wwPDB X-ray Structure Validation Summary Report (i)

Dec 21, 2021 – 12:12 PM JST

PDB ID	:	6K9E
Title	:	The A form apo structure of NrS-1 C terminal region-CTR(305-718)
Authors	:	Chen, X.; Gan, J.
Deposited on	:	2019-06-14
Resolution	:	2.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

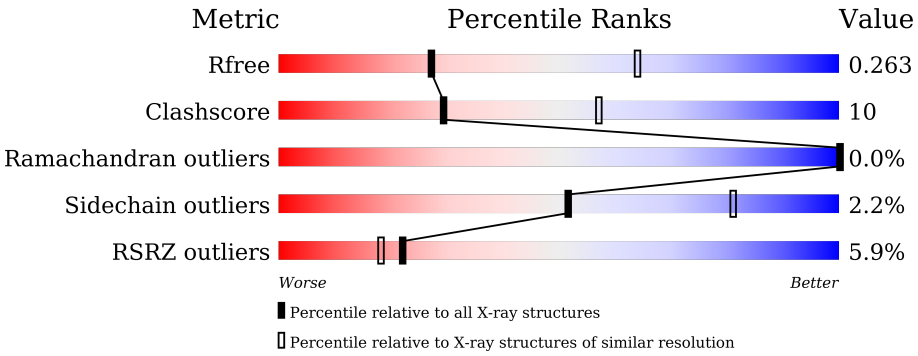
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.25
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	415	7% 75% 20%
1	B	415	5% 72% 25%
1	C	415	6% 78% 16%
1	D	415	4% 76% 21%
1	E	415	7% 75% 21%
1	F	415	5% 75% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	801	-	-	X	-

2 Entry composition (i)

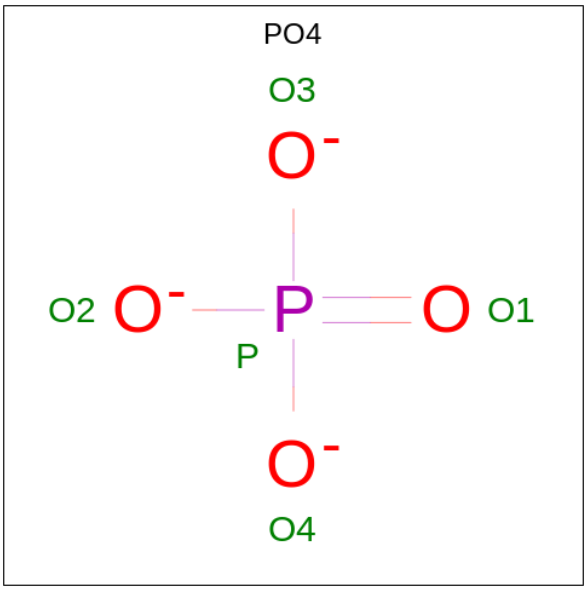
There are 2 unique types of molecules in this entry. The entry contains 19411 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Primase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3226	2101	526	588	11			
1	B	404	Total	C	N	O	S	0	0	0
			3260	2123	531	595	11			
1	C	401	Total	C	N	O	S	0	0	0
			3211	2093	525	583	10			
1	D	404	Total	C	N	O	S	0	0	0
			3237	2111	529	587	10			
1	E	402	Total	C	N	O	S	0	0	0
			3213	2095	526	581	11			
1	F	404	Total	C	N	O	S	0	0	0
			3234	2107	529	587	11			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



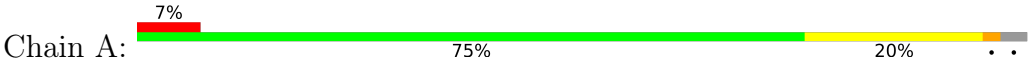
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0

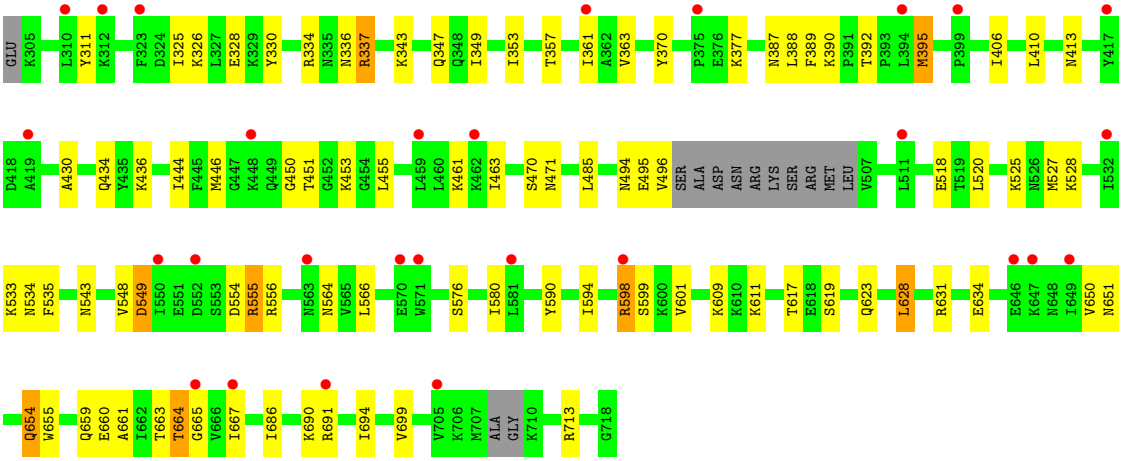
3 Residue-property plots (i)

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: Primase

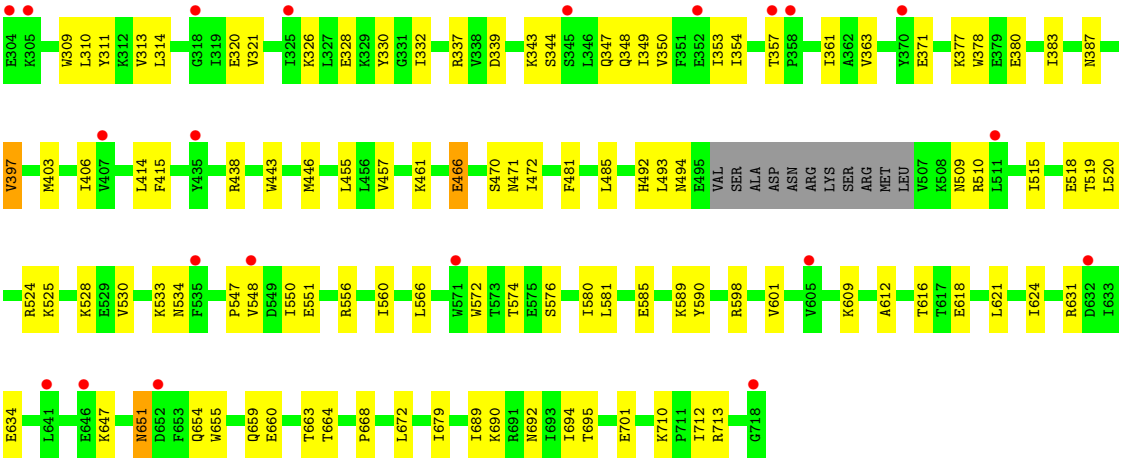
Chain A:





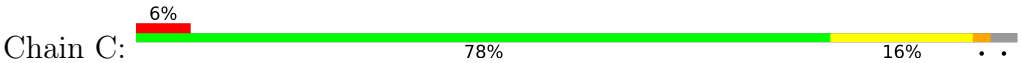
• Molecule 1: Primase

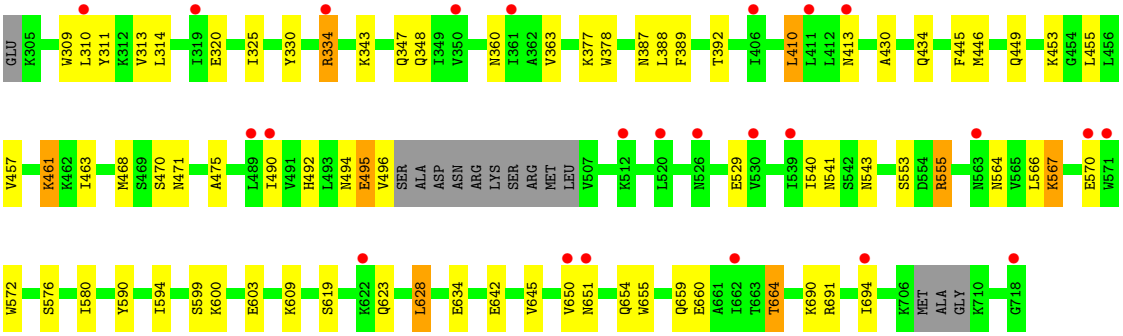
Chain B:



