKS	PB6-O56	-3.72	1.40	1.54
3	A	502	IHP	P4-O14	3.47	1.65	1.59
3	A	502	IHP	P3-O13	3.35	1.65	1.59
3	A	502	IHP	P6-O36	3.25	1.67	1.54
2	A	501	ZKS	PA6-O16	-3.03	1.52	1.60
2	A	501	ZKS	PB6-O76	-2.88	1.43	1.54
2	A	501	ZKS	C2-C3	2.82	1.58	1.52
2	B	501	ZKS	C1-C6	-2.72	1.46	1.52
2	B	501	ZKS	PA5-O15	2.69	1.64	1.59
2	B	501	ZKS	PA3-O23	-2.62	1.44	1.54
3	A	502	IHP	C6-C1	2.50	1.57	1.52
3	A	502	IHP	C6-C5	2.50	1.57	1.52
3	A	502	IHP	O16-C6	2.44	1.53	1.44
2	A	501	ZKS	PA2-O42	-2.33	1.45	1.54
2	A	501	ZKS	PA2-O12	2.25	1.63	1.59
2	B	501	ZKS	PA5-O35	-2.15	1.46	1.54
2	A	501	ZKS	PA1-O31	-2.15	1.46	1.54
2	B	501	ZKS	PA4-O24	-2.10	1.46	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ZKS	O46-PA6-O16	9.68	122.01	102.48
3	A	502	IHP	O16-P6-O26	-7.63	79.95	109.39
2	A	501	ZKS	O46-PA6-O16	6.35	115.28	102.48
3	A	502	IHP	O46-P6-O16	-5.49	81.38	105.99
3	A	502	IHP	O36-P6-O16	-4.50	85.83	105.99
2	B	501	ZKS	O16-C6-C1	-3.75	99.85	108.69
