



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2025 – 12:25 PM JST

PDB ID : 8ZRS / pdb\_00008zrs  
Title : Crystal structure of Skd3, AAA+ only  
Authors : Lee, S.; Lee, C.  
Deposited on : 2024-06-05  
Resolution : 3.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

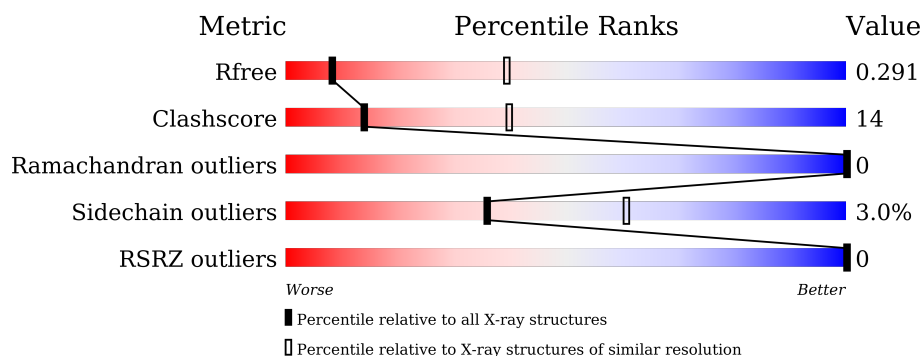
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	A	362	<div> <div>54%</div> <div>22%</div> <div>•</div> <div>23%</div> </div>
1	B	362	<div> <div>57%</div> <div>24%</div> <div>•</div> <div>17%</div> </div>
1	C	362	<div> <div>57%</div> <div>25%</div> <div>•</div> <div>17%</div> </div>
1	D	362	<div> <div>58%</div> <div>23%</div> <div>•</div> <div>17%</div> </div>
1	E	362	<div> <div>53%</div> <div>23%</div> <div>•</div> <div>23%</div> </div>
1	F	362	<div> <div>56%</div> <div>23%</div> <div>•</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	362	
1	H	362	
1	I	362	
1	J	362	
1	K	362	
1	L	362	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28287 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 Caseinolytic peptidase B protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2275	1455	403	409	8			
1	B	301	Total	C	N	O	S	0	0	0
			2465	1570	444	443	8			
1	C	301	Total	C	N	O	S	0	0	0
			2470	1572	447	443	8			
1	D	299	Total	C	N	O	S	0	0	0
			2446	1559	439	440	8			
1	E	280	Total	C	N	O	S	0	0	0
			2287	1461	407	411	8			
1	F	291	Total	C	N	O	S	0	0	0
			2378	1513	427	430	8			
1	G	266	Total	C	N	O	S	0	0	0
			2172	1392	387	386	7			
1	H	288	Total	C	N	O	S	0	0	0
			2354	1504	421	421	8			
1	I	295	Total	C	N	O	S	0	0	0
			2413	1538	432	435	8			
1	J	293	Total	C	N	O	S	0	0	0
			2397	1530	428	431	8			
1	K	269	Total	C	N	O	S	0	0	0
			2193	1404	391	391	7			
1	L	291	Total	C	N	O	S	0	0	0
			2377	1513	429	427	8			

There are 12 discrepancies between the modelled and reference sequences:

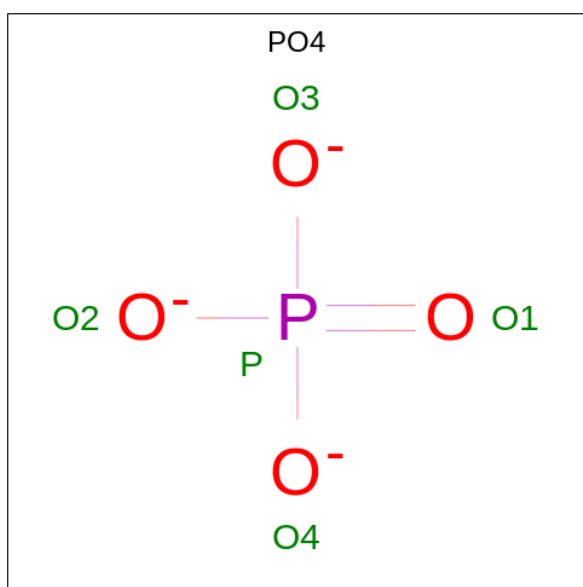
Chain	Residue	Modelled	Actual	Comment	Reference
A	294	SER	-	expression tag	UNP A0A8M3AT32
B	294	SER	-	expression tag	UNP A0A8M3AT32
C	294	SER	-	expression tag	UNP A0A8M3AT32
D	294	SER	-	expression tag	UNP A0A8M3AT32
E	294	SER	-	expression tag	UNP A0A8M3AT32

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Chain	Residue	Modelled	Actual	Comment	Reference
F	294	SER	-	expression tag	UNP A0A8M3AT32
G	294	SER	-	expression tag	UNP A0A8M3AT32
H	294	SER	-	expression tag	UNP A0A8M3AT32
I	294	SER	-	expression tag	UNP A0A8M3AT32
J	294	SER	-	expression tag	UNP A0A8M3AT32
K	294	SER	-	expression tag	UNP A0A8M3AT32
L	294	SER	-	expression tag	UNP A0A8M3AT32

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0

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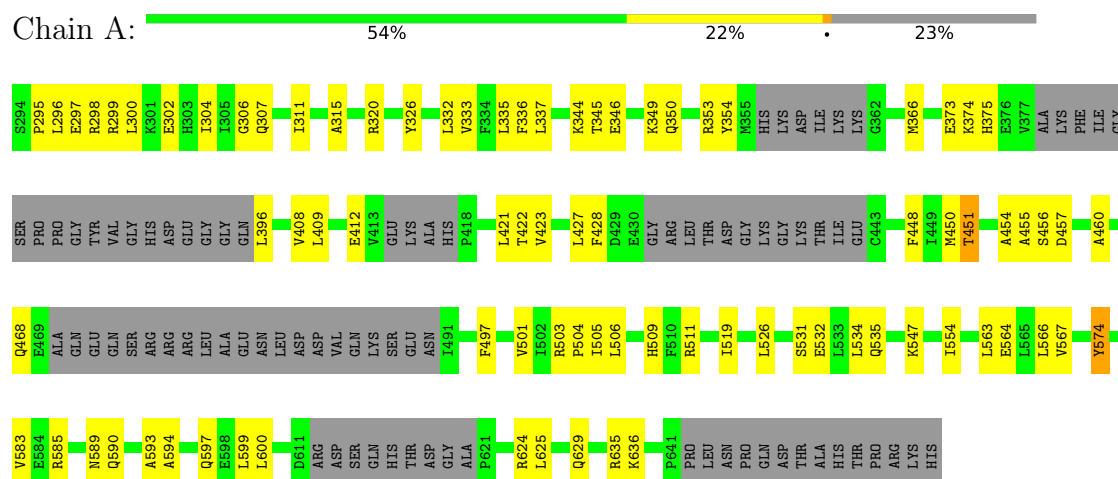
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		

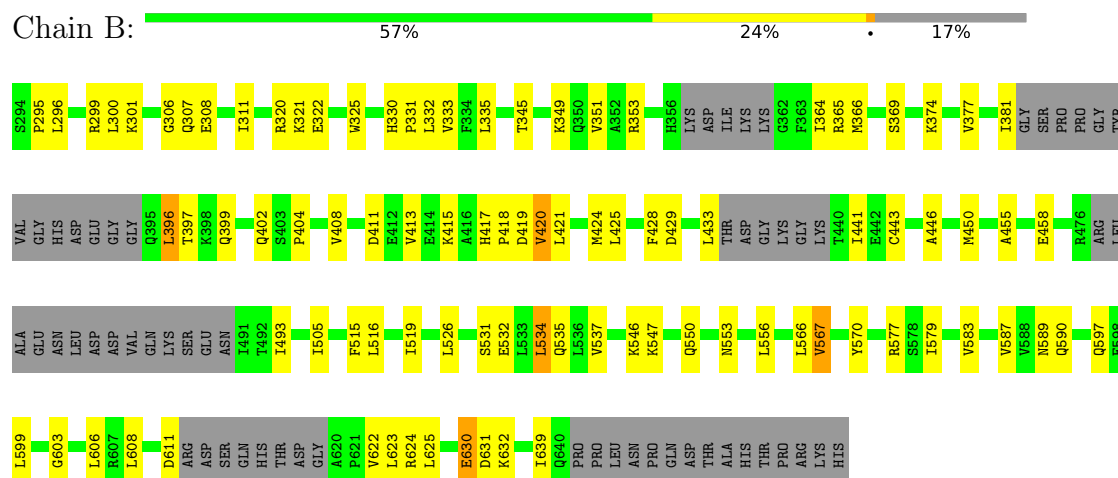
### 3 Residue-property plots [i](#)

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: Caseinolytic peptidase B protein homolog

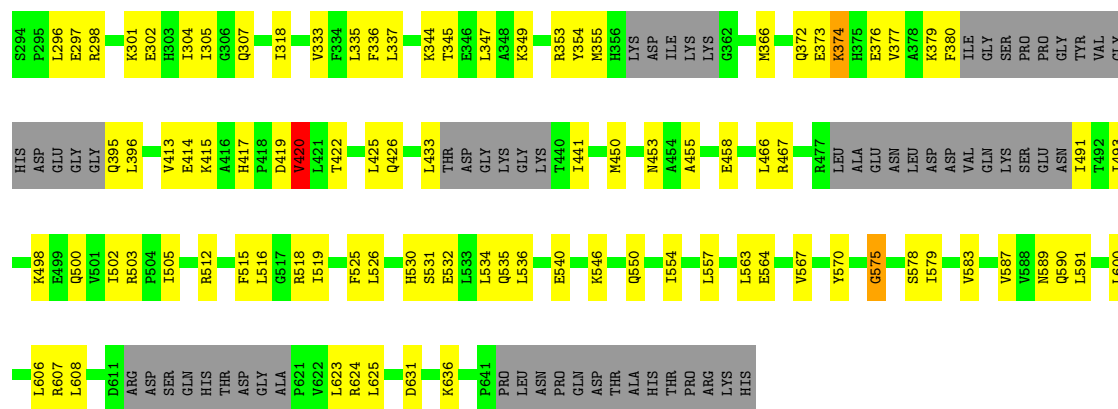


#### • Molecule 1: Caseinolytic peptidase B protein homolog



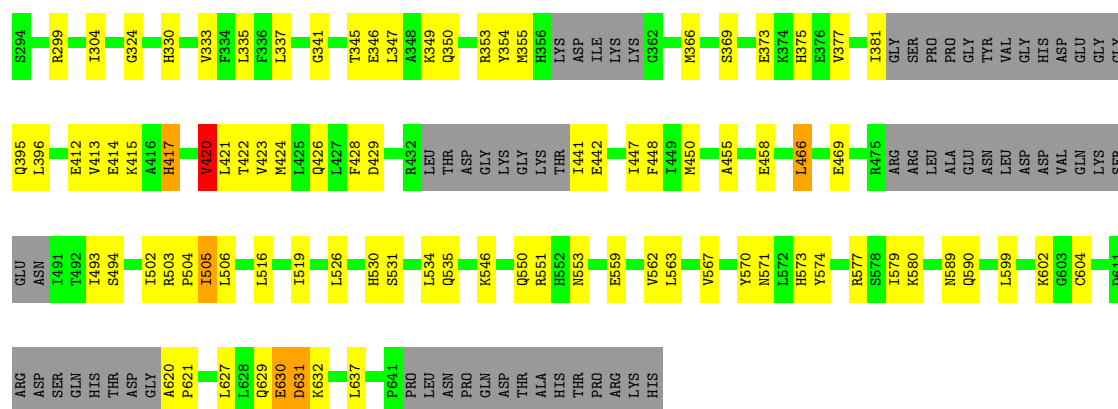
#### • Molecule 1: Caseinolytic peptidase B protein homolog





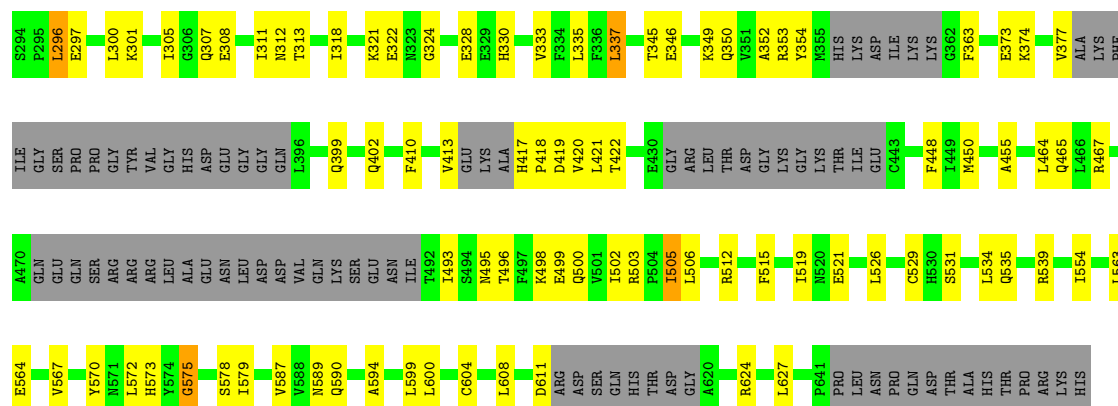
• Molecule 1: Caseinolytic peptidase B protein homolog