• Molecule 1: Primase

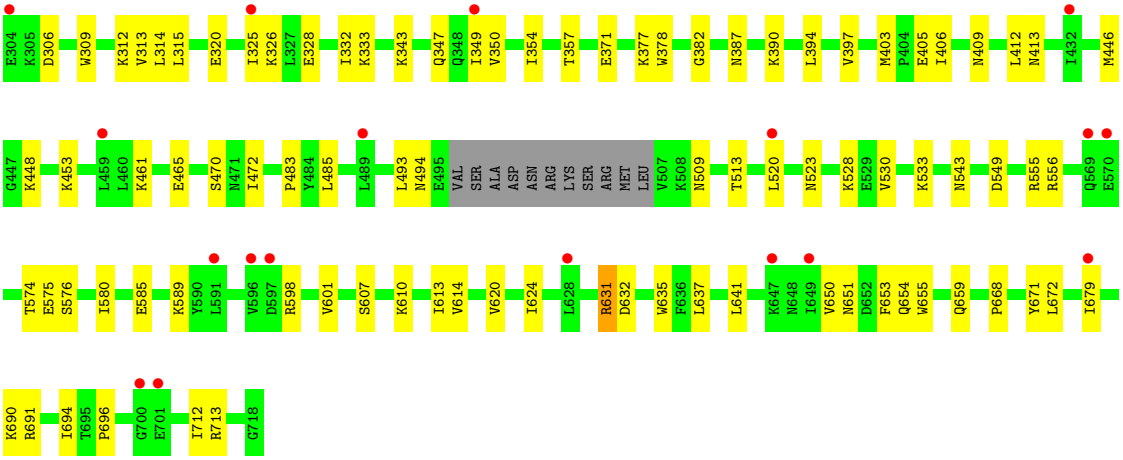
Chain C:





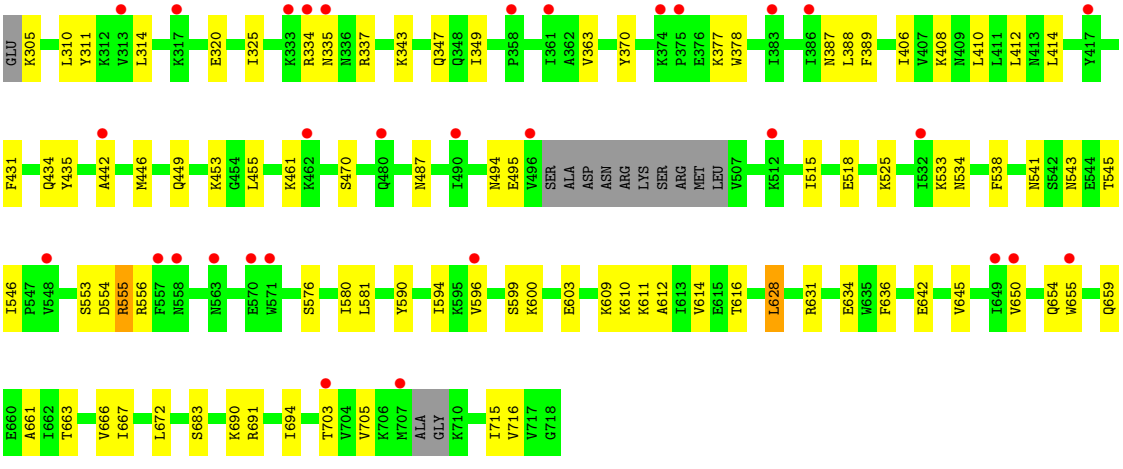
• Molecule 1: Primase

Chain D:



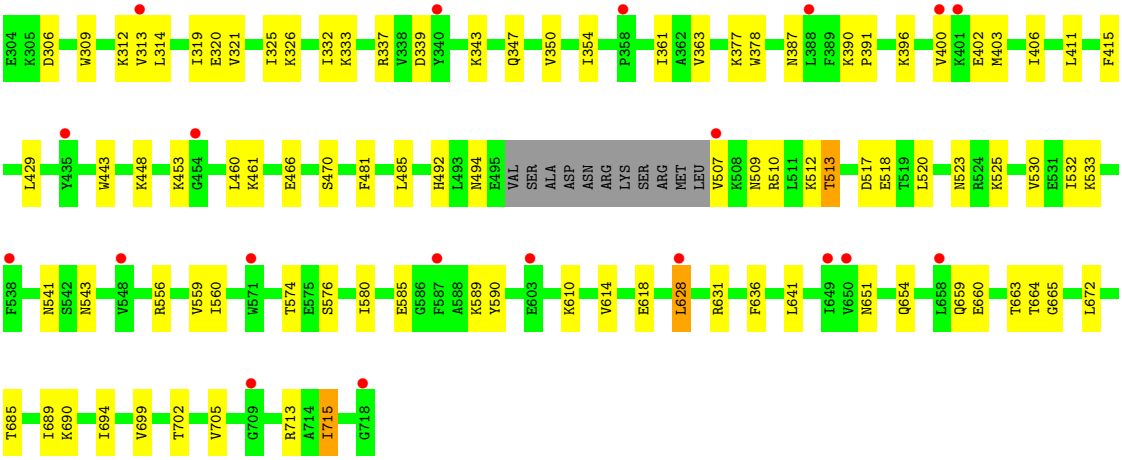
• Molecule 1: Primase

Chain E:



• Molecule 1: Primase

Chain F:


E304 K305 D306 W309 K312 V313 L314 I319 E320 V321 I325 K326 I332 K333 R337 V338 D339 Y340 K343 Q347 V350 I354 P358 I361 A362 V363 K377 W378 N387 L388 F389 K390 P391 K396 V400 K401 E402 M403 I406 L411 F415
L429 Y435 W443 K448 K453 G454 L460 K461 E466 S470 F481 L485 H492 L493 N494 E495 VAL SER ALA ASP ASN ARG LYS SER ARG MET LEU V507 K508 N509 R510 L511 K512 T513 D517 E518 T519 L520 N523 R524 K525 V530 E531 I532 K533
P538 N541 S542 N543 V548 R556 V559 I560 W571 T574 E575 S576 I580 E585 Q586 F587 A588 K589 Y590 E603 K610 V614 E618 L628 R631 F636 L641 I649 V650 N651 Q654 L658 Q659 E660 T663 T664 G665 L672
T685 I689 K690 I694 V699 T702 V705 G709 R713 A714 I715 G718

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	159.69Å 159.91Å 159.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.90 29.69 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.5 (29.69-2.90) 87.1 (29.69-2.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.236 , 0.264 0.236 , 0.263	Depositor DCC
R_{free} test set	4057 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , -38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.059 for -h,l,k 0.058 for -k,-h,-l 0.059 for l,-k,h 0.437 for l,h,k 0.437 for k,l,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	19411	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	0.33	0/3292	0.55	0/4465
1	B	0.39	2/3327 (0.1%)	0.57	0/4505
1	C	0.33	0/3277	0.53	1/4446 (0.0%)
1	D	0.37	0/3304	0.55	0/4479
1	E	0.33	0/3279	0.53	0/4447
1	F	0.47	2/3301 (0.1%)	0.55	0/4476
All	All	0.37	4/19780 (0.0%)	0.55	1/26818 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	518	GLU	CD-OE1	-13.35	1.10	1.25
1	F	518	GLU	CD-OE2	-11.04	1.13	1.25
1	B	701	GLU	CD-OE1	-5.20	1.20	1.25
1	B	701	GLU	CD-OE2	-5.09	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	410	LEU	CA-CB-CG	5.53	128.03	115.30

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	3226	0	3251	75	0
1	B	3260	0	3313	83	0
1	C	3211	0	3236	73	0
1	D	3237	0	3276	66	0
1	E	3213	0	3239	67	0
1	F	3234	0	3271	66	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	1	0
2	E	5	0	0	1	0
All	All	19411	0	19586	371	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 10.