2	B	501	ZKS	C1-C6-C5	3.16	117.33	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ZKS	O31-PA1-O11	-2.99	92.60	105.99
2	A	501	ZKS	O16-C6-C1	-2.96	101.71	108.69
2	A	501	ZKS	O21-PA1-O31	2.89	118.70	107.64
2	B	501	ZKS	O11-PA1-O41	-2.89	98.25	109.39
3	A	502	IHP	O46-P6-O26	2.82	121.71	110.68
2	A	501	ZKS	O11-PA1-O41	-2.77	98.68	109.39
2	B	501	ZKS	O31-PA1-O11	-2.74	93.74	105.99
3	A	502	IHP	O42-P2-O32	2.68	117.87	107.64
2	B	501	ZKS	O21-PA1-O31	2.68	117.86	107.64
2	A	501	ZKS	O13-PA3-O43	-2.61	99.30	109.39
3	A	502	IHP	O36-P6-O26	2.50	120.46	110.68
3	A	502	IHP	O15-P5-O25	-2.43	100.02	109.39
3	A	502	IHP	O11-P1-O21	-2.41	100.11	109.39
2	B	501	ZKS	O22-PA2-O42	2.39	116.75	107.64
2	A	501	ZKS	O31-PA1-O41	2.36	119.91	110.68
2	B	501	ZKS	O16-C6-C5	2.29	114.08	108.69
3	A	502	IHP	O44-P4-O34	2.26	116.28	107.64
3	A	502	IHP	O13-P3-O23	-2.24	100.75	109.39
2	A	501	ZKS	O56-PB6-O46	-2.22	97.18	104.64
2	B	501	ZKS	PA6-O16-C6	-2.22	111.34	119.41
2	B	501	ZKS	O24-PA4-O44	2.17	115.95	107.64