Chain D: 58% 23% 17%



• Molecule 1: Caseinolytic peptidase B protein homolog

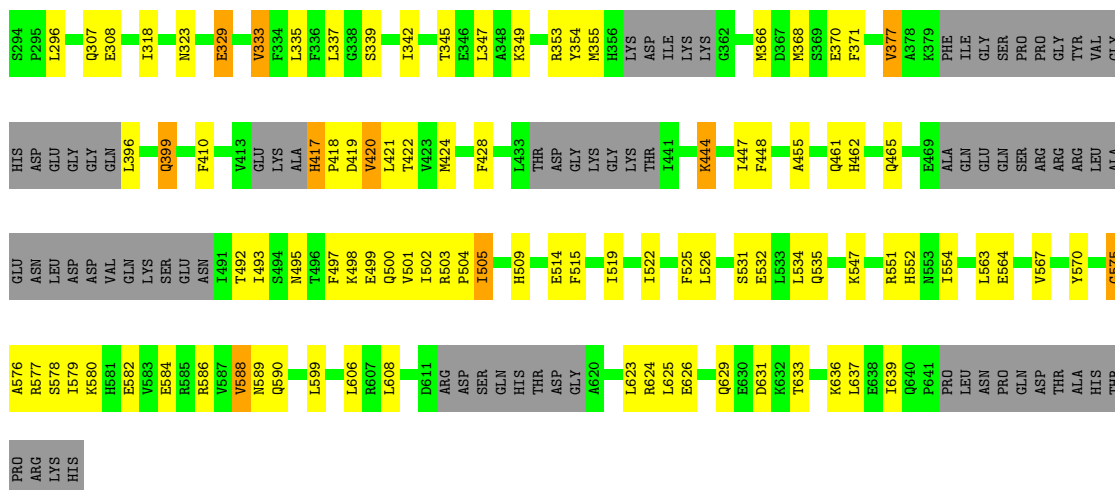
Chain E: 53% 23% 23%



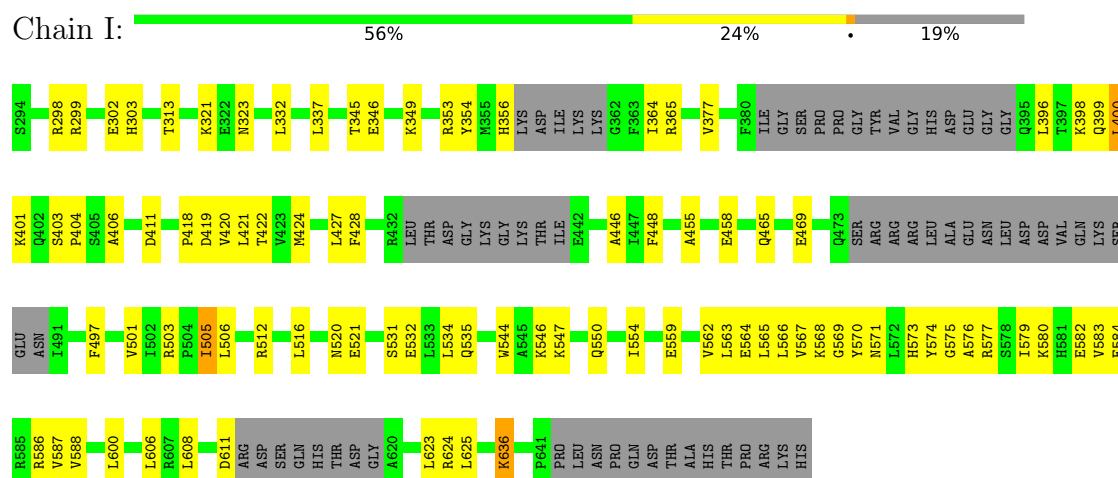
• Molecule 1: Caseinolytic peptidase B protein homolog

Chain F: 56% 23% 20%

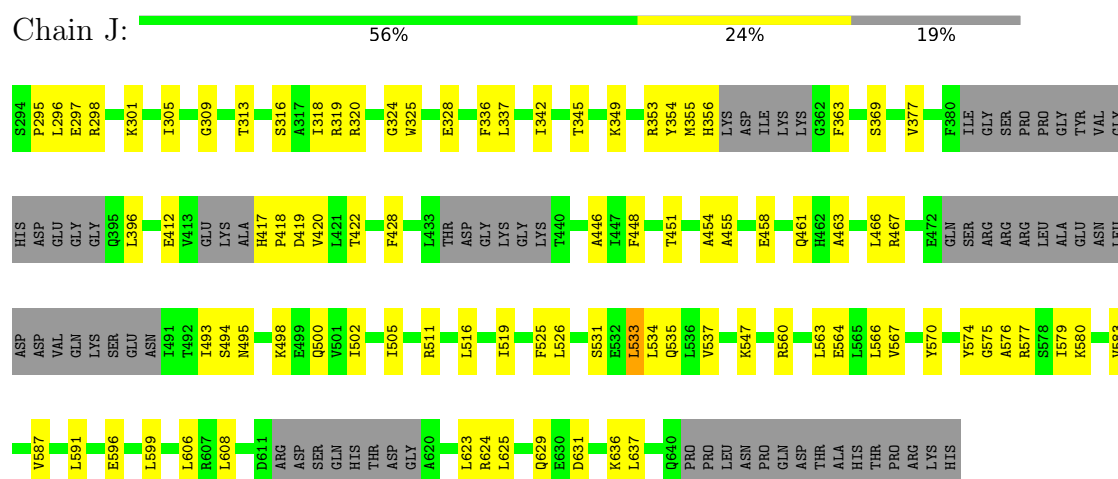




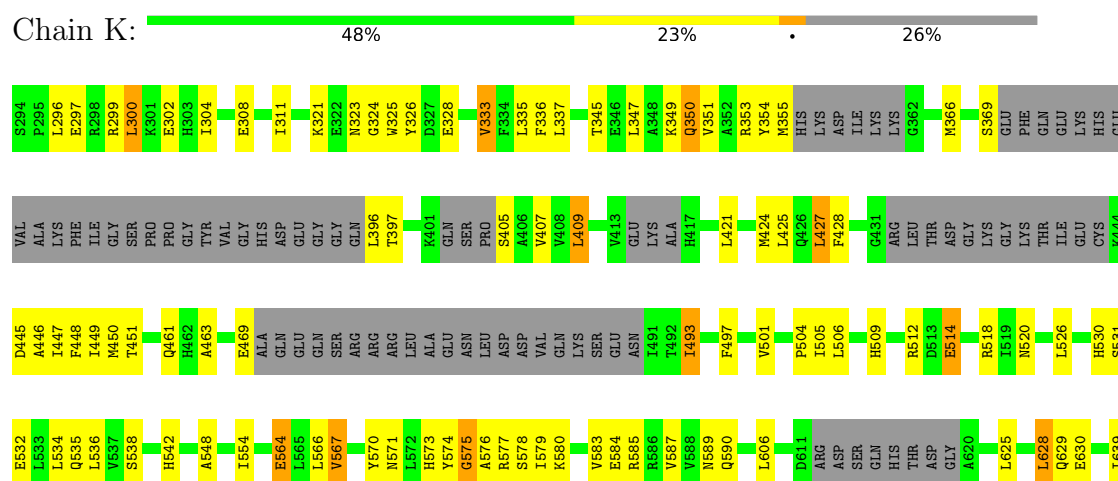
• Molecule 1: Caseinolytic peptidase B protein homolog



• Molecule 1: Caseinolytic peptidase B protein homolog



• Molecule 1: Caseinolytic peptidase B protein homolog





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.86Å 172.41Å 140.87Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	14.90 – 3.39 14.90 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.8 (14.90-3.39) 91.4 (14.90-3.39)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.229 , 0.284 0.274 , 0.291	Depositor DCC
$R_{free}$ test set	71081 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.0	Xtriage
Anisotropy	0.975	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 17.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.077 for l,k,-h-l 0.077 for -h-l,k,h 0.439 for h,-k,-h-l 0.076 for l,-k,h 0.078 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0507e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4

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	0.56	0/2313	0.98	1/3108 (0.0%)
1	B	0.51	0/2506	0.95	3/3367 (0.1%)
1	C	0.53	0/2512	0.96	7/3374 (0.2%)
1	D	0.55	0/2488	0.97	4/3344 (0.1%)
1	E	0.52	0/2326	0.96	2/3128 (0.1%)
1	F	0.51	0/2418	0.92	1/3249 (0.0%)
1	G	0.59	0/2207	0.98	3/2968 (0.1%)
1	H	0.59	0/2394	0.98	3/3218 (0.1%)
1	I	0.58	0/2455	1.01	4/3300 (0.1%)
1	J	0.59	0/2437	0.98	4/3275 (0.1%)
1	K	0.66	0/2228	1.10	5/2994 (0.2%)
1	L	0.51	0/2417	0.93	2/3248 (0.1%)
All	All	0.56	0/28701	0.98	39/38573 (0.1%)

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	420	VAL	N-CA-C	-9.90	98.74	112.50
1	D	420	VAL	N-CA-C	-8.38	100.67	113.16
1	B	631	ASP	N-CA-C	-7.44	104.20	113.20
1	D	631	ASP	N-CA-C	-6.98	104.63	113.01
1	H	377	VAL	N-CA-C	-6.89	102.43	111.05

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	2275	0	2320	60	0
1	B	2465	0	2510	73	0
1	C	2470	0	2515	65	0
1	D	2446	0	2486	60	0
1	E	2287	0	2324	68	0
1	F	2378	0	2412	61	0
1	G	2172	0	2223	80	0
1	H	2354	0	2399	83	0
1	I	2413	0	2446	81	0
1	J	2397	0	2435	81	0
1	K	2193	0	2243	71	0
1	L	2377	0	2417	66	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	1	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	1	0
All	All	28287	0	28730	805	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 14.

The worst 5 of 805 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:I:377:VAL:HG22	1:I:420:VAL:HG23	1.19	1.13
1:I:547:LYS:NZ	1:J:328:GLU:CG	2.20	1.04
1:J:324:GLY:HA2	1:J:328:GLU:OE2	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:547:LYS:NZ	1:J:328:GLU:HG2	1.76	1.00
1:I:503:ARG:NH1	1:I:516:LEU:CD1	2.24	0.99

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	264/362 (73%)	260 (98%)	4 (2%)	0	100	100
1	B	289/362 (80%)	281 (97%)	8 (3%)	0	100	100
1	C	289/362 (80%)	280 (97%)	9 (3%)	0	100	100
1	D	287/362 (79%)	278 (97%)	9 (3%)	0	100	100
1	E	266/362 (74%)	260 (98%)	6 (2%)	0	100	100
1	F	279/362 (77%)	273 (98%)	6 (2%)	0	100	100
1	G	250/362 (69%)	246 (98%)	4 (2%)	0	100	100
1	H	274/362 (76%)	266 (97%)	8 (3%)	0	100	100
1	I	283/362 (78%)	276 (98%)	7 (2%)	0	100	100
1	J	279/362 (77%)	272 (98%)	7 (2%)	0	100	100
1	K	253/362 (70%)	246 (97%)	7 (3%)	0	100	100
1	L	279/362 (77%)	272 (98%)	7 (2%)	0	100	100
All	All	3292/4344 (76%)	3210 (98%)	82 (2%)	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	249/318 (78%)	241 (97%)	8 (3%)	34	59
1	B	267/318 (84%)	260 (97%)	7 (3%)	41	64
1	C	268/318 (84%)	262 (98%)	6 (2%)	47	68
1	D	265/318 (83%)	259 (98%)	6 (2%)	45	67
1	E	249/318 (78%)	242 (97%)	7 (3%)	38	62
1	F	258/318 (81%)	249 (96%)	9 (4%)	31	56
1	G	236/318 (74%)	223 (94%)	13 (6%)	18	44
1	H	256/318 (80%)	246 (96%)	10 (4%)	27	53
1	I	261/318 (82%)	258 (99%)	3 (1%)	70	81
1	J	260/318 (82%)	256 (98%)	4 (2%)	60	76
1	K	238/318 (75%)	223 (94%)	15 (6%)	15	40
1	L	257/318 (81%)	253 (98%)	4 (2%)	58	75
All	All	3064/3816 (80%)	2972 (97%)	92 (3%)	36	61

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	329	GLU
1	J	466	LEU
1	H	370	GLU
1	H	588	VAL
1	K	350	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	590	GLN
1	I	465	GLN
1	H	461	GLN
1	I	399	GLN

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Mol	Chain	Res	Type
1	J	417	HIS

### 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](#)

12 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	PO4	C	701	-	4,4,4	0.94	0	6,6,6	0.36	0
2	PO4	G	701	-	4,4,4	0.94	0	6,6,6	0.38	0
2	PO4	A	701	-	4,4,4	0.93	0	6,6,6	0.51	0
2	PO4	L	701	-	4,4,4	0.96	0	6,6,6	0.37	0
2	PO4	K	701	-	4,4,4	0.94	0	6,6,6	0.43	0
2	PO4	F	701	-	4,4,4	0.92	0	6,6,6	0.52	0
2	PO4	B	701	-	4,4,4	0.93	0	6,6,6	0.44	0
2	PO4	I	701	-	4,4,4	0.92	0	6,6,6	0.50	0
2	PO4	H	701	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	D	701	-	4,4,4	0.94	0	6,6,6	0.47	0
2	PO4	E	701	-	4,4,4	0.96	0	6,6,6	0.45	0
2	PO4	J	701	-	4,4,4	0.92	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

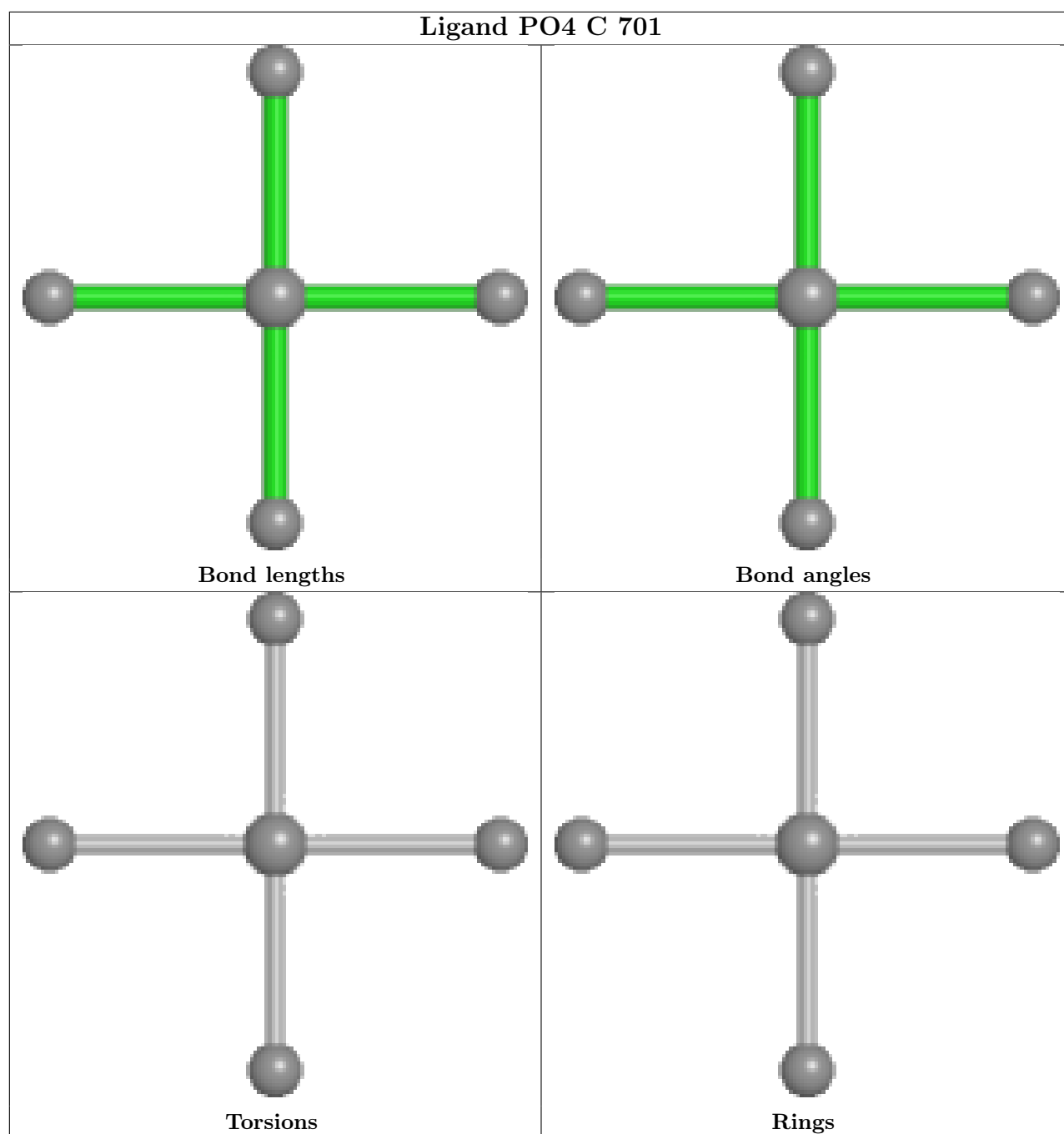
There are no torsion outliers.