The worst 5 of 371 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:C:410:LEU:HD12	1:C:580:ILE:HG21	1.35	1.09
1:B:509:ASN:HB3	1:C:495:GLU:HG2	1.39	1.04
1:D:509:ASN:CB	1:E:495:GLU:OE1	2.08	1.01
1:D:325:ILE:CD1	1:E:349:ILE:HD11	1.91	0.99
1:D:325:ILE:HD12	1:E:349:ILE:HD11	1.45	0.94

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	396/415 (95%)	386 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	400/415 (96%)	387 (97%)	12 (3%)	1 (0%)	41 71
1	C	395/415 (95%)	384 (97%)	11 (3%)	0	100 100
1	D	400/415 (96%)	388 (97%)	12 (3%)	0	100 100
1	E	396/415 (95%)	385 (97%)	11 (3%)	0	100 100
1	F	400/415 (96%)	389 (97%)	11 (3%)	0	100 100
All	All	2387/2490 (96%)	2319 (97%)	67 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	651	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	349/378 (92%)	339 (97%)	10 (3%)	42 76
1	B	355/378 (94%)	347 (98%)	8 (2%)	50 80
1	C	346/378 (92%)	338 (98%)	8 (2%)	50 80
1	D	348/378 (92%)	341 (98%)	7 (2%)	55 82
1	E	345/378 (91%)	339 (98%)	6 (2%)	60 86
1	F	349/378 (92%)	342 (98%)	7 (2%)	55 82
All	All	2092/2268 (92%)	2046 (98%)	46 (2%)	52 81

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	494	ASN
1	E	628	LEU
1	D	549	ASP
1	D	672	LEU
1	E	683	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	494	ASN
1	F	471	ASN
1	D	409	ASN
1	F	360	ASN
1	D	360	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	A	801	-	4,4,4	1.05	0	6,6,6	0.57	0
2	PO4	C	801	-	4,4,4	1.05	0	6,6,6	0.42	0
2	PO4	D	801	-	4,4,4	1.00	0	6,6,6	0.50	0
2	PO4	B	801	-	4,4,4	0.99	0	6,6,6	0.49	0
2	PO4	C	802	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	E	801	-	4,4,4	1.01	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

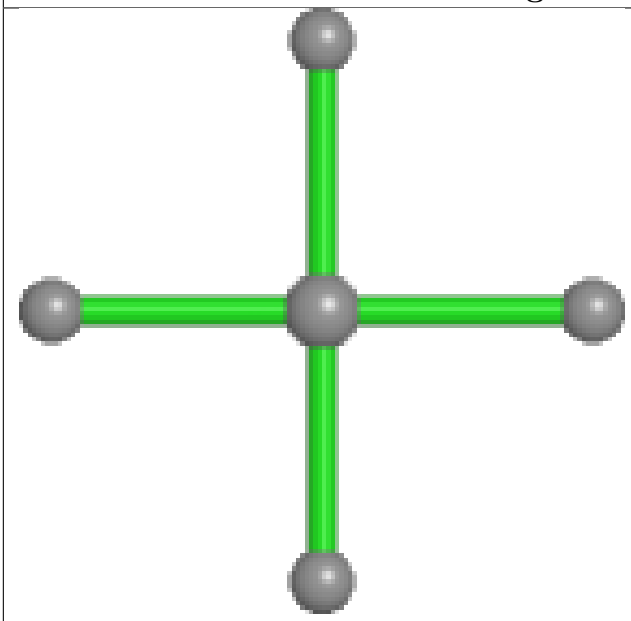
There are no ring outliers.

5 monomers are involved in 6 short contacts:

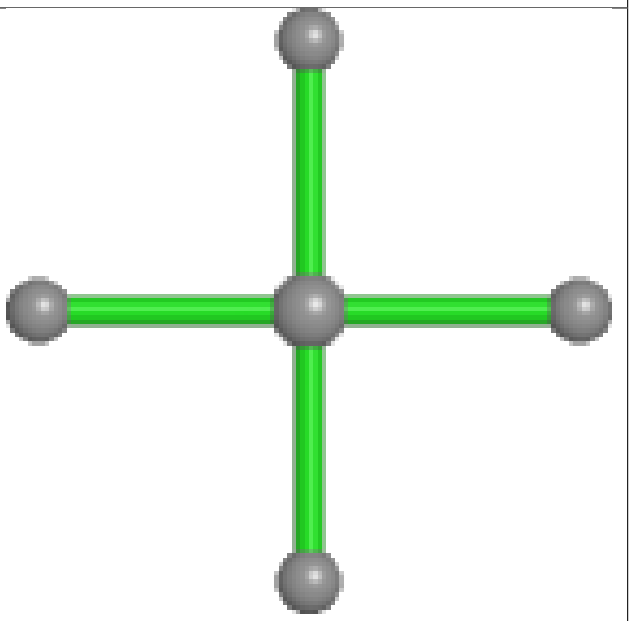
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PO4	2	0
2	D	801	PO4	1	0
2	B	801	PO4	1	0
2	C	802	PO4	1	0
2	E	801	PO4	1	0

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 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.