3	A	502	IHP	O16-C6-C5	2.14	113.72	108.69
2	B	501	ZKS	O21-PA1-O41	2.14	119.04	110.68
3	A	502	IHP	O45-P5-O35	2.13	115.76	107.64
3	A	502	IHP	O43-P3-O33	2.04	115.44	107.64
2	B	501	ZKS	O12-C2-C3	2.04	113.50	108.69
2	B	501	ZKS	O33-PA3-O23	2.04	115.43	107.64
2	B	501	ZKS	O31-PA1-O41	2.03	118.62	110.68
2	A	501	ZKS	O33-PA3-O23	2.03	115.38	107.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ZKS	C2-O12-PA2-O32
2	A	501	ZKS	C3-O13-PA3-O43
2	A	501	ZKS	C5-O15-PA5-O45
2	B	501	ZKS	C3-O13-PA3-O43
2	B	501	ZKS	C5-O15-PA5-O45
3	A	502	IHP	C5-O15-P5-O25
2	A	501	ZKS	C2-O12-PA2-O42
2	A	501	ZKS	C5-O15-PA5-O35

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Mol	Chain	Res	Type	Atoms
2	A	501	ZKS	C6-O16-PA6-O36
2	A	501	ZKS	C4-O14-PA4-O34
2	B	501	ZKS	C4-O14-PA4-O34
2	B	501	ZKS	PA6-O46-PB6-O76
2	B	501	ZKS	C5-O15-PA5-O35
3	A	502	IHP	C2-C3-O13-P3
3	A	502	IHP	C6-O16-P6-O46

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ZKS	2	0