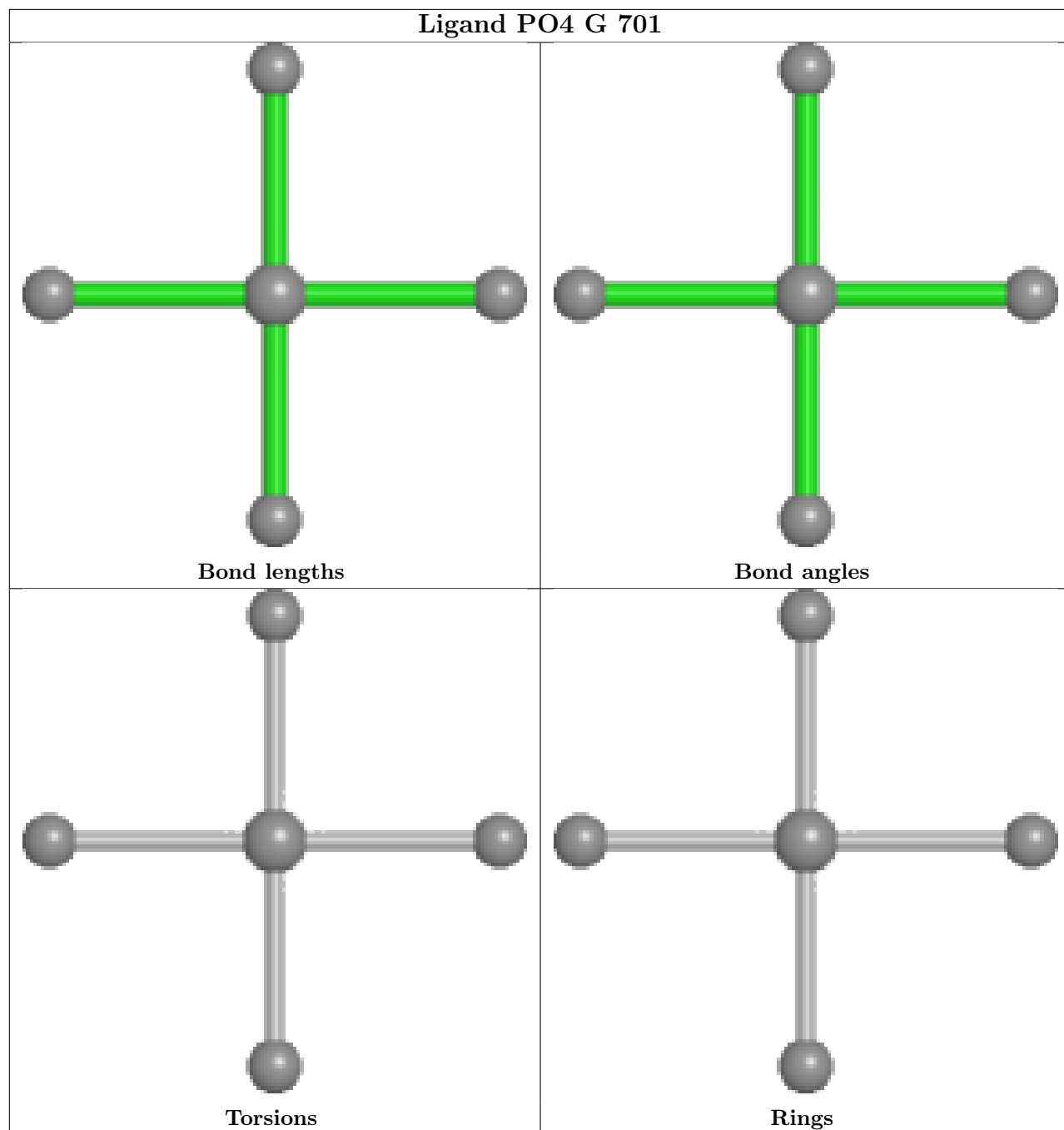
There are no ring outliers.

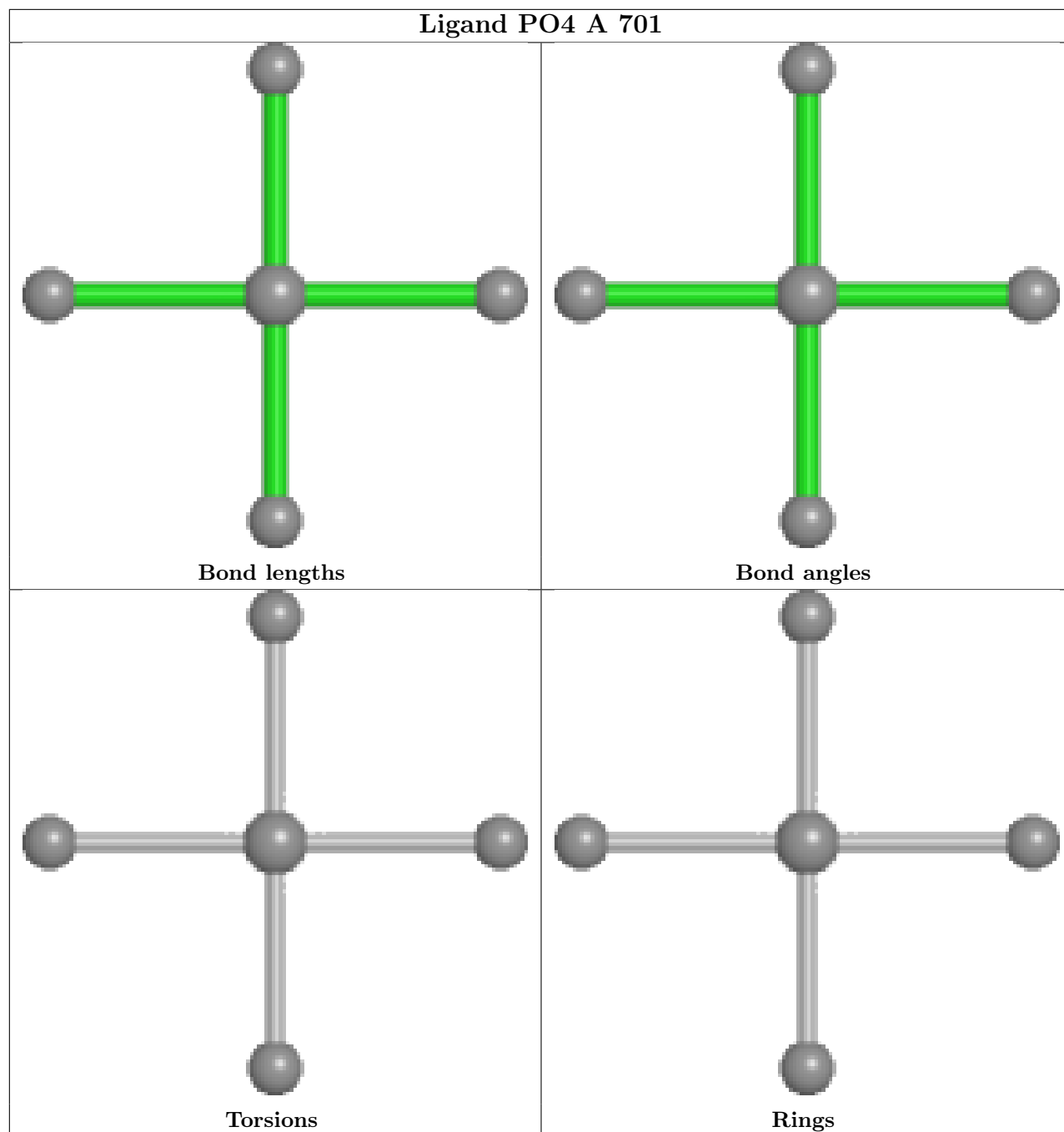
6 monomers are involved in 6 short contacts:

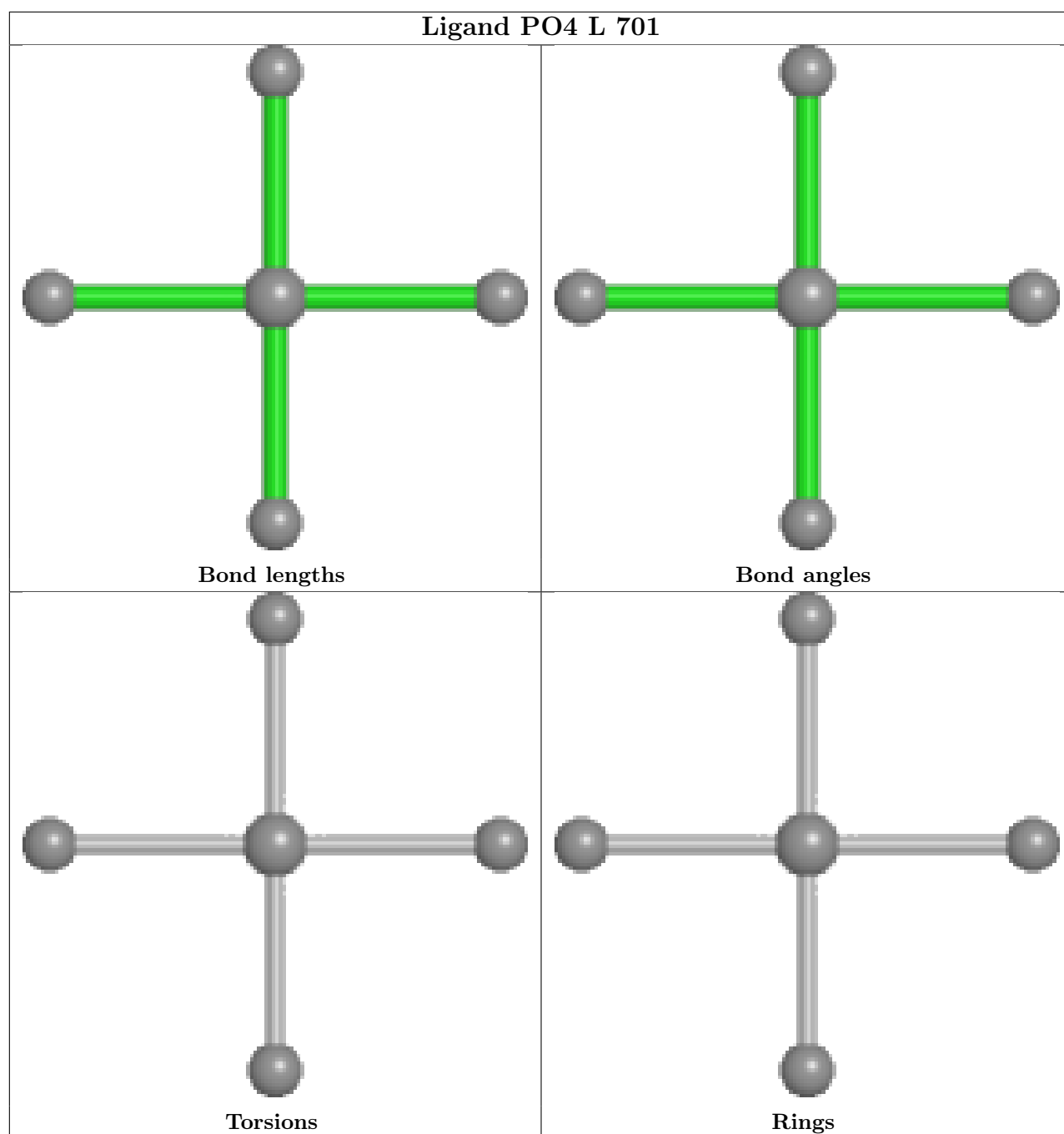
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	PO4	1	0
2	L	701	PO4	1	0
2	F	701	PO4	1	0
2	B	701	PO4	1	0
2	I	701	PO4	1	0
2	D	701	PO4	1	0