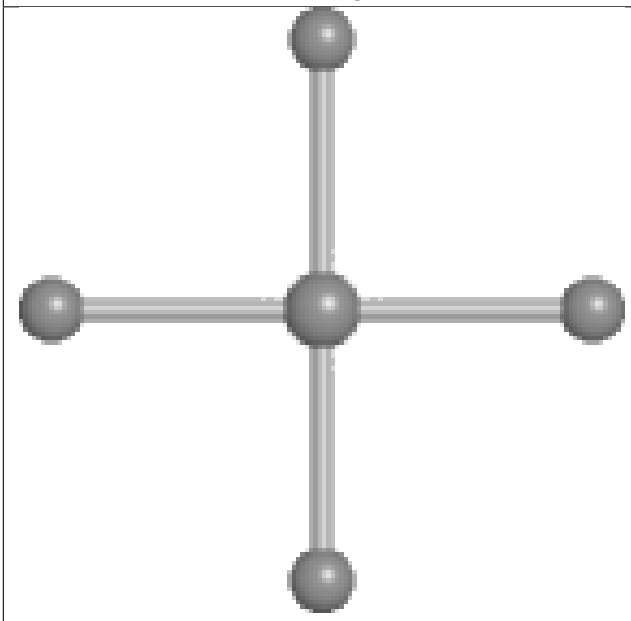
Ligand PO4 A 801



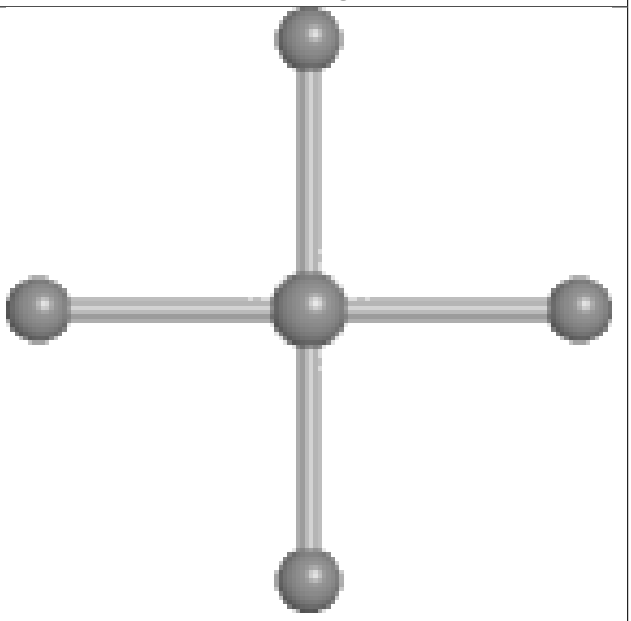
Bond lengths



Bond angles

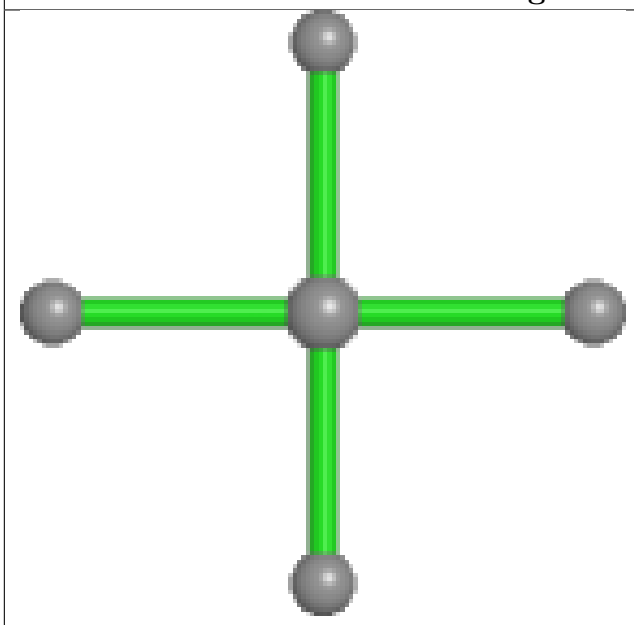


Torsions

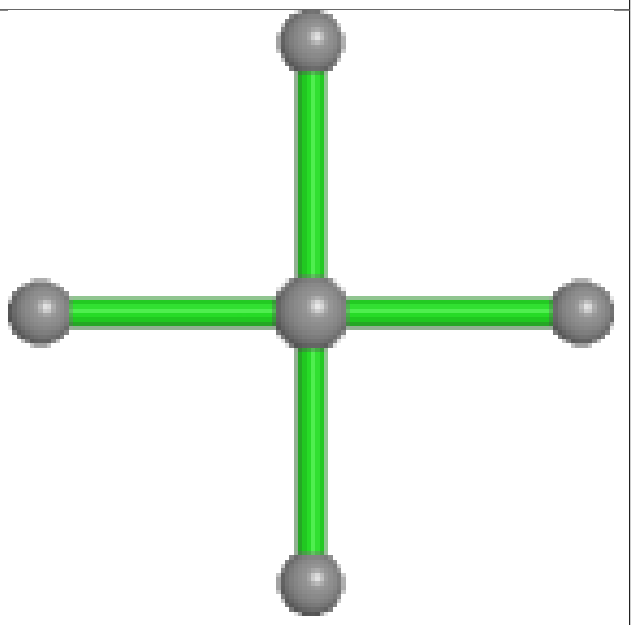


Rings

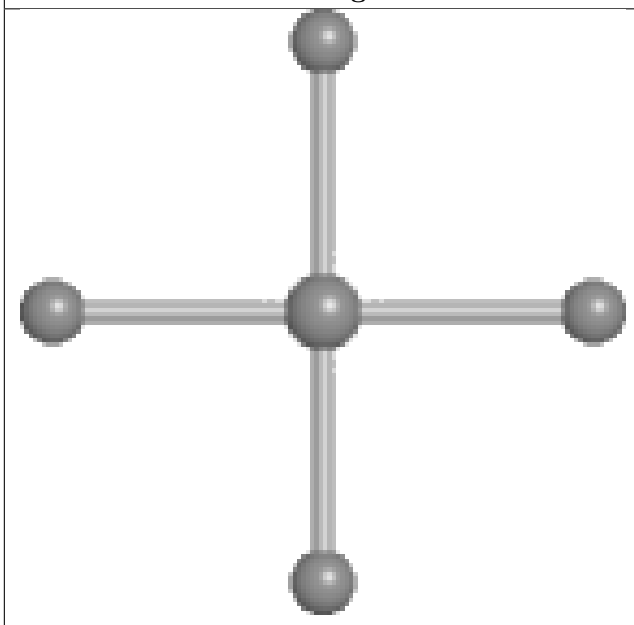
Ligand PO4 C 801



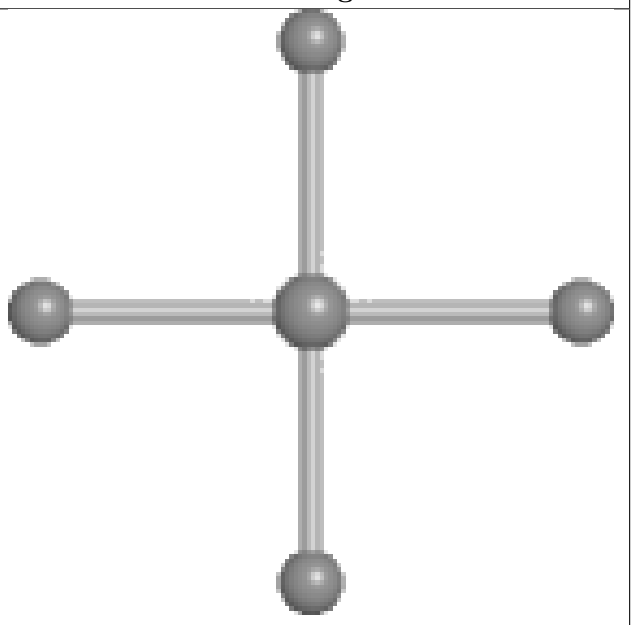
Bond lengths



Bond angles

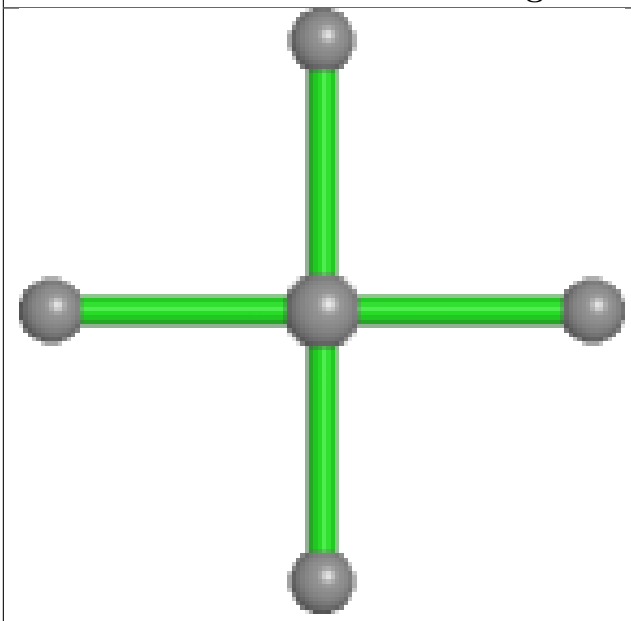


Torsions

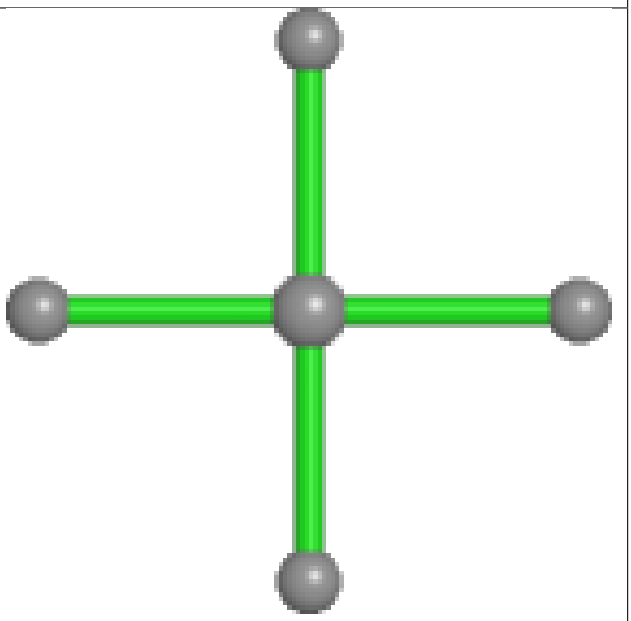


Rings

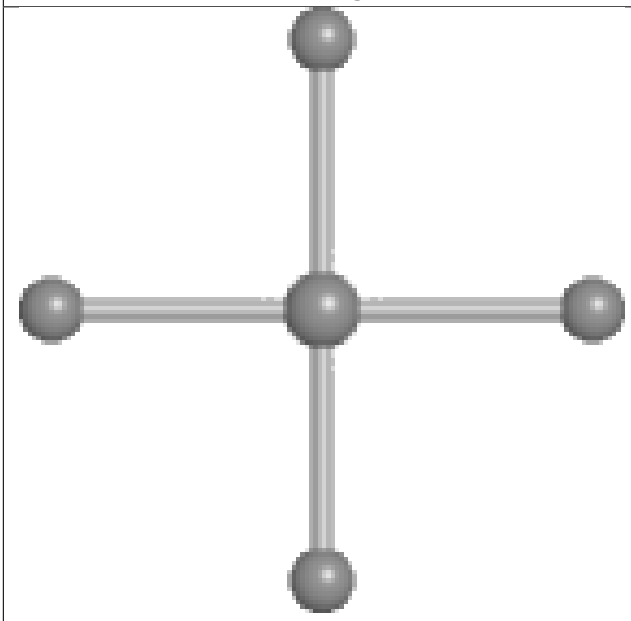
Ligand PO4 D 801



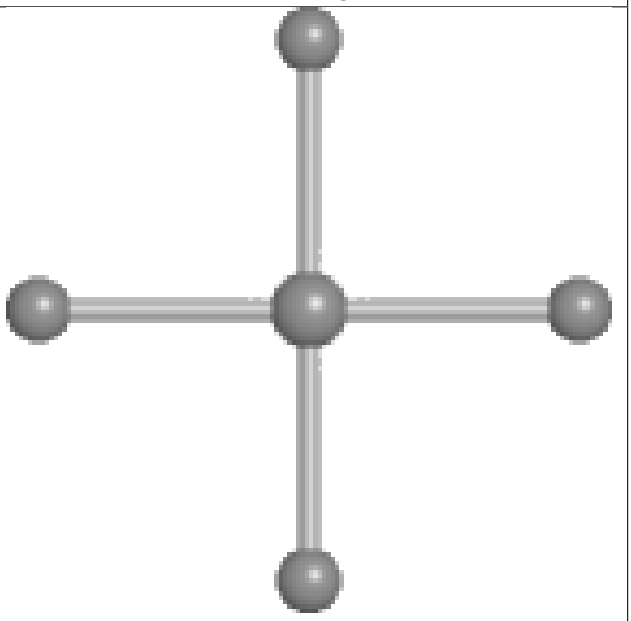