2	A	501	ZKS	1	0
3	A	502	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 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 ZKS B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ZKS A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand IHP A 502

Bond lengths

Bond angles

Torsions

Rings
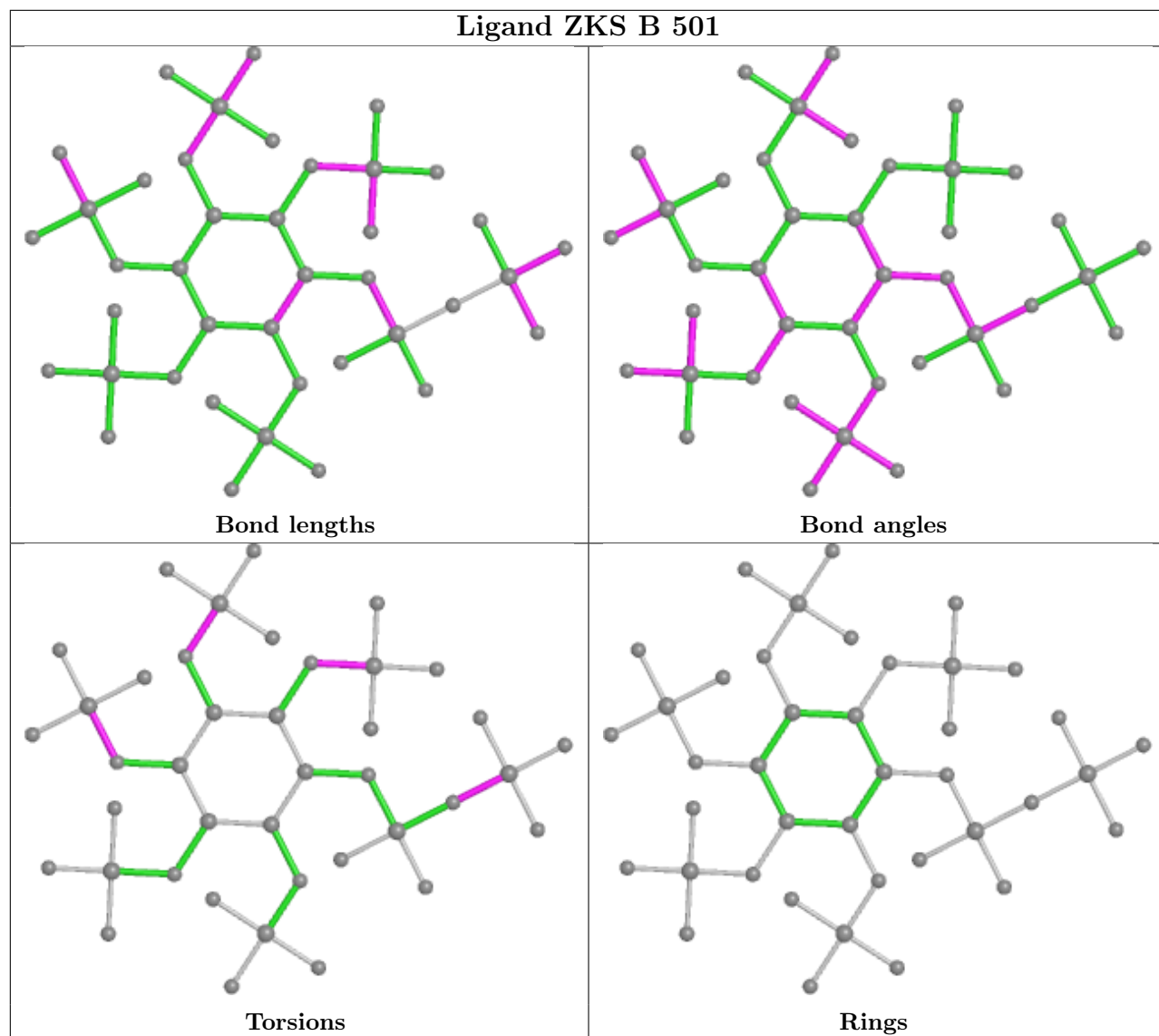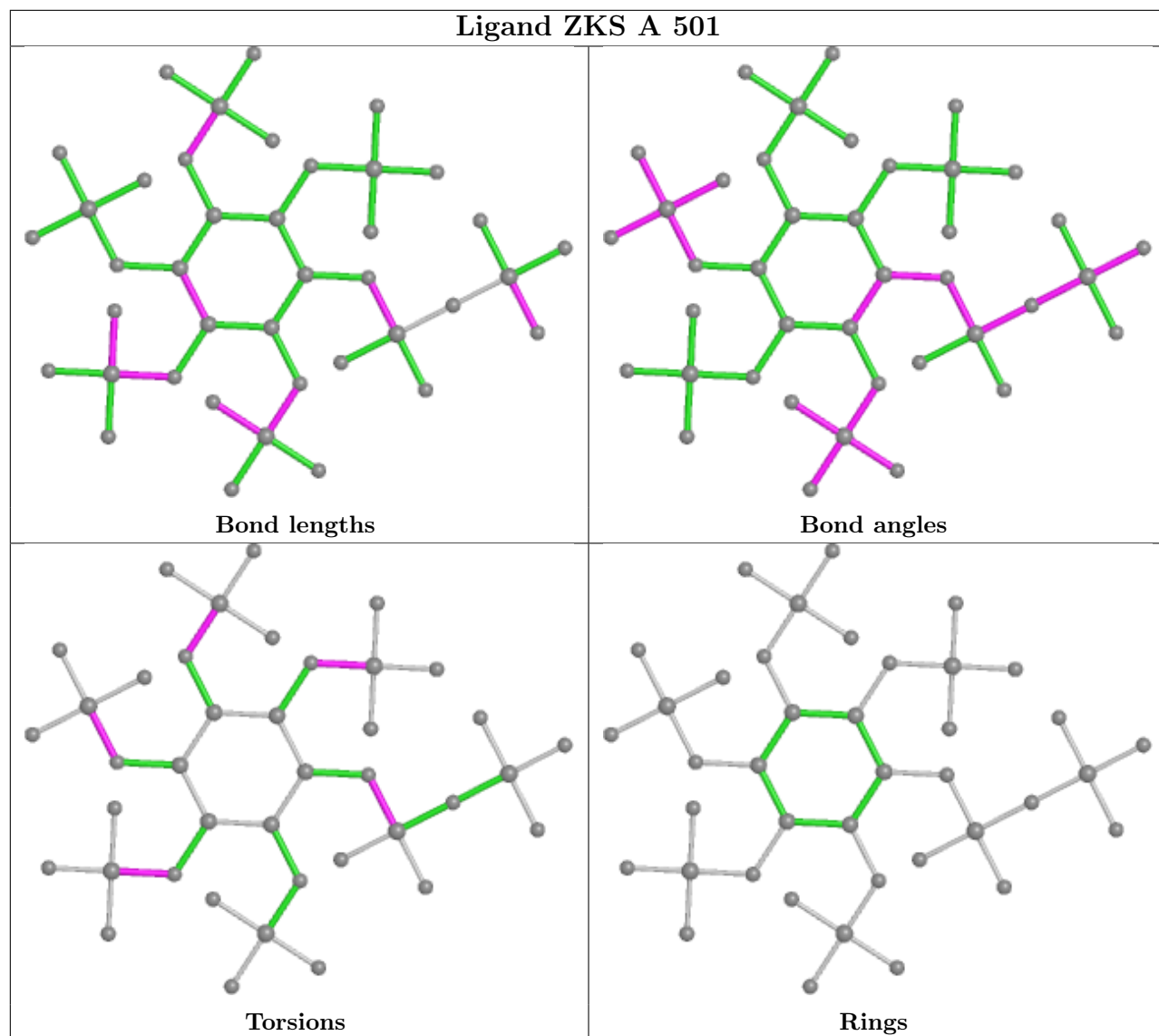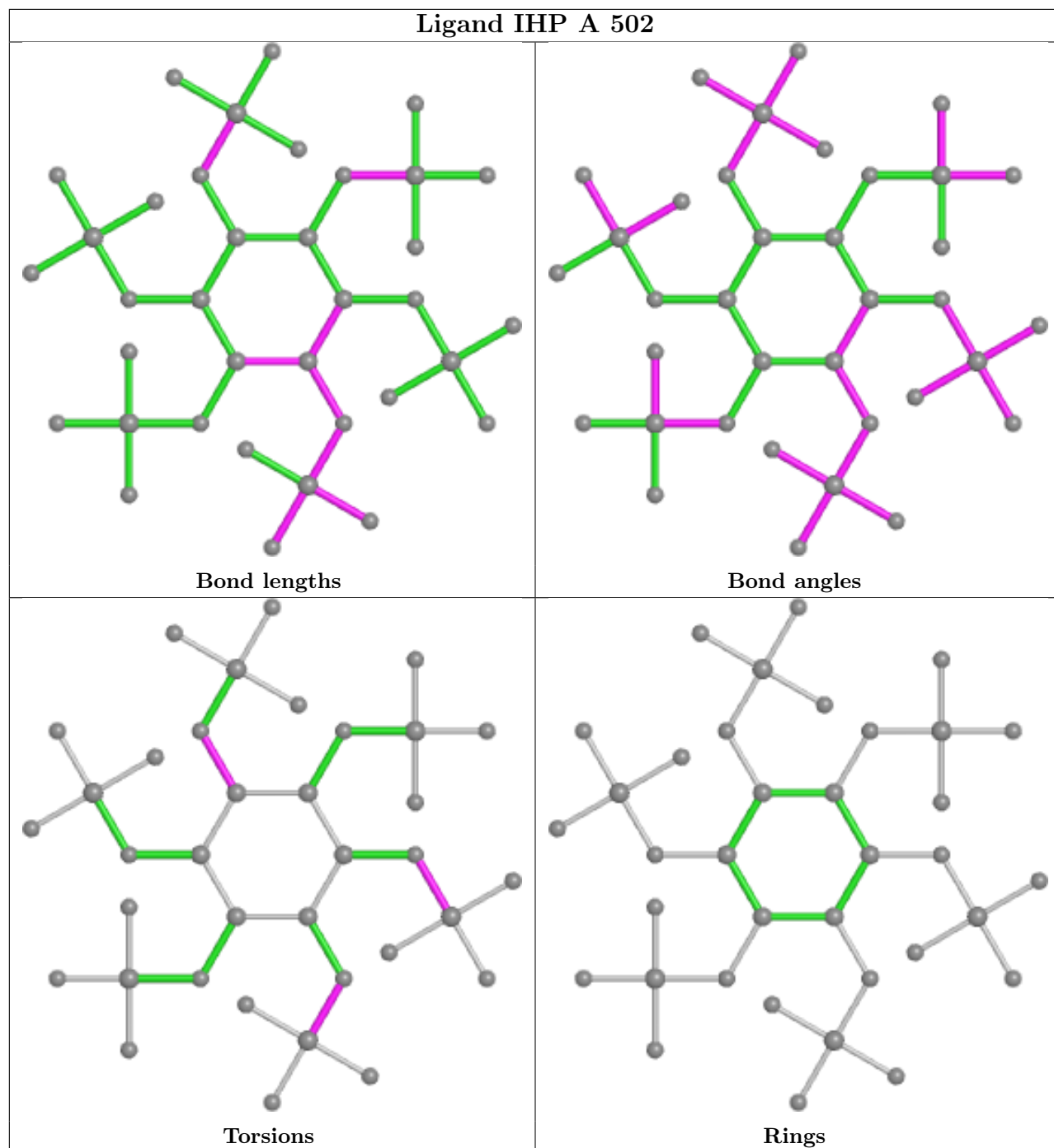
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	154/171 (90%)	-0.36	3 (1%)	66	74	10, 22, 49, 73	0
1	B	153/171 (89%)	-0.23	6 (3%)	39	49	12, 22, 62, 88	0
All	All	307/342 (89%)	-0.29	9 (2%)	51	60	10, 22, 54, 88	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	GLY	4.0
1	B	125	ASN	3.2
1	B	201	SER	3.2
1	B	202	SER	3.2
1	B	119	ASN	3.2
1	B	123	PHE	2.8
1	A	126	ILE	2.6
1	A	123	PHE	2.1
1	A	185	ALA	2.0

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IHP	A	502	36/36	0.90	0.36	61,79,108,113	0