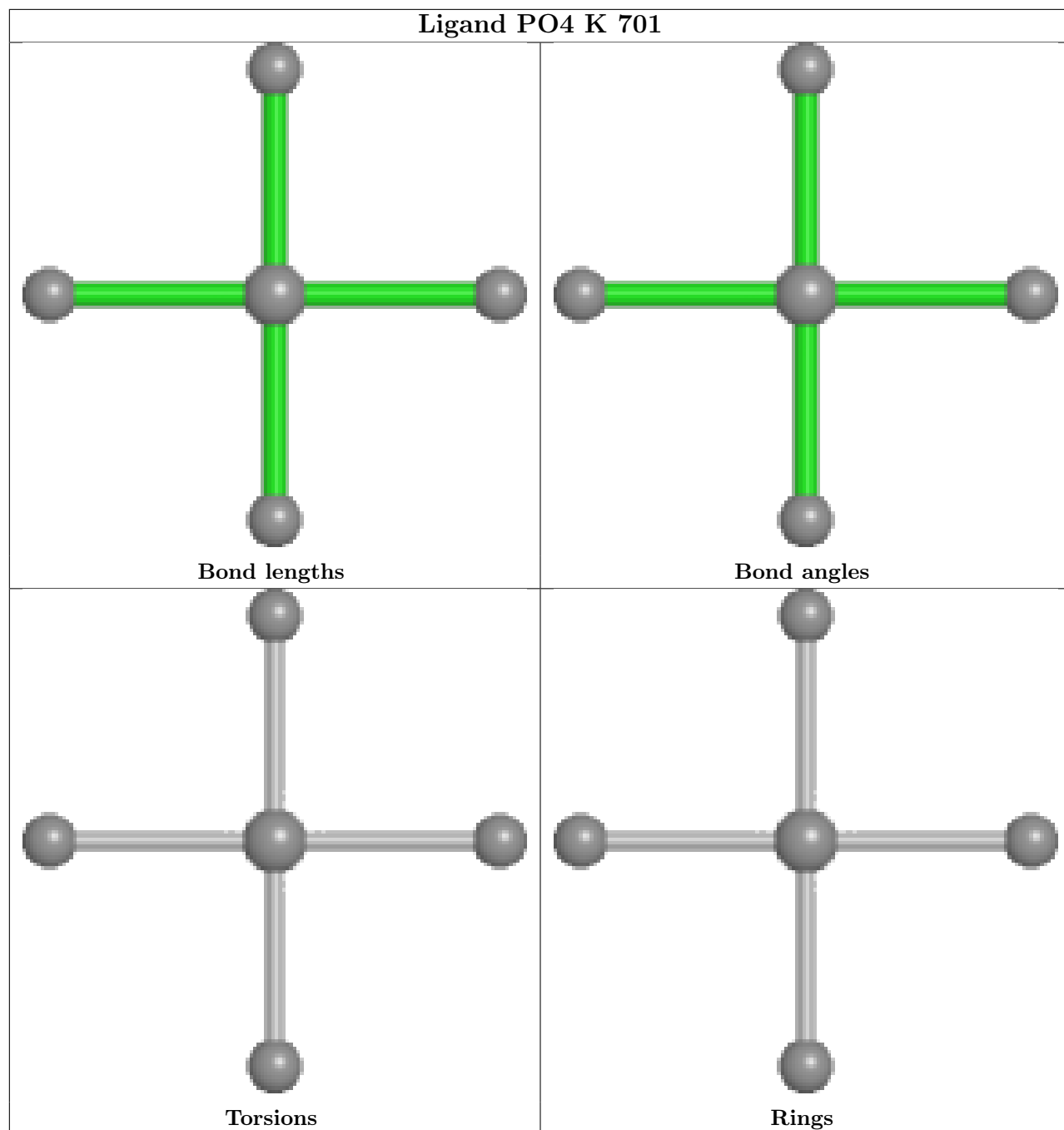
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