Bond lengths



Bond angles

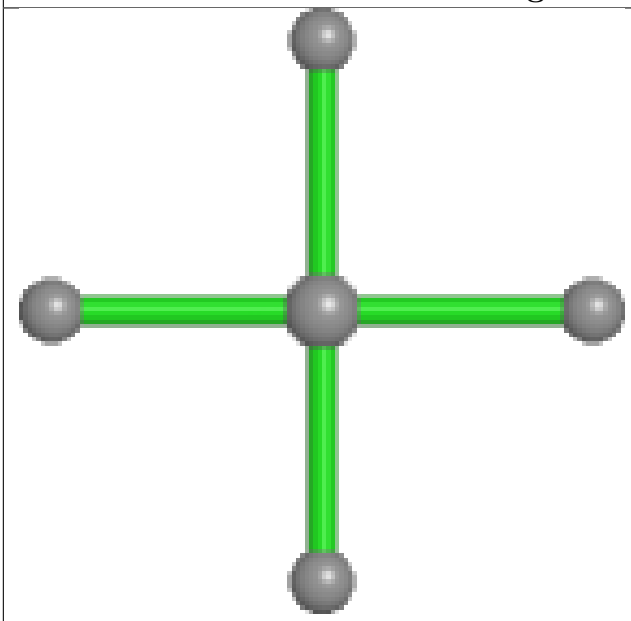


Torsions

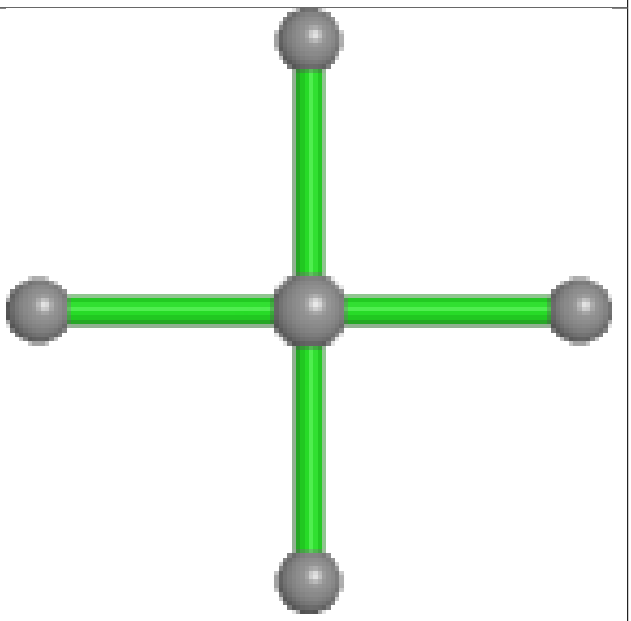


Rings

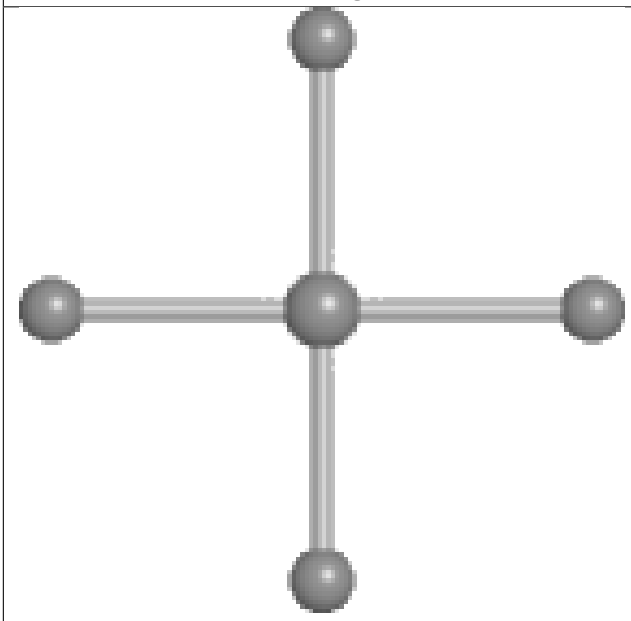
Ligand PO4 B 801



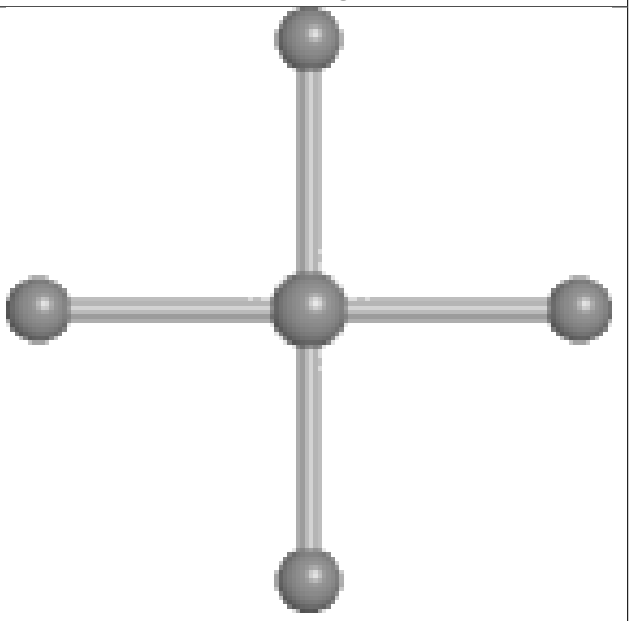
Bond lengths



Bond angles

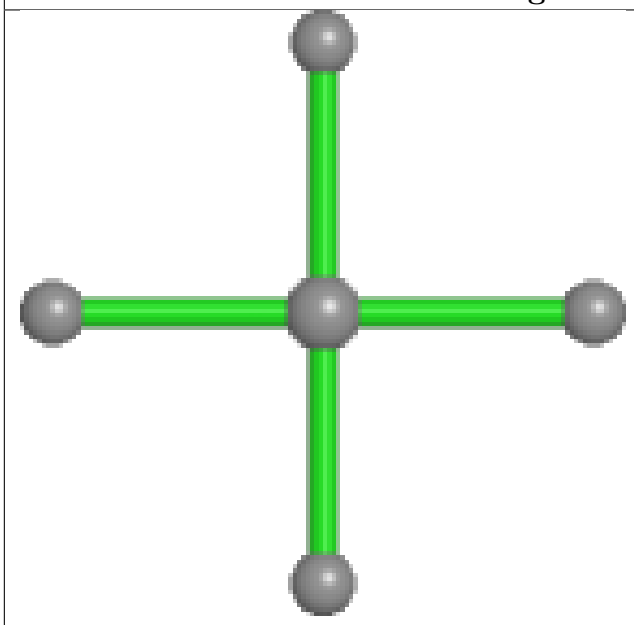


Torsions

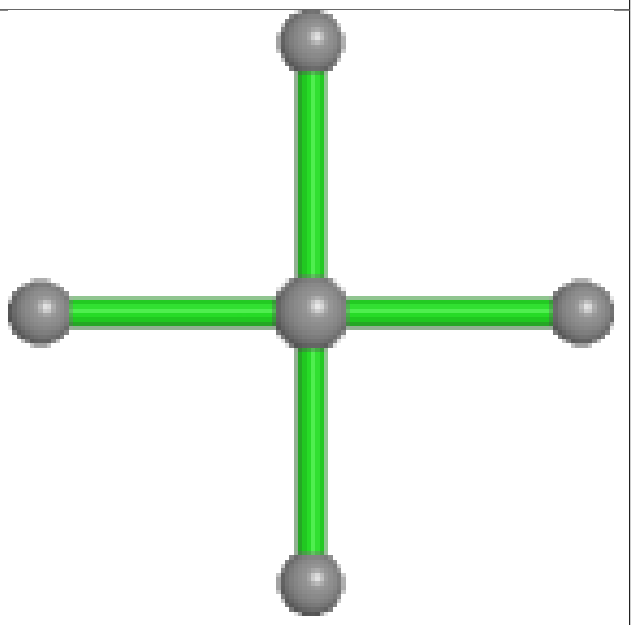


Rings

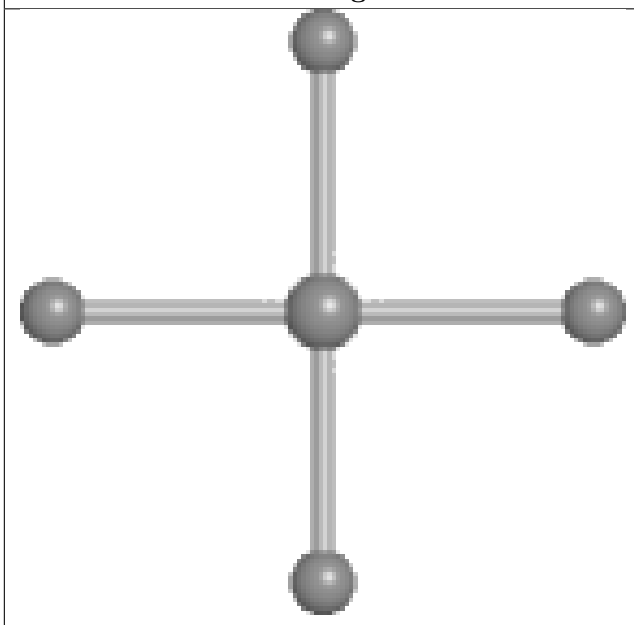
Ligand PO4 C 802



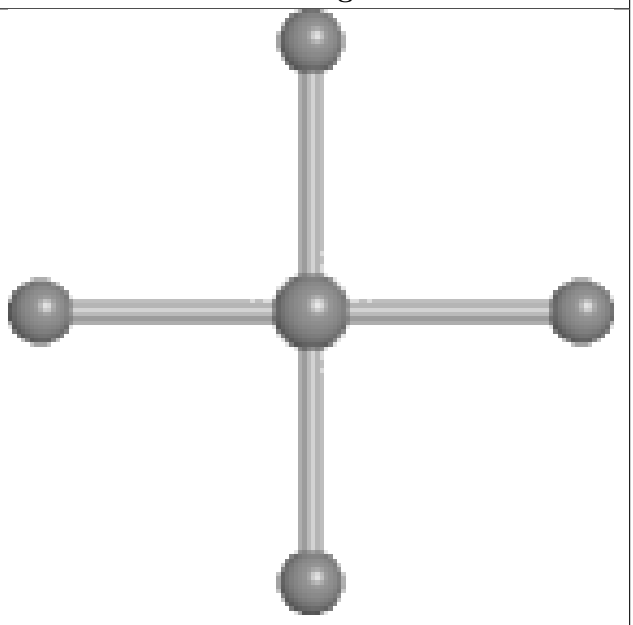
Bond lengths



Bond angles

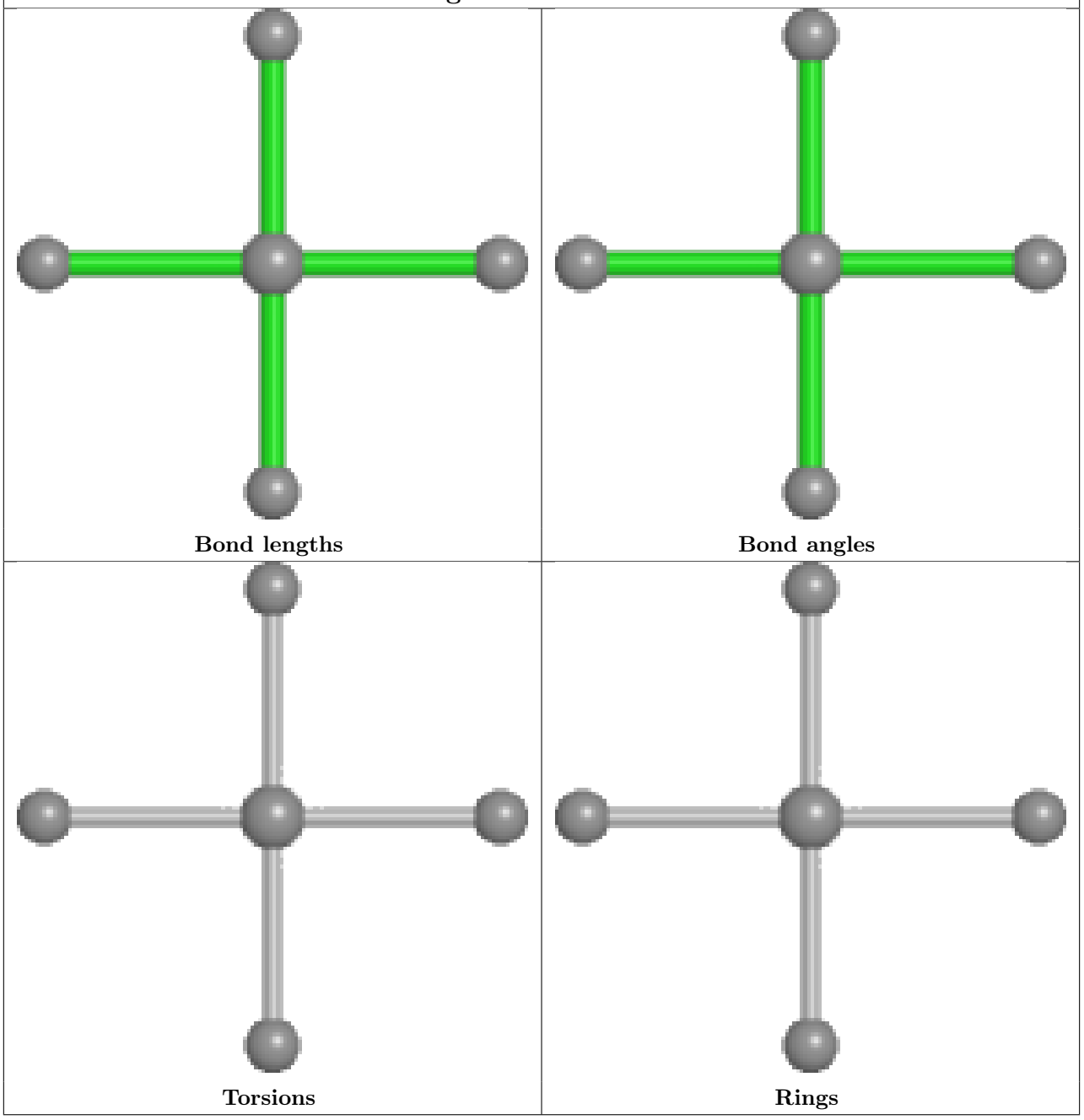


Torsions



Rings

Ligand PO4 E 801