2	ZKS	B	501	40/40	0.98	0.10	21,59,92,102	0
2	ZKS	A	501	40/40	0.98	0.09	16,42,72,76	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.
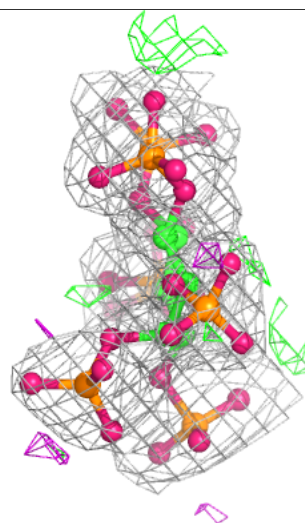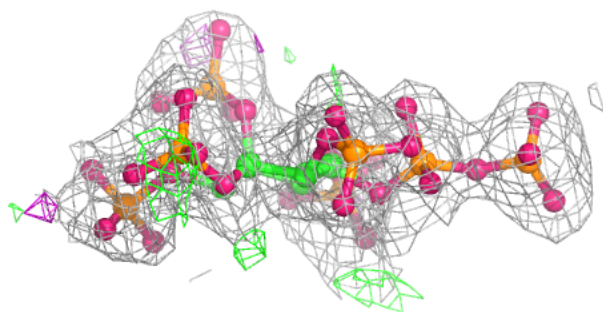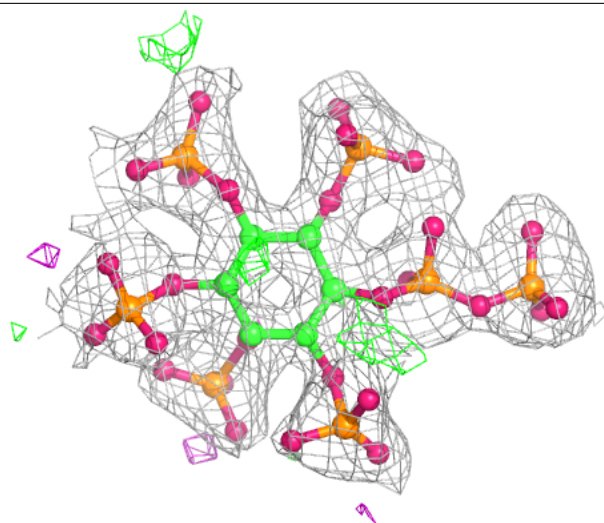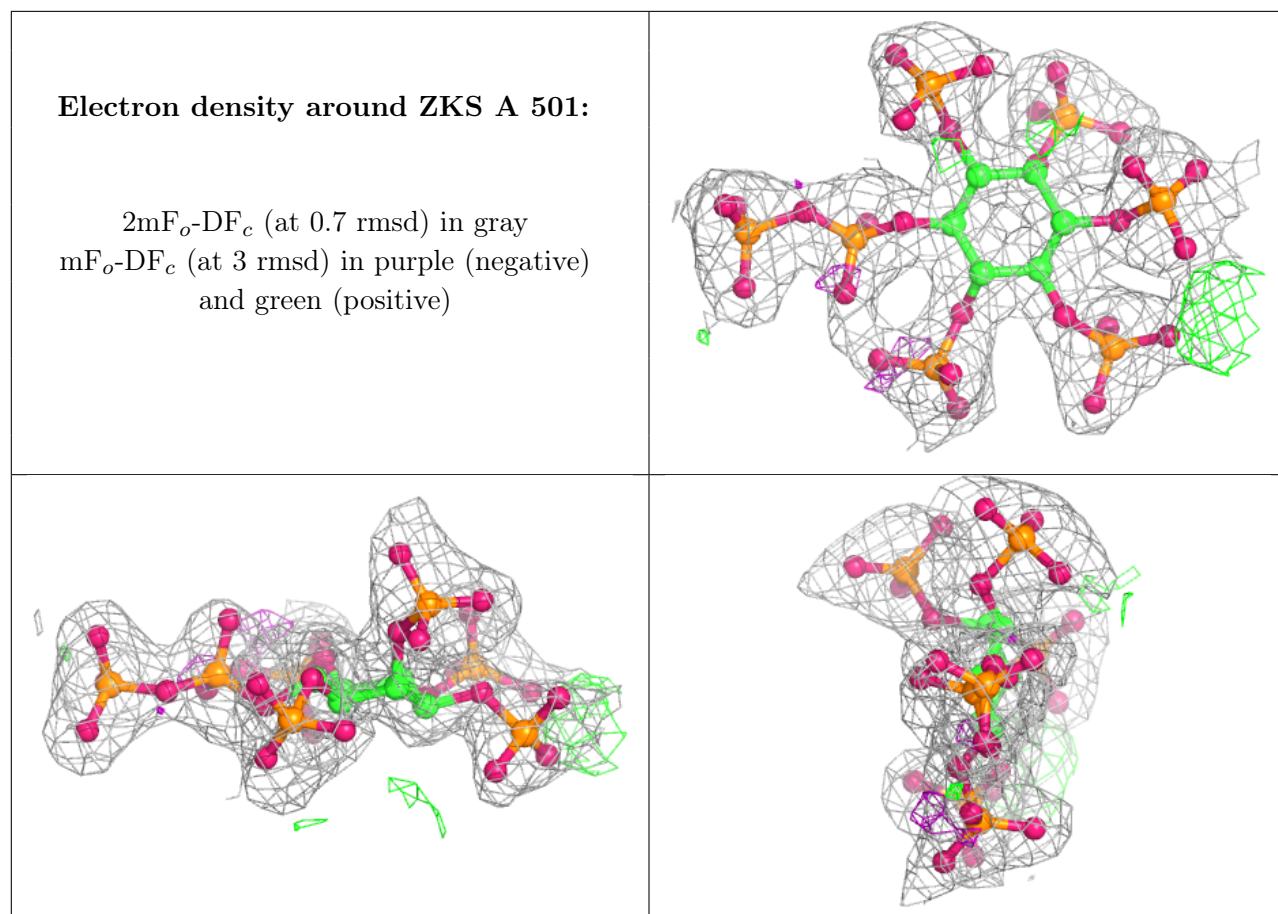