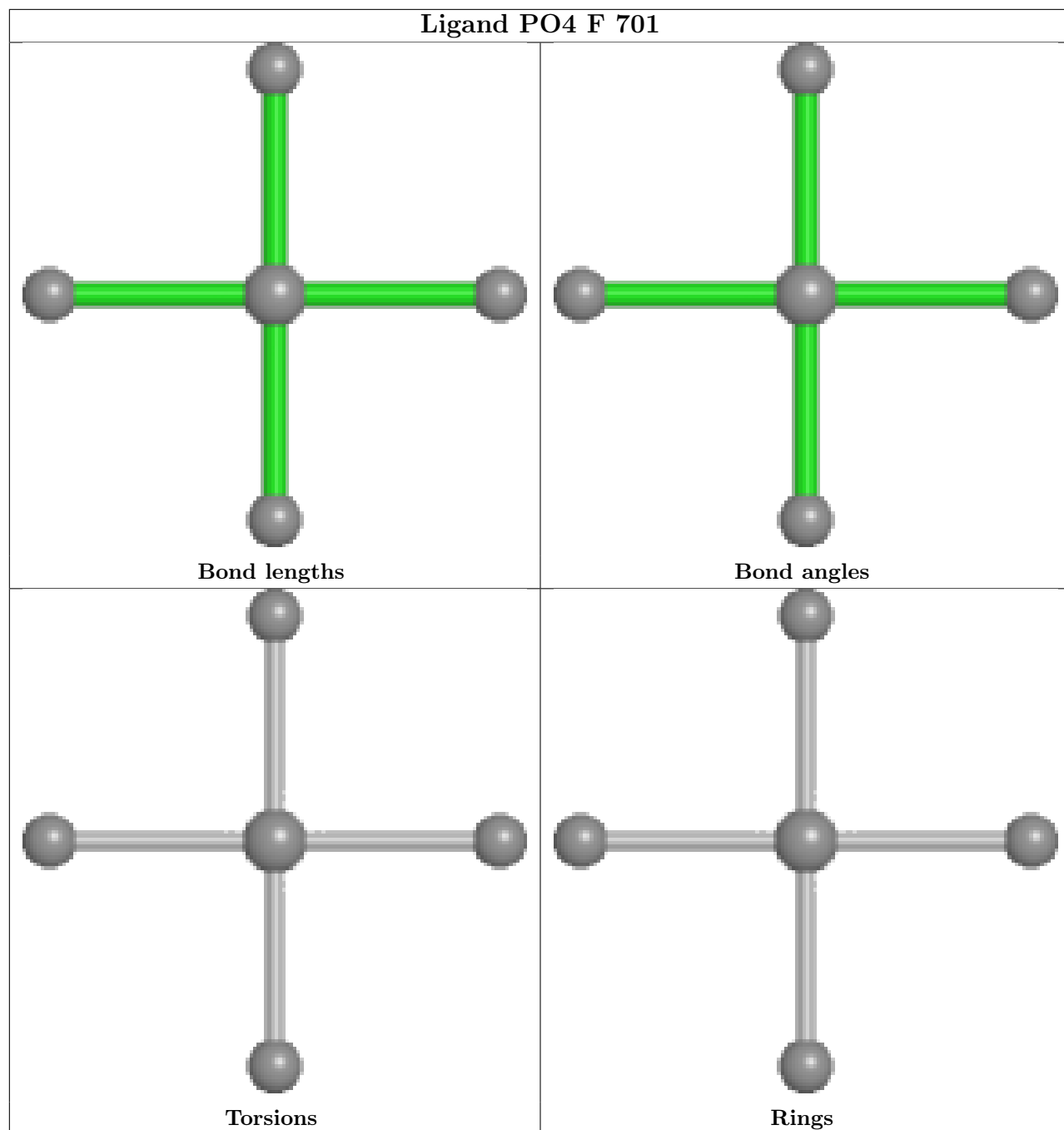




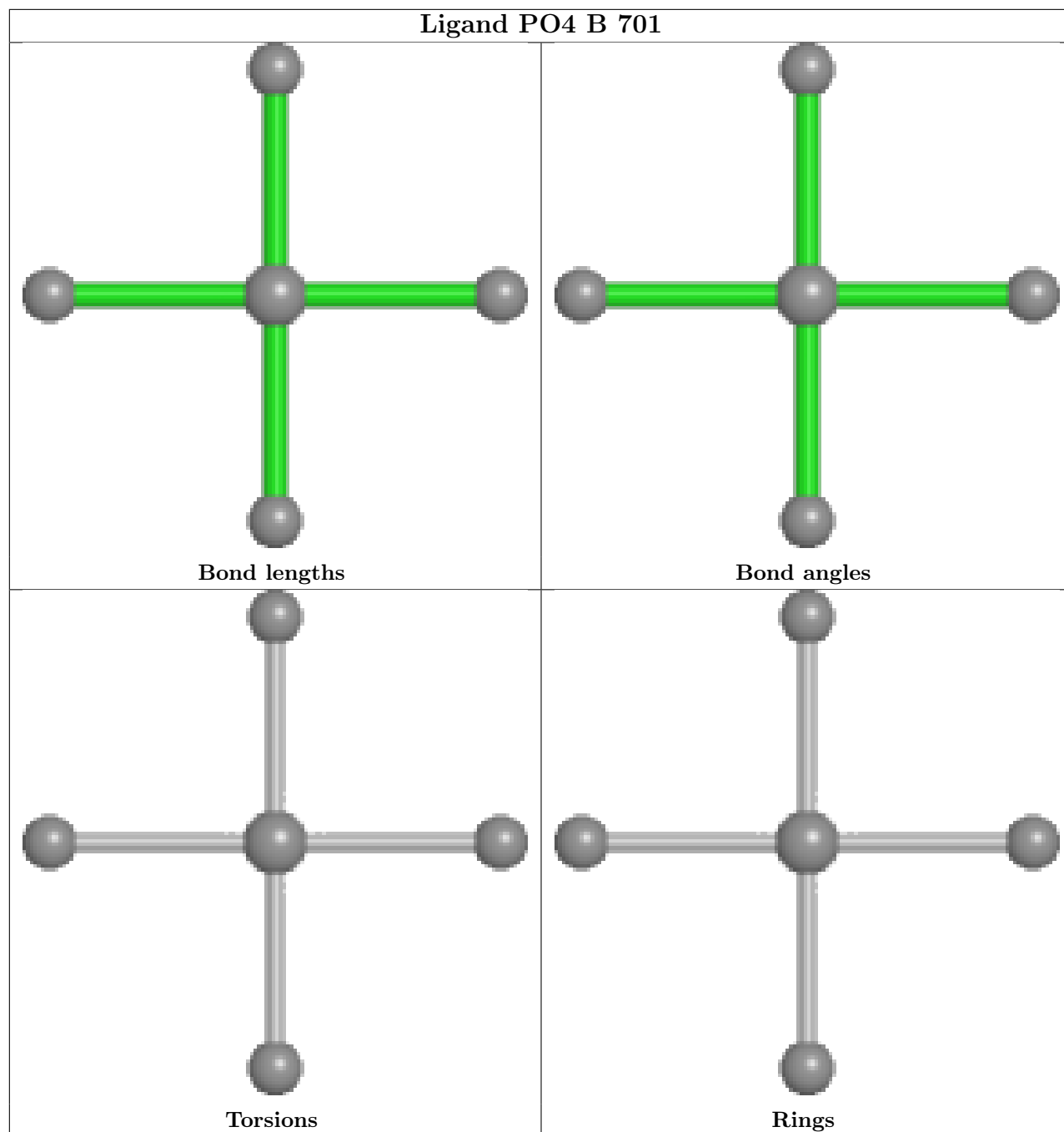


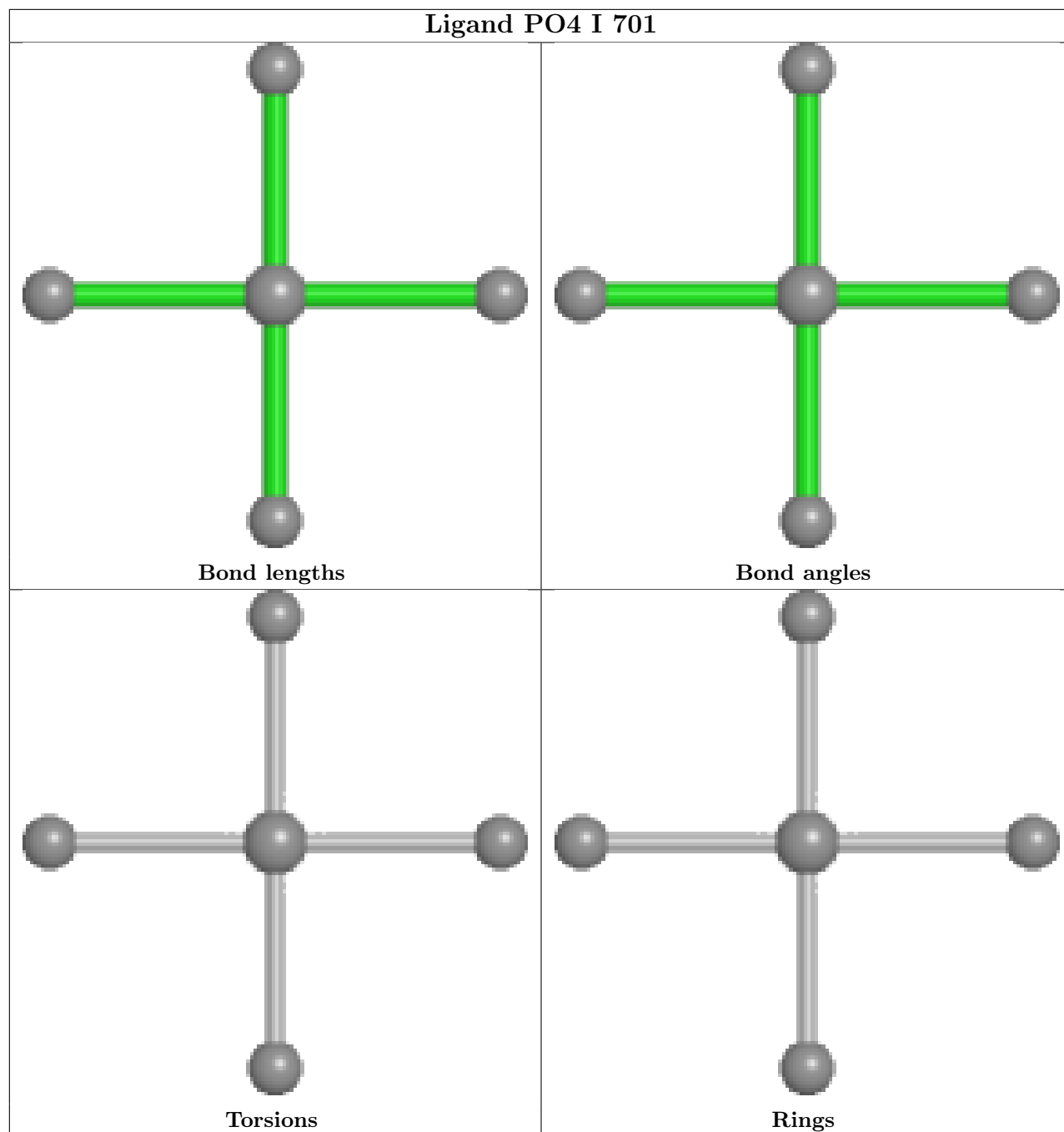


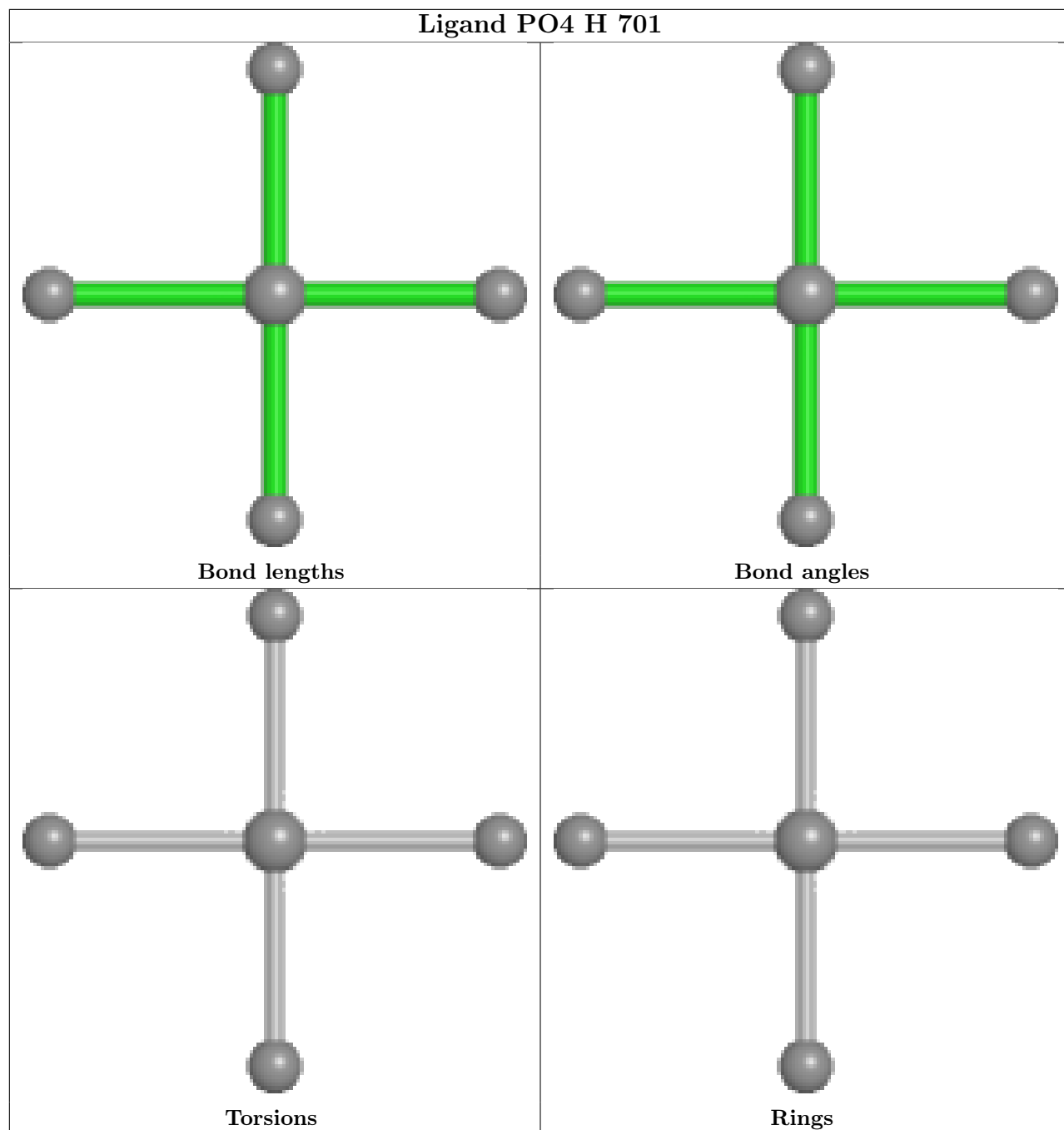


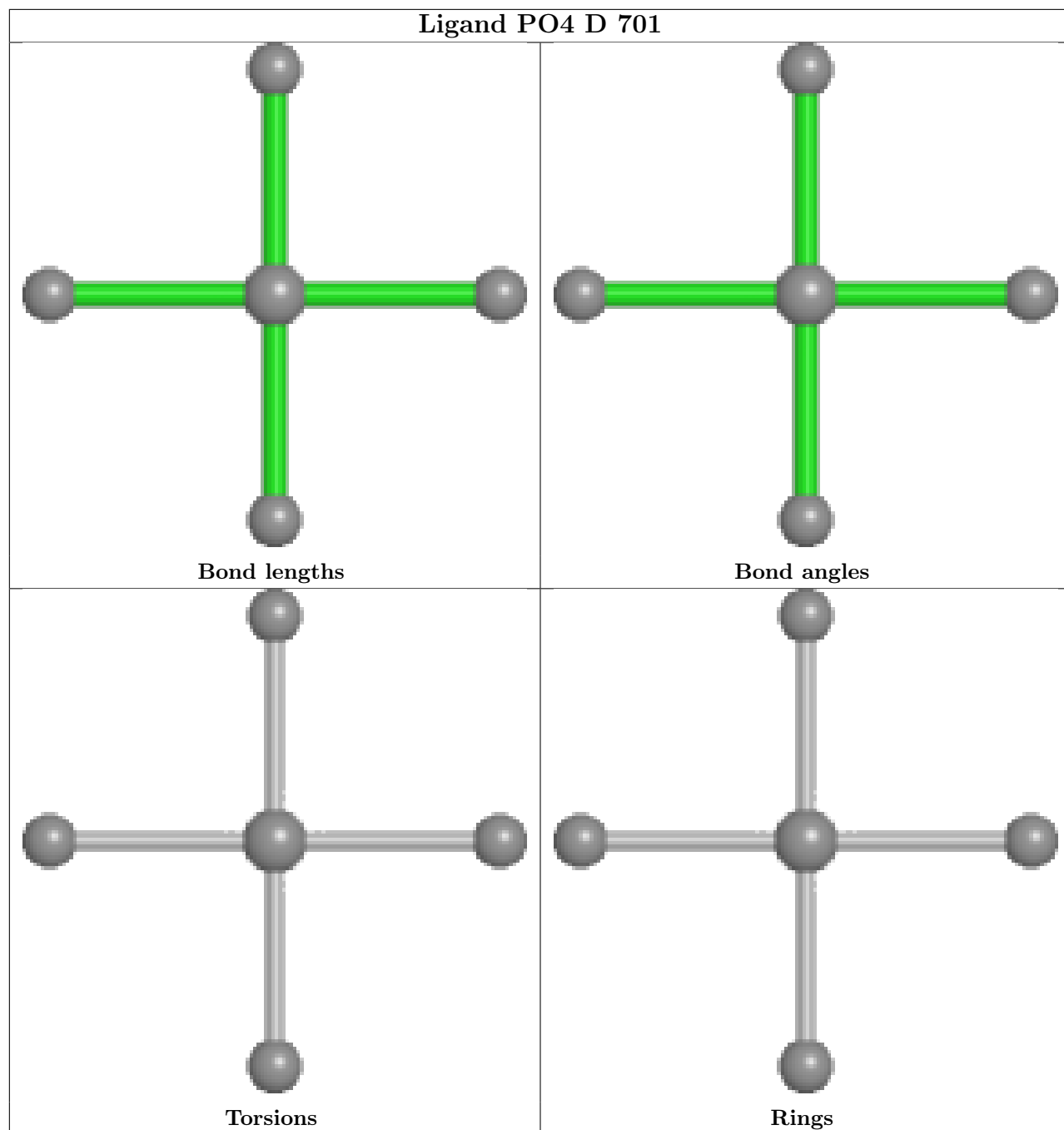


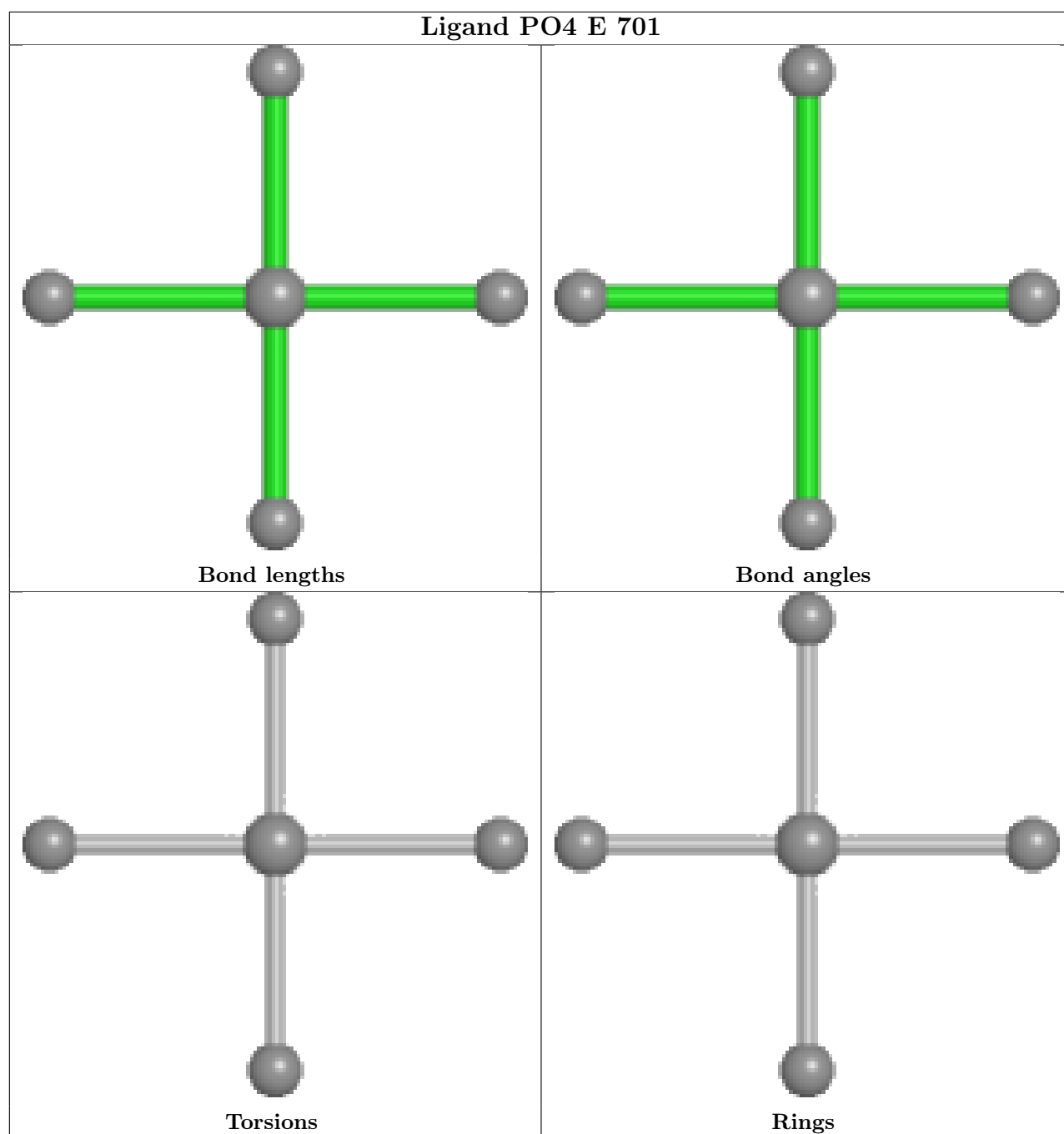


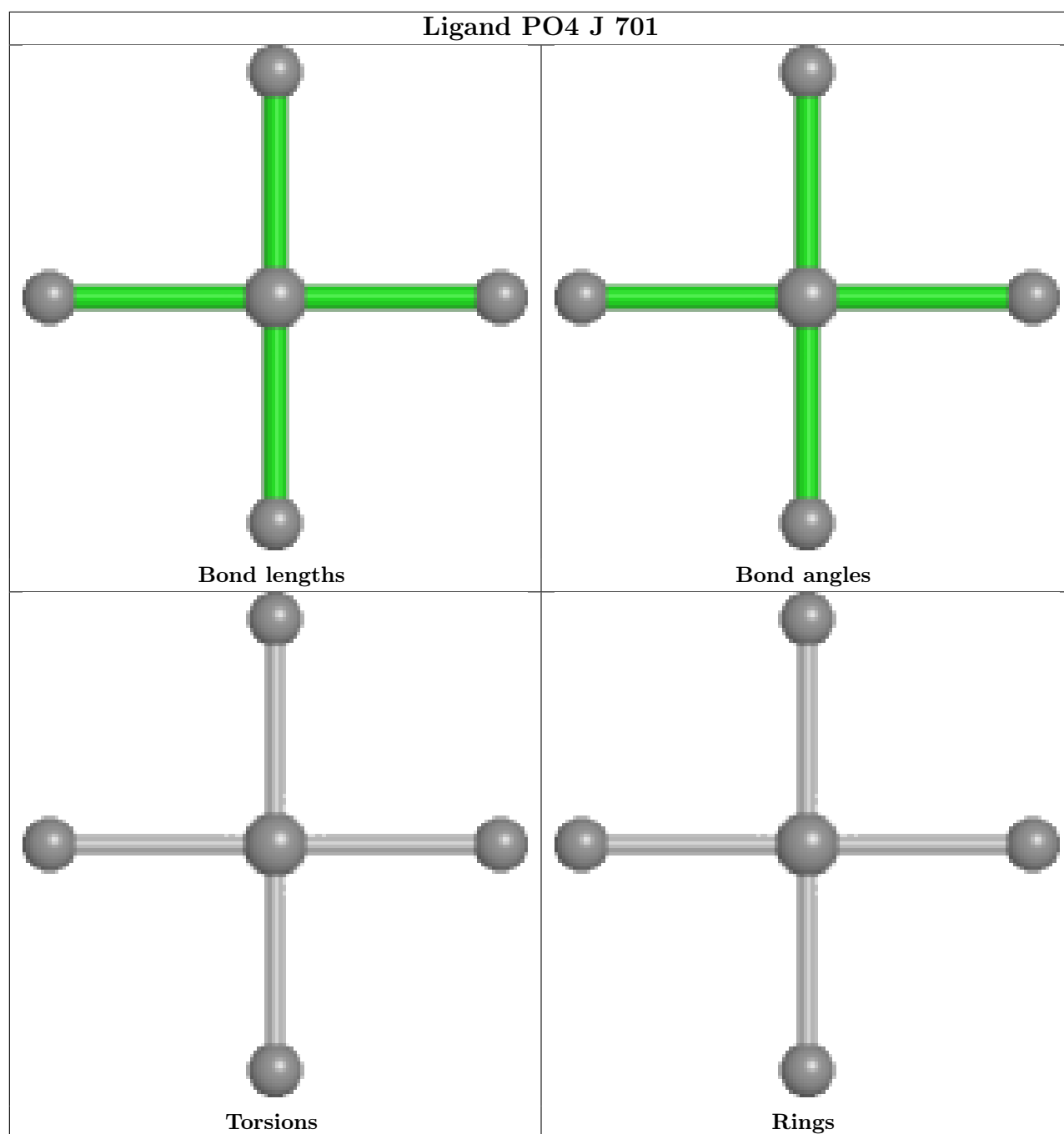












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	278/362 (76%)	-0.81	0 100 100	52, 96, 163, 228	0
1	B	301/362 (83%)	-1.04	0 100 100	45, 79, 130, 166	0
1	C	301/362 (83%)	-1.04	0 100 100	44, 78, 124, 156	0
1	D	299/362 (82%)	-1.05	0 100 100	45, 74, 128, 198	0
1	E	280/362 (77%)	-0.76	0 100 100	50, 98, 164, 241	0
1	F	291/362 (80%)	-0.91	0 100 100	42, 82, 129, 186	0
1	G	266/362 (73%)	-0.67	0 100 100	45, 113, 182, 259	0
1	H	288/362 (79%)	-0.91	0 100 100	51, 96, 146, 193	0
1	I	295/362 (81%)	-1.03	0 100 100	41, 76, 126, 198	0
1	J	293/362 (80%)	-0.86	0 100 100	50, 96, 148, 195	0
1	K	269/362 (74%)	-0.69	0 100 100	48, 111, 181, 227	0
1	L	291/362 (80%)	-1.02	0 100 100	46, 82, 124, 177	0
All	All	3452/4344 (79%)	-0.90	0 100 100	41, 88, 155, 259	0

There are no RSRZ outliers to report.