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^{th} 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^2)	Q<0.9
1	A	402/415 (96%)	0.67	28 (6%)	16	12	32, 40, 49, 80	0
1	B	404/415 (97%)	0.63	21 (5%)	27	23	32, 40, 48, 61	0
1	C	401/415 (96%)	0.65	24 (5%)	21	18	33, 40, 48, 71	0
1	D	404/415 (97%)	0.65	18 (4%)	33	29	32, 40, 48, 70	0
1	E	402/415 (96%)	0.69	31 (7%)	13	10	32, 40, 48, 71	0
1	F	404/415 (97%)	0.66	20 (4%)	28	25	33, 40, 48, 64	0
All	All	2417/2490 (97%)	0.66	142 (5%)	22	18	32, 40, 49, 80	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	570	GLU	7.3
1	E	496	VAL	5.7
1	F	718	GLY	5.4
1	C	361	ILE	4.9
1	E	361	ILE	4.4

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 (i)

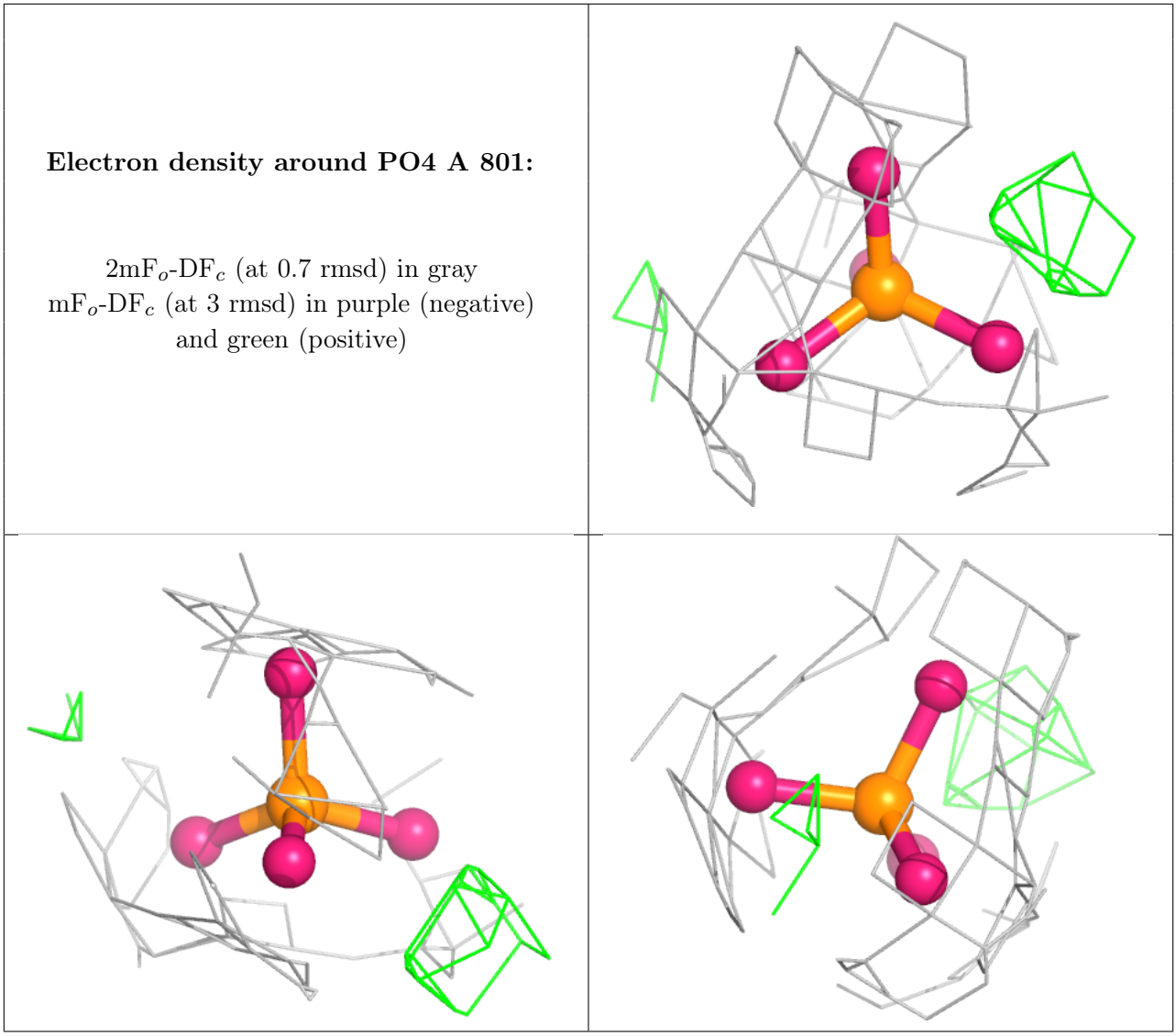
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	PO4	A	801	5/5	0.91	0.19	35,36,65,65	0
2	PO4	B	801	5/5	0.92	0.18	35,35,36,42	0
2	PO4	C	801	5/5	0.92	0.21	35,36,88,88	0
2	PO4	D	801	5/5	0.92	0.20	35,36,91,98	0
2	PO4	E	801	5/5	0.92	0.15	35,36,45,105	0
2	PO4	C	802	5/5	0.96	0.14	35,36,39,42	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.

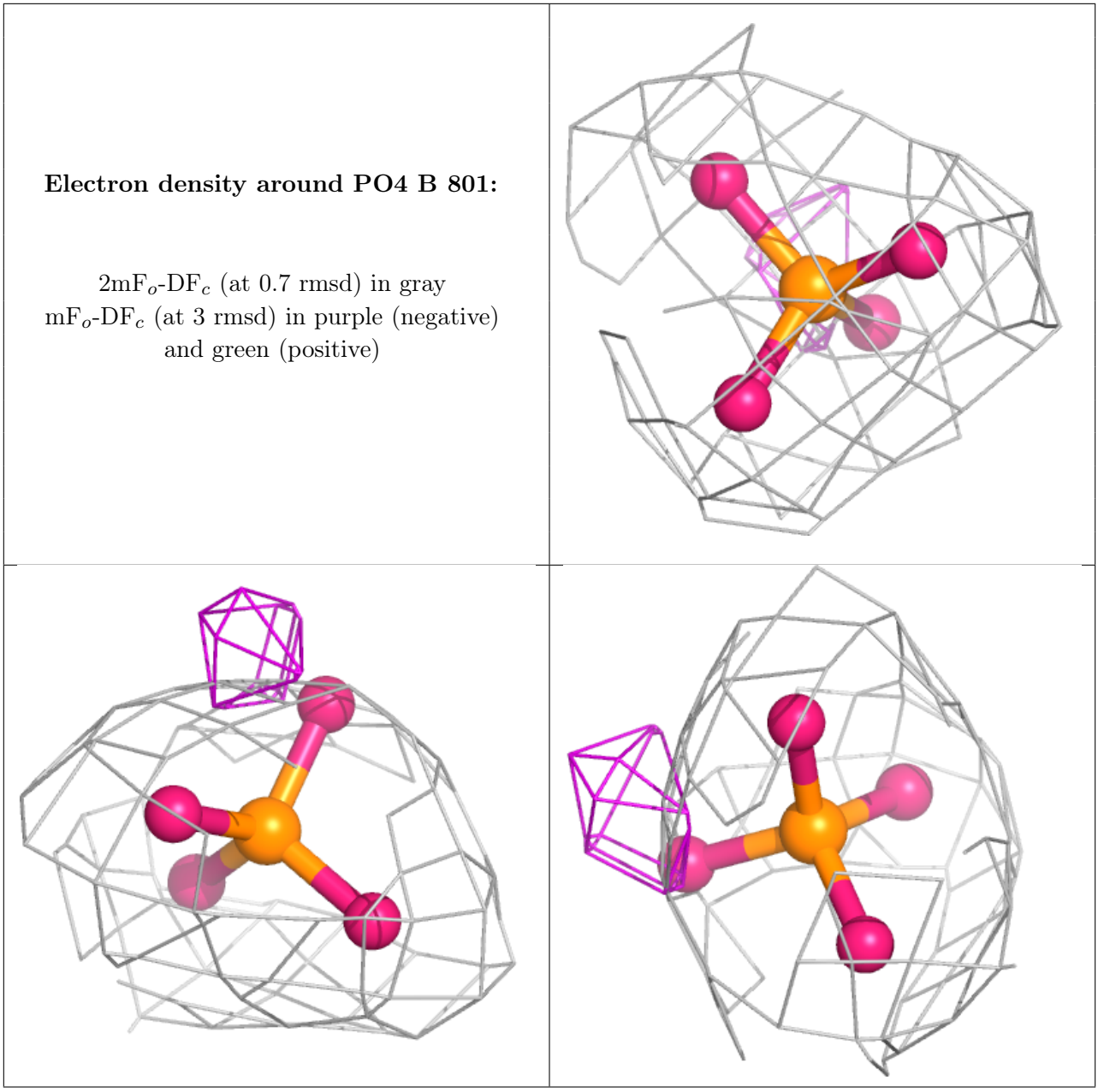
Electron density around PO4 A 801:

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



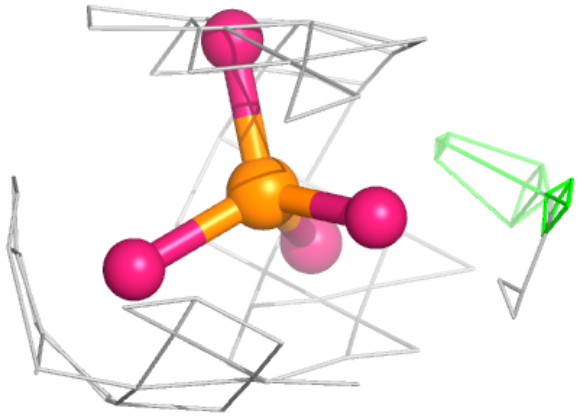
Electron density around PO4 B 801:

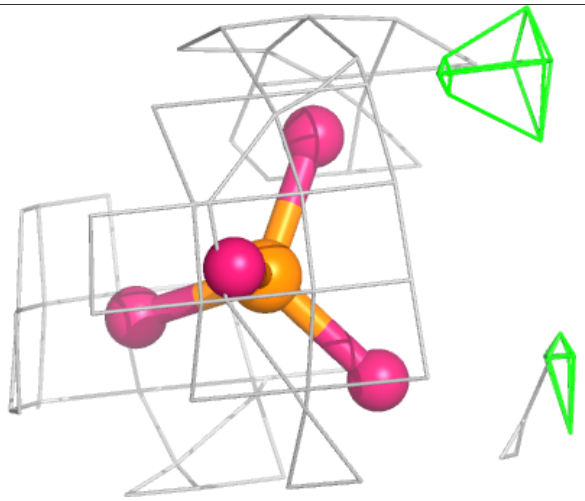
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

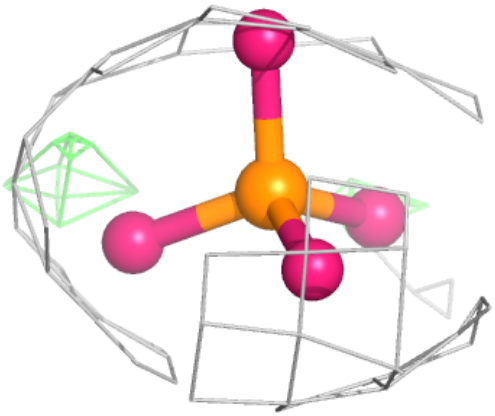


Electron density around PO4 C 801:

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

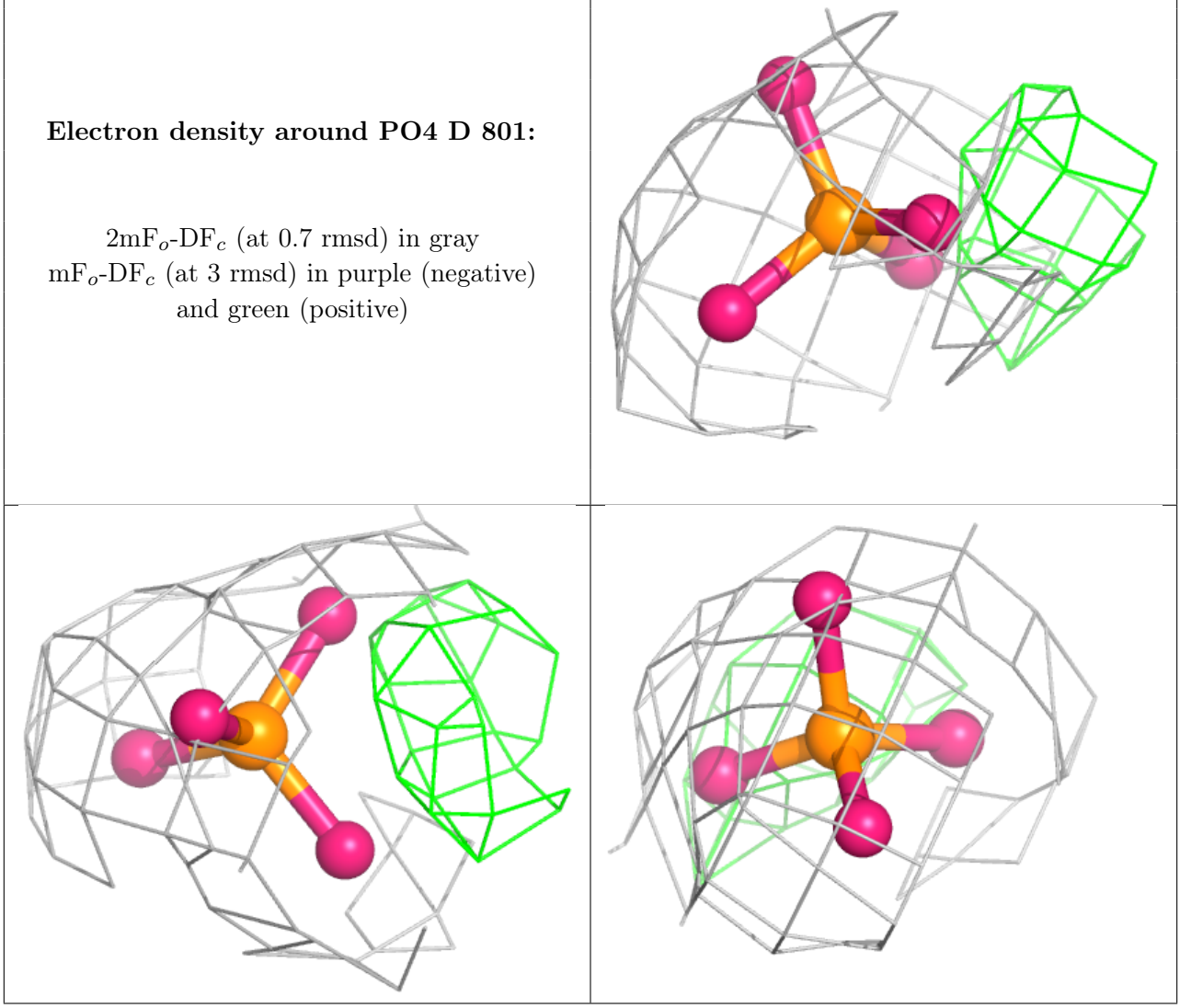