Electron density around IHP A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
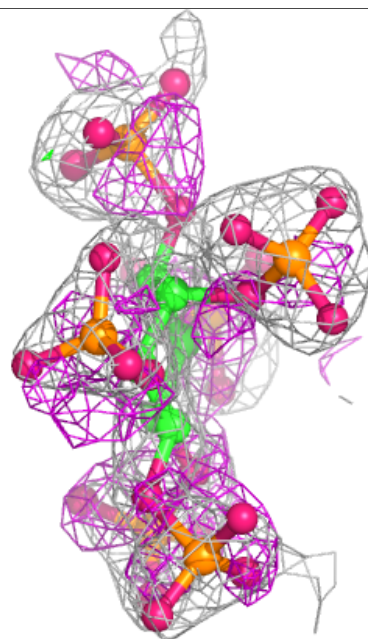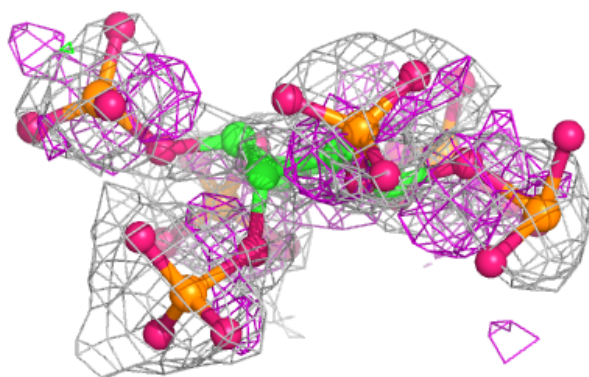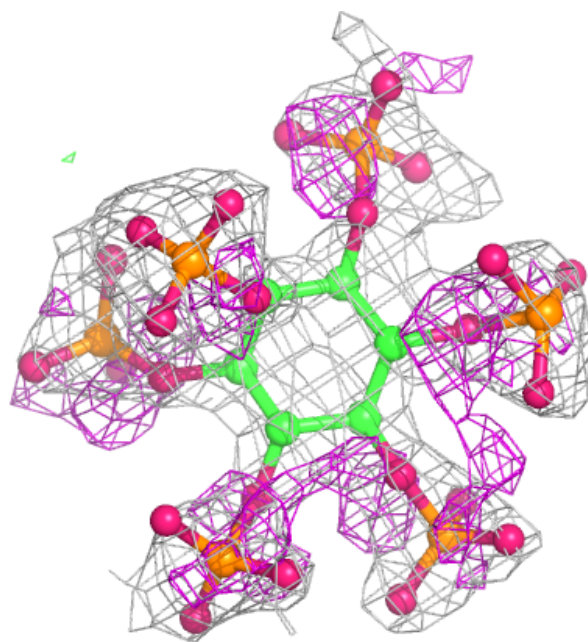
Electron density around ZKS B 501:

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

Electron density around ZKS A 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.