### 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

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.

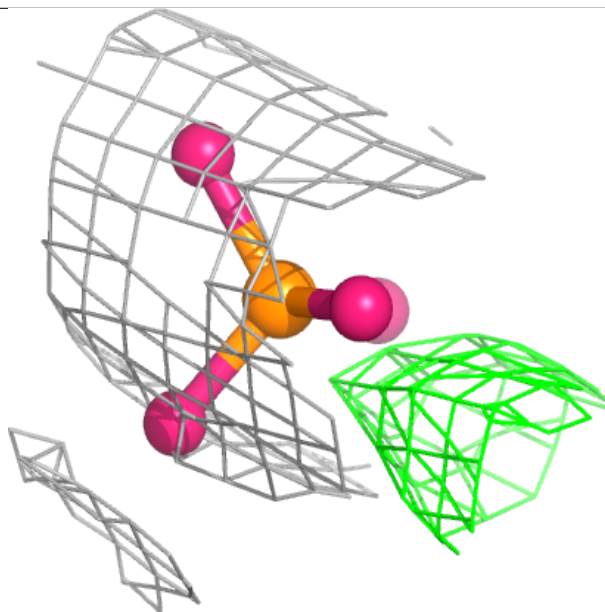
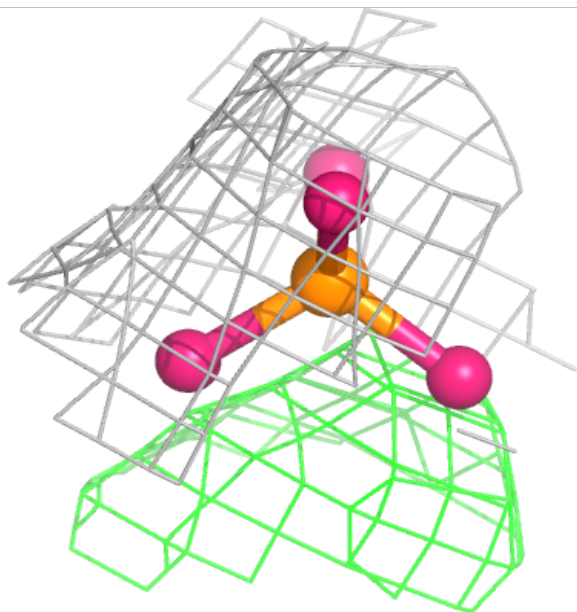
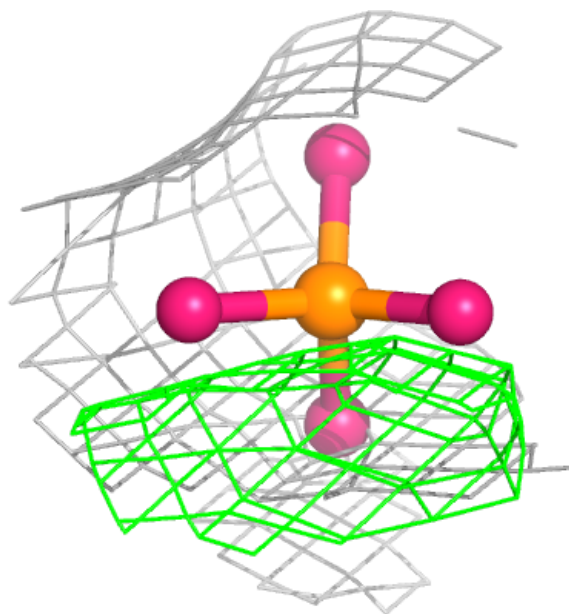
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	G	701	5/5	0.94	0.07	190,190,191,191	0
2	PO4	K	701	5/5	0.94	0.07	152,152,152,153	0
2	PO4	E	701	5/5	0.96	0.05	120,122,124,125	0
2	PO4	L	701	5/5	0.96	0.06	95,98,102,103	0
2	PO4	J	701	5/5	0.97	0.06	134,134,135,136	0
2	PO4	F	701	5/5	0.97	0.05	97,98,101,102	0
2	PO4	D	701	5/5	0.97	0.04	102,103,106,107	0
2	PO4	A	701	5/5	0.98	0.04	177,178,178,179	0
2	PO4	H	701	5/5	0.98	0.05	137,138,138,141	0
2	PO4	I	701	5/5	0.98	0.05	98,99,102,103	0
2	PO4	C	701	5/5	0.99	0.04	93,96,99,103	0
2	PO4	B	701	5/5	0.99	0.05	101,104,107,109	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.



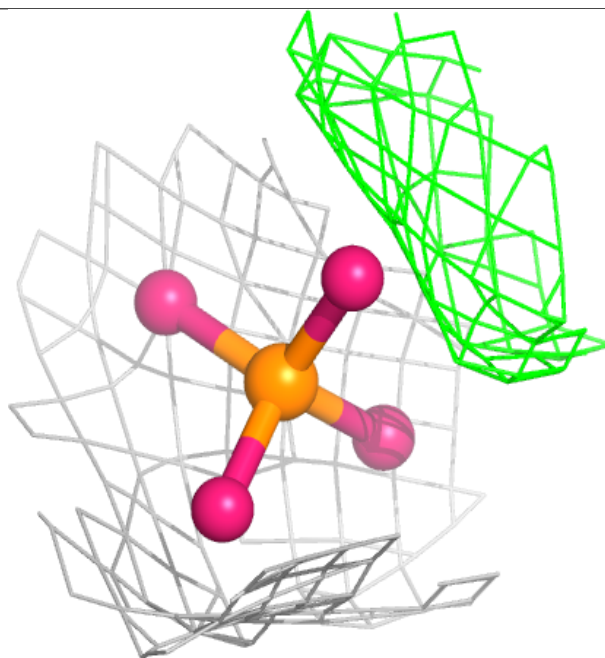
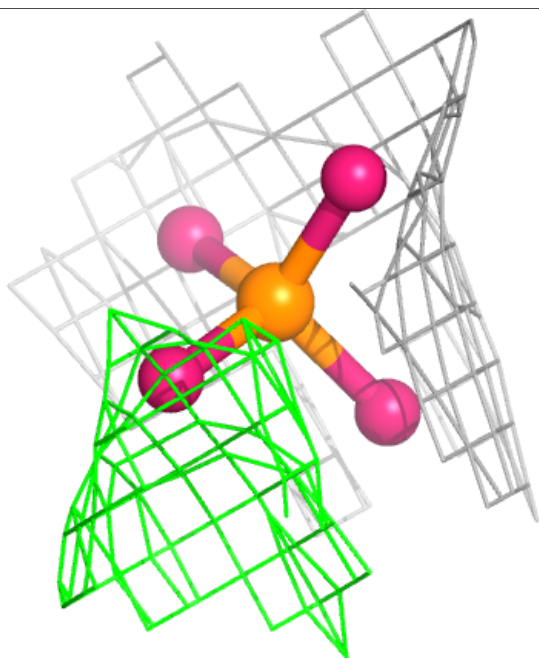
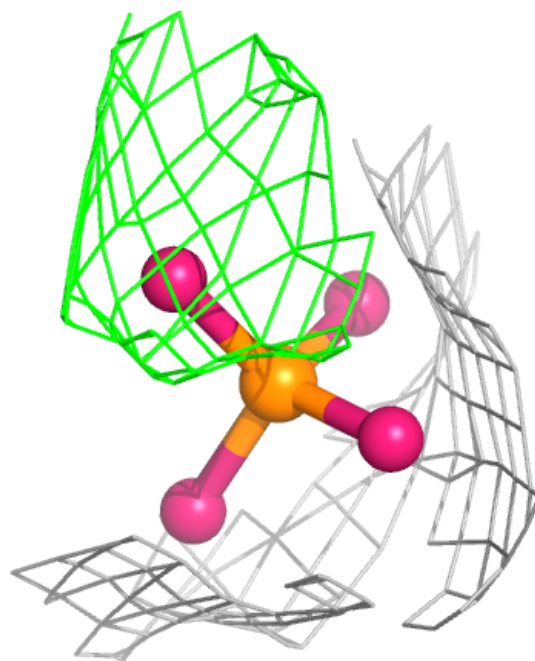
**Electron density around PO4 G 701:**

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



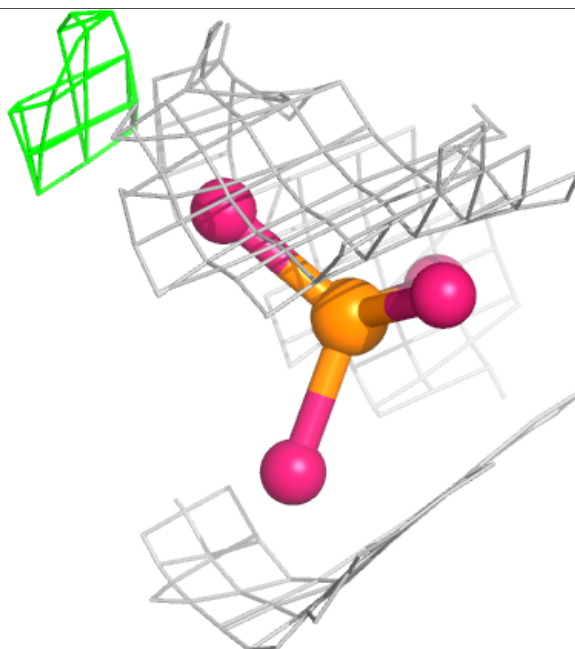
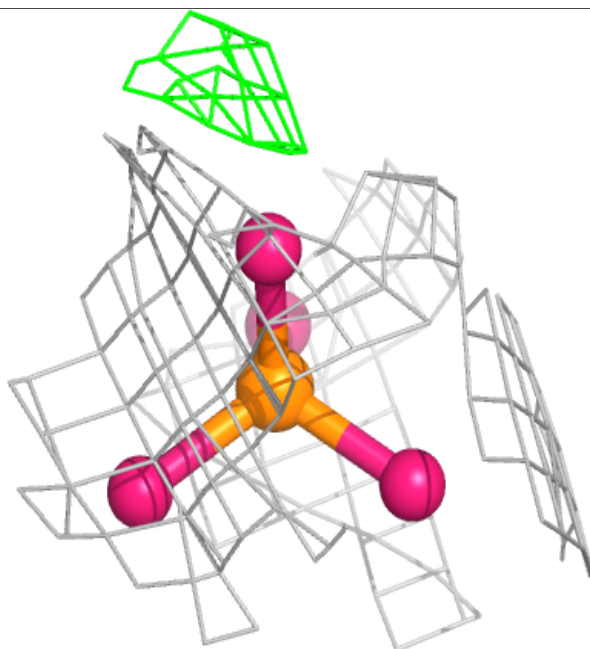
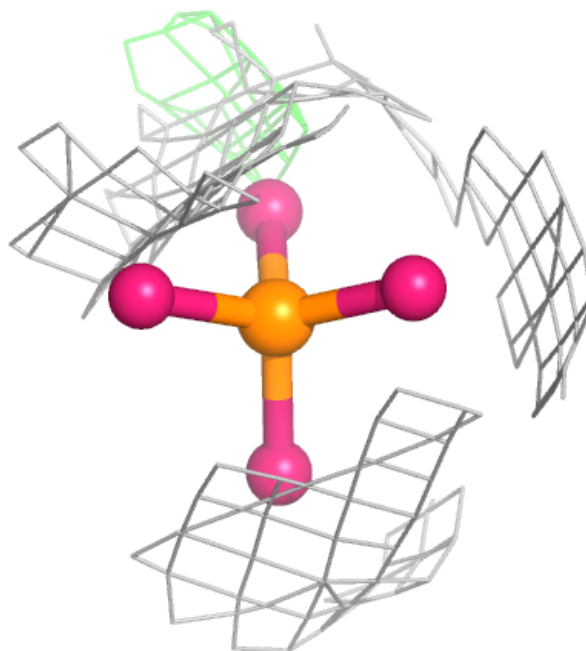
**Electron density around PO4 K 701:**

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



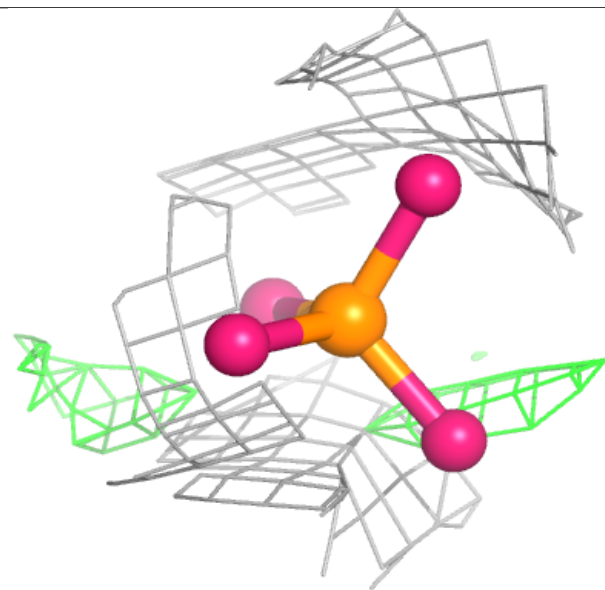
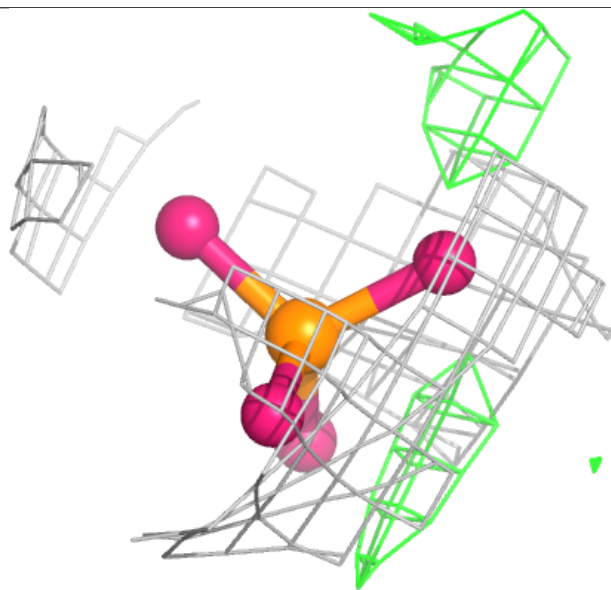
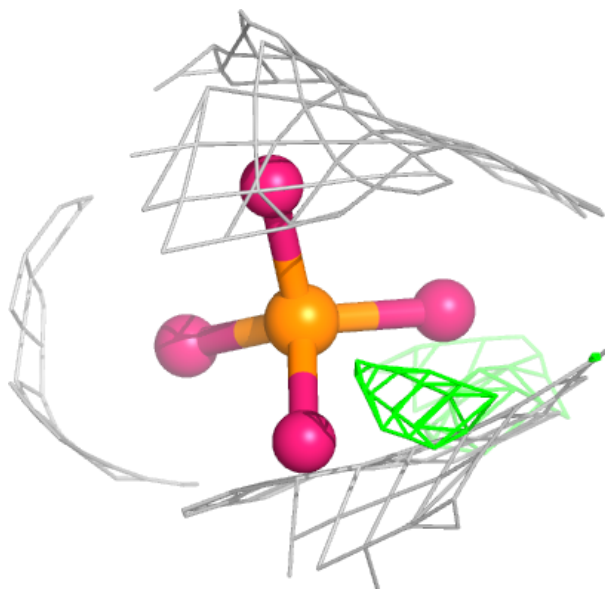
**Electron density around PO4 E 701:**

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



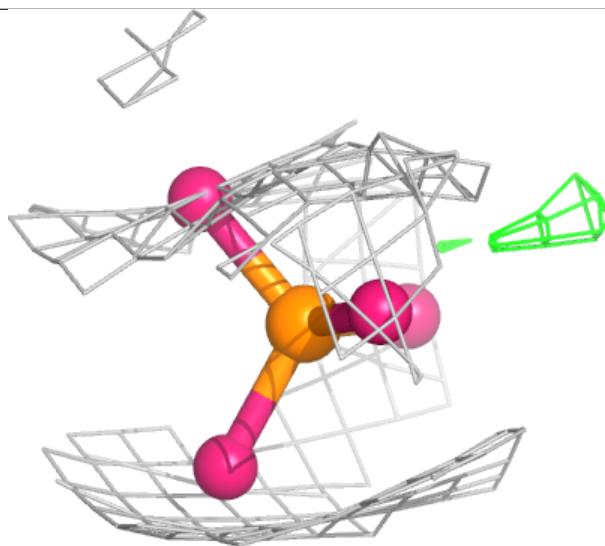
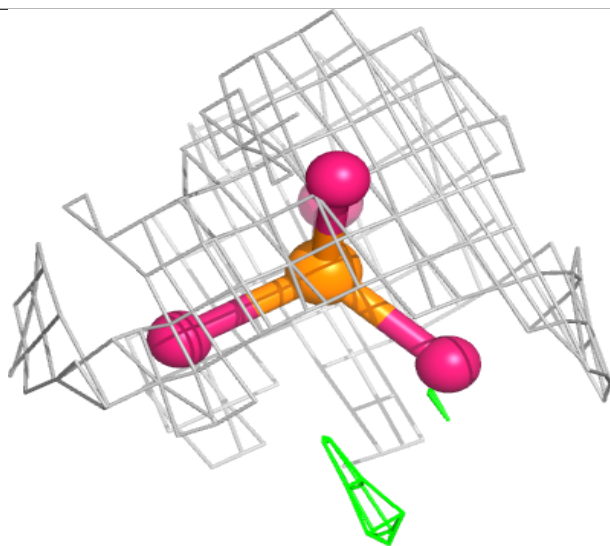
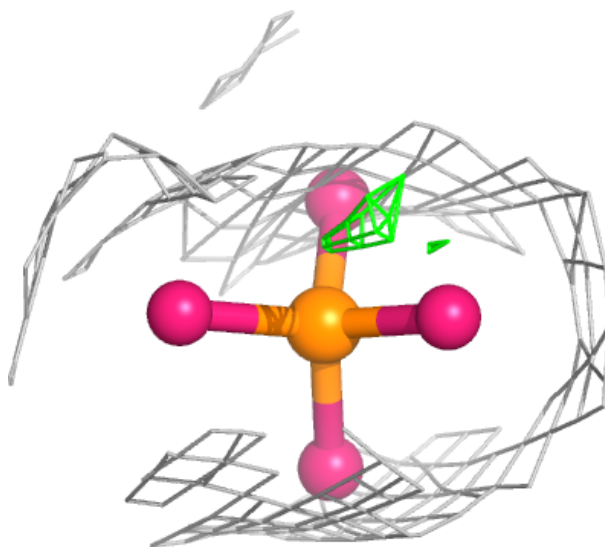
**Electron density around PO4 L 701:**

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



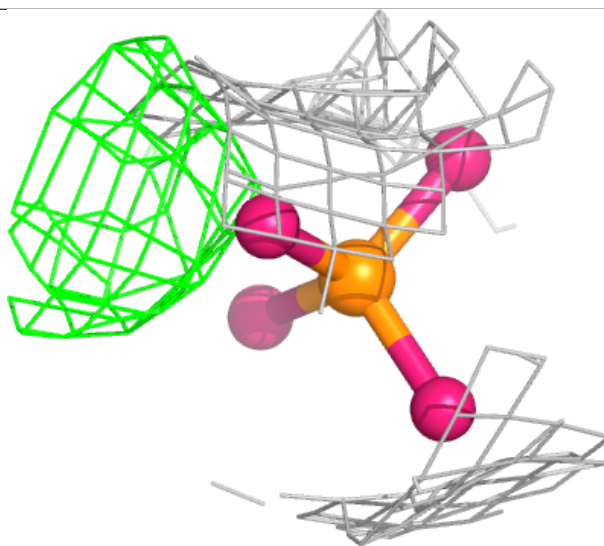
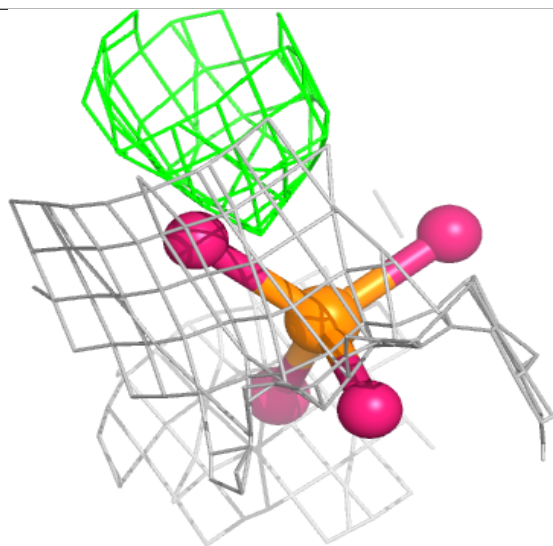
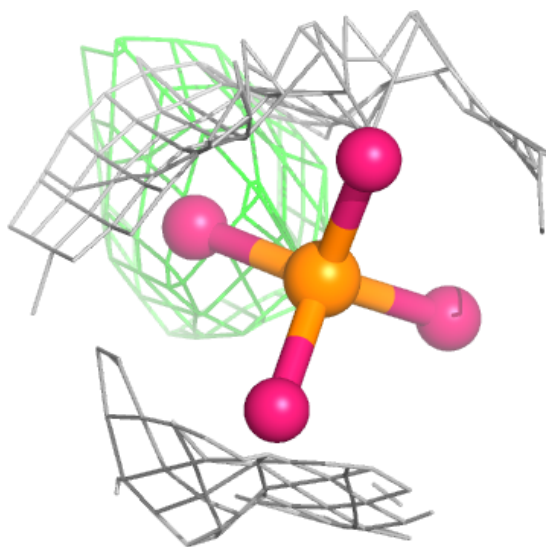
**Electron density around PO4 J 701:**

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



**Electron density around PO4 F 701:**

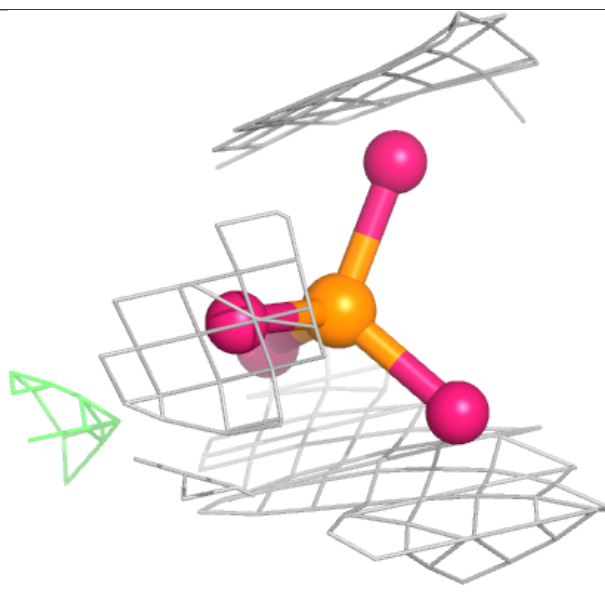
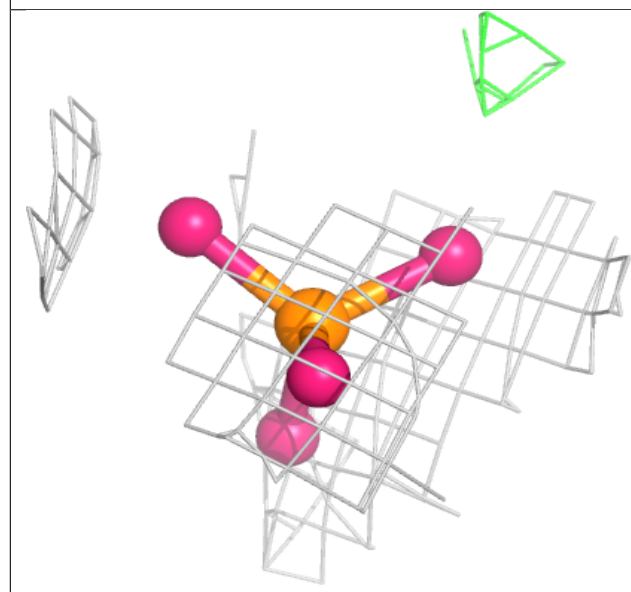
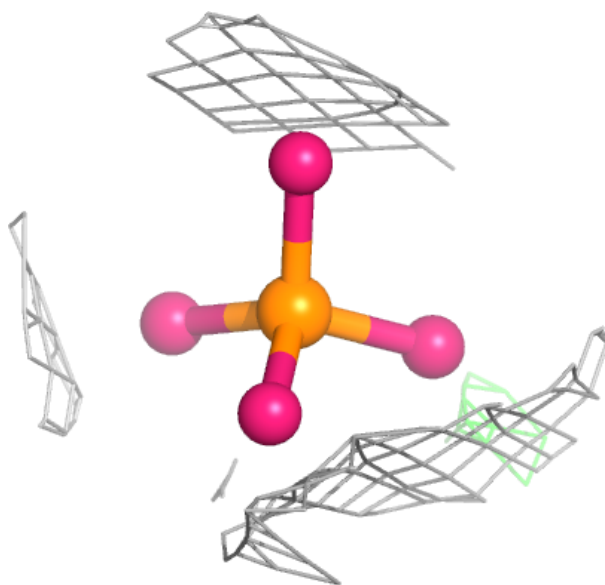
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





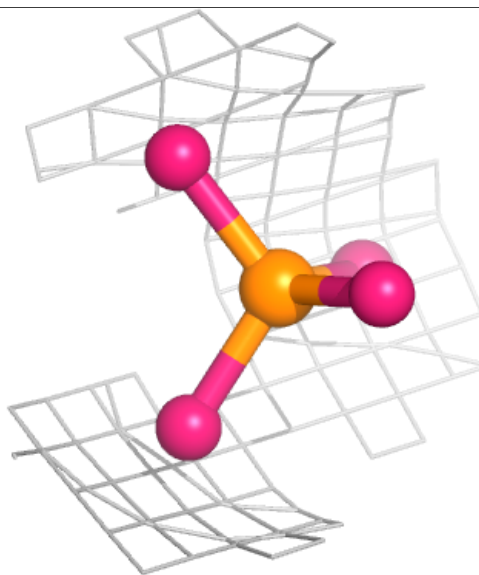
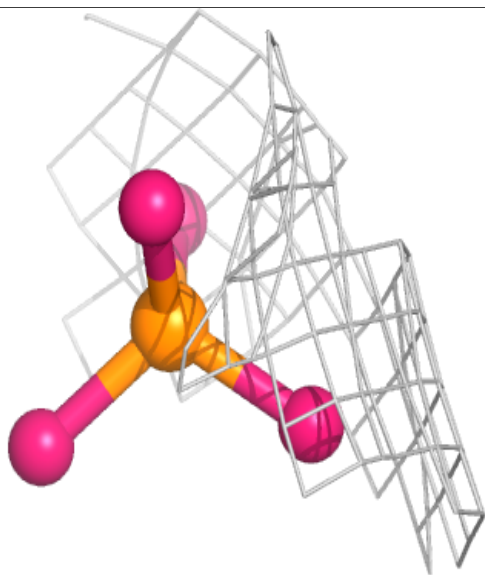
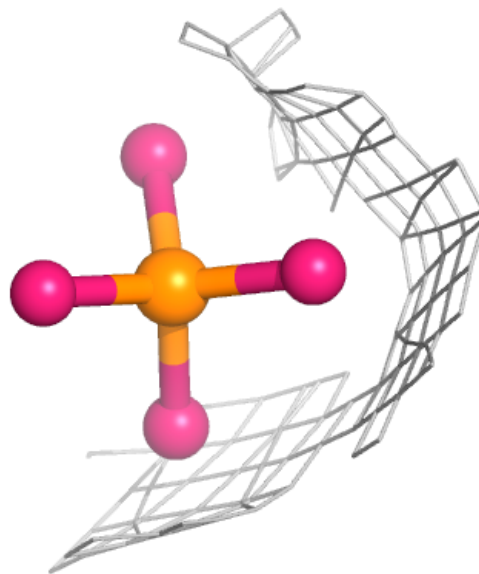
**Electron density around PO4 D 701:**

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



**Electron density around PO4 A 701:**

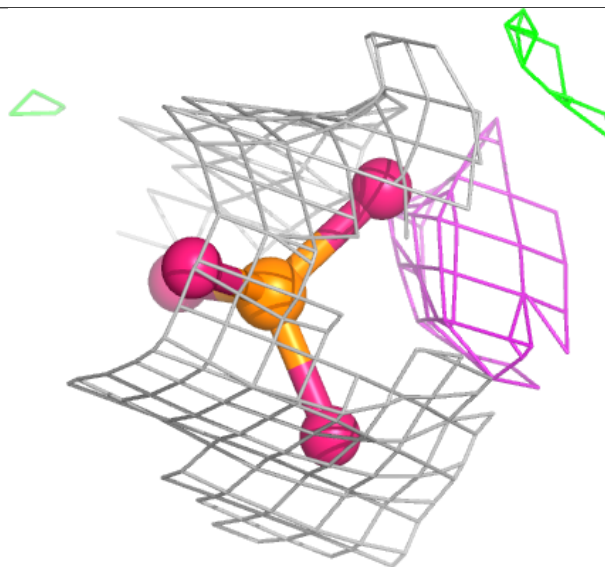
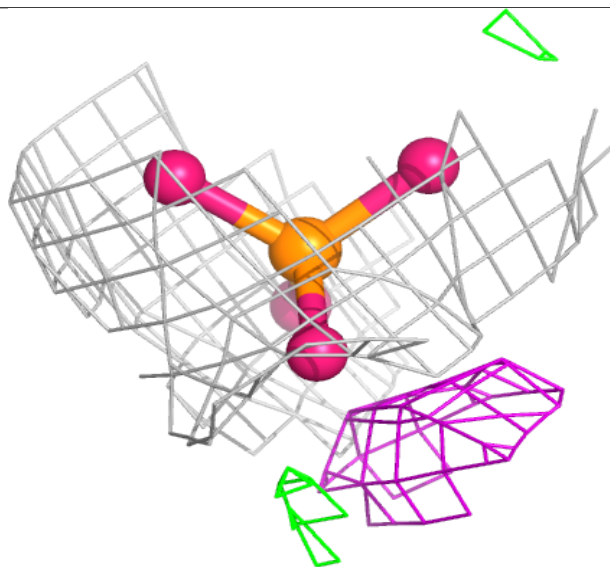
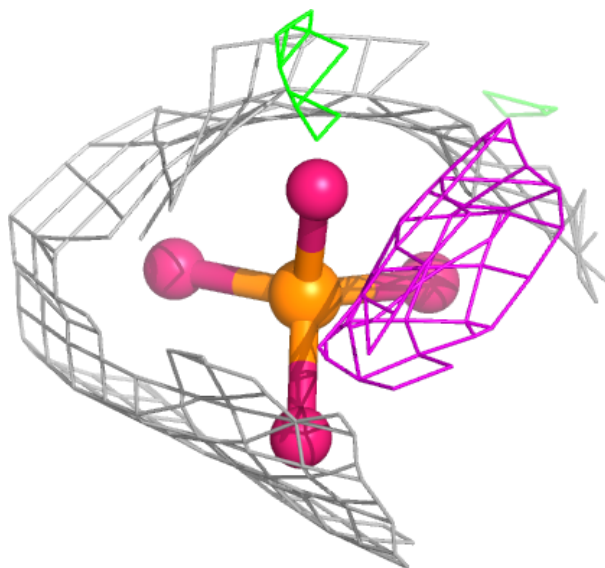
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





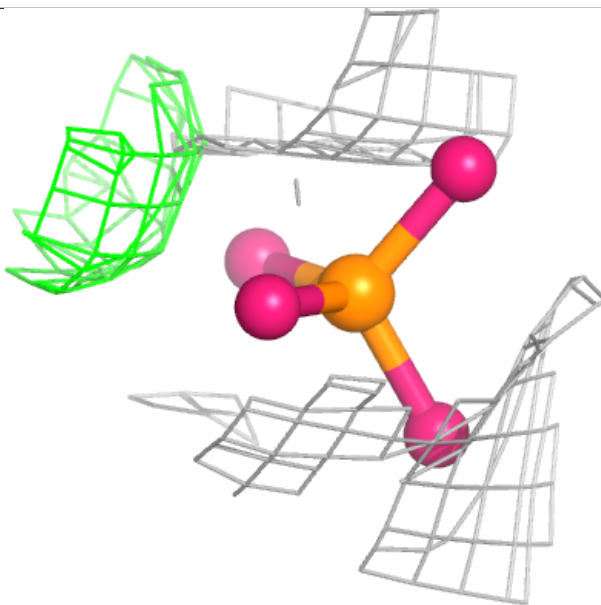
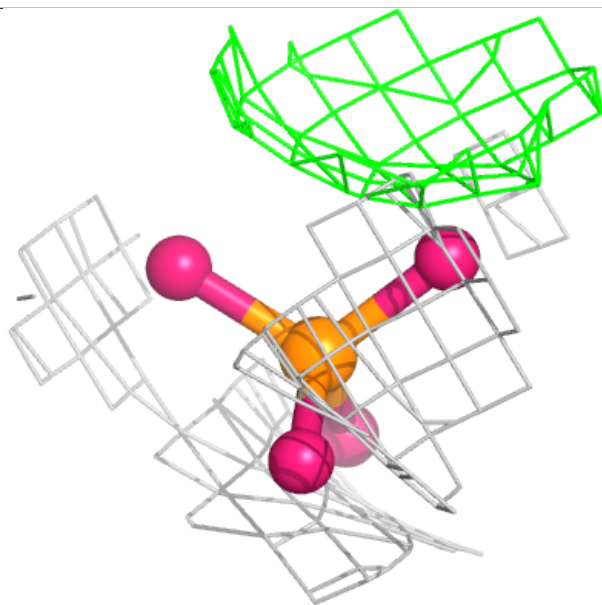
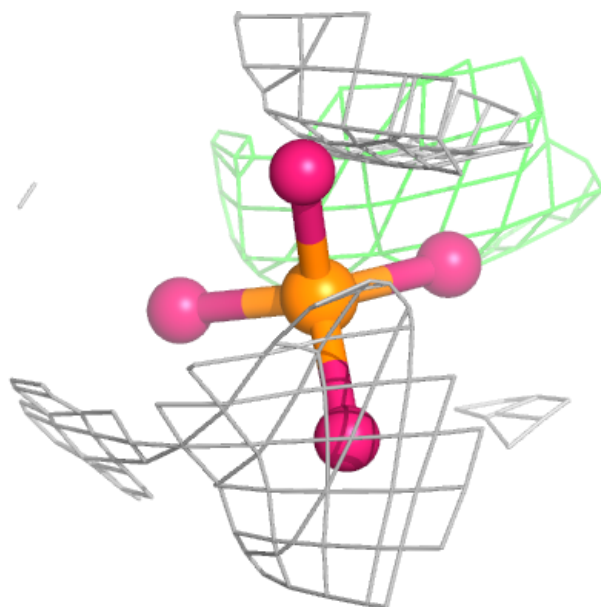
**Electron density around PO4 H 701:**

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



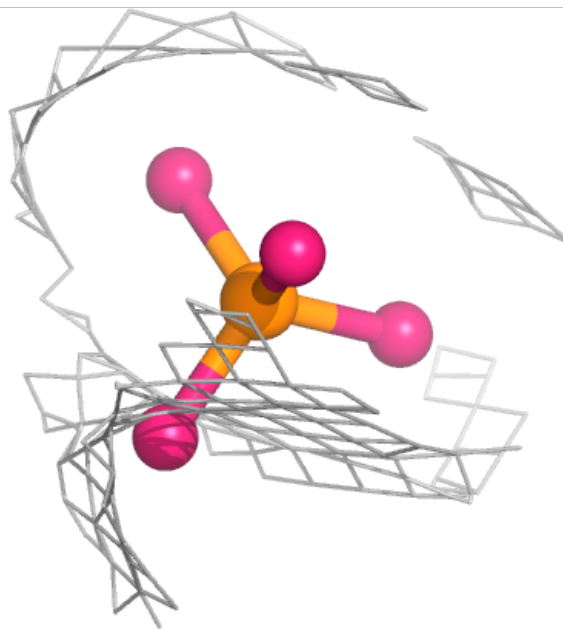
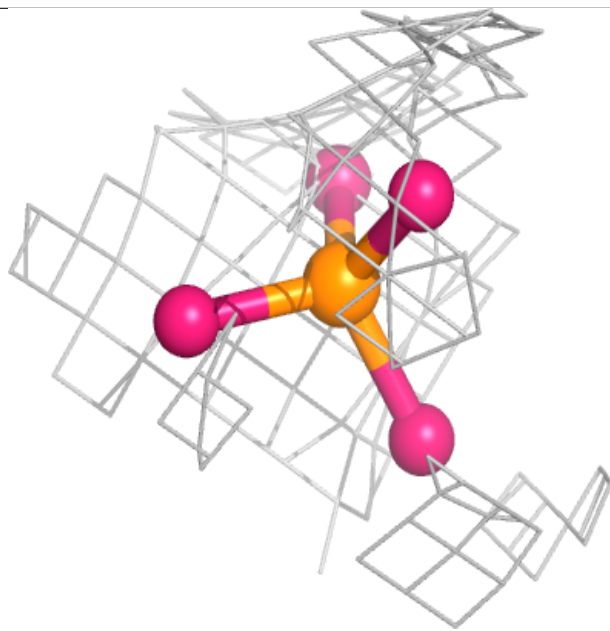
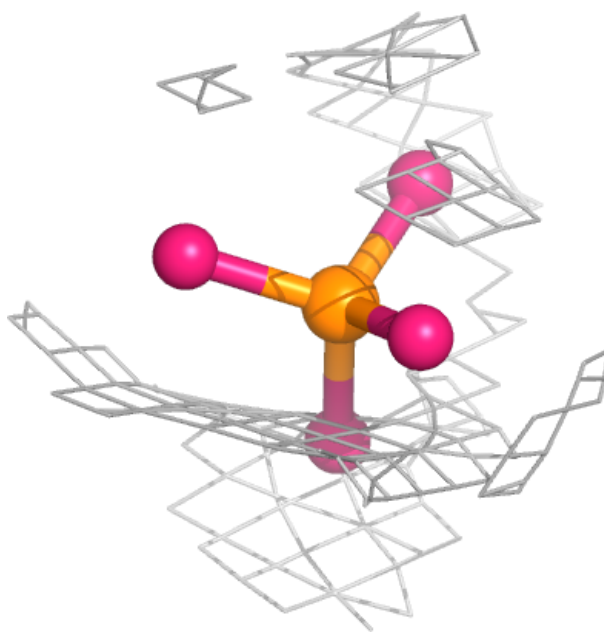
**Electron density around PO4 I 701:**

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



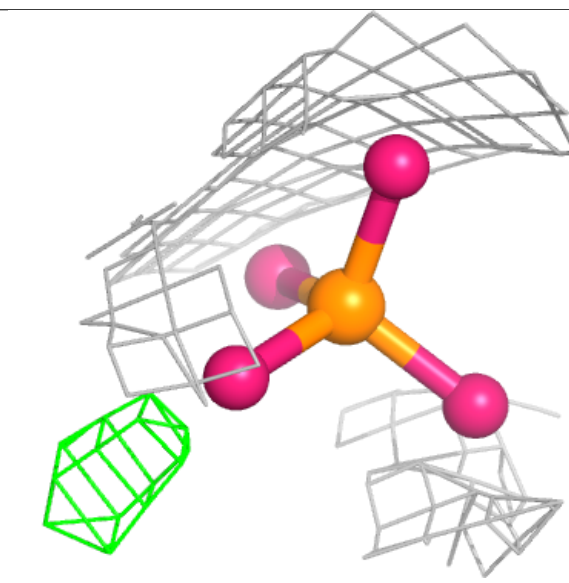
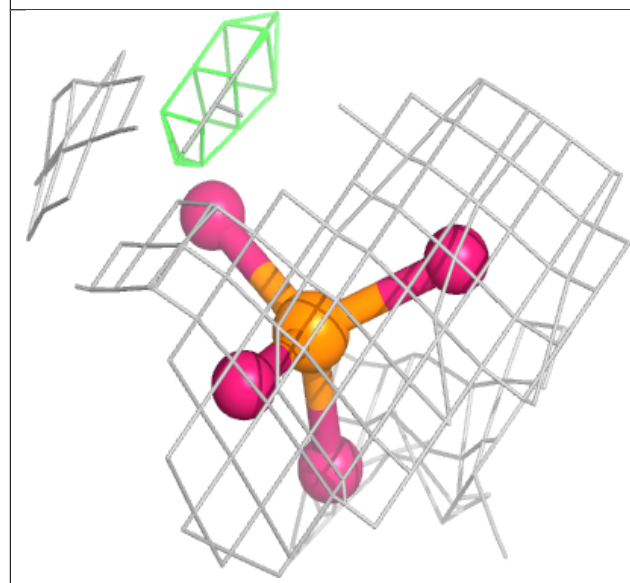
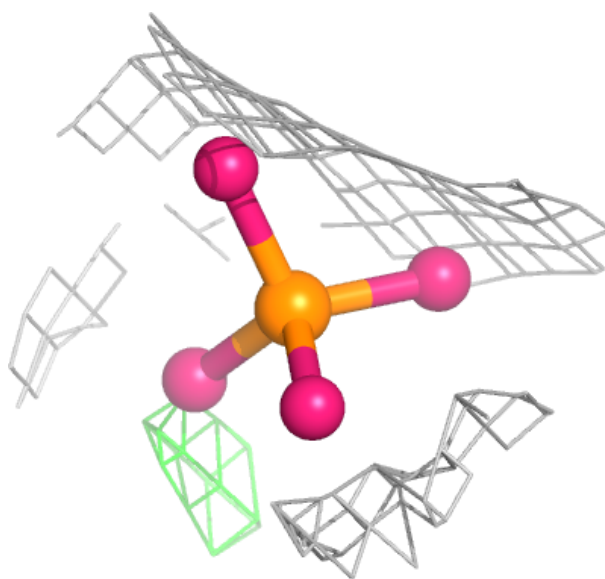
**Electron density around PO4 C 701:**

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



**Electron density around PO4 B 701:**

$2mF_o-DF_c$  (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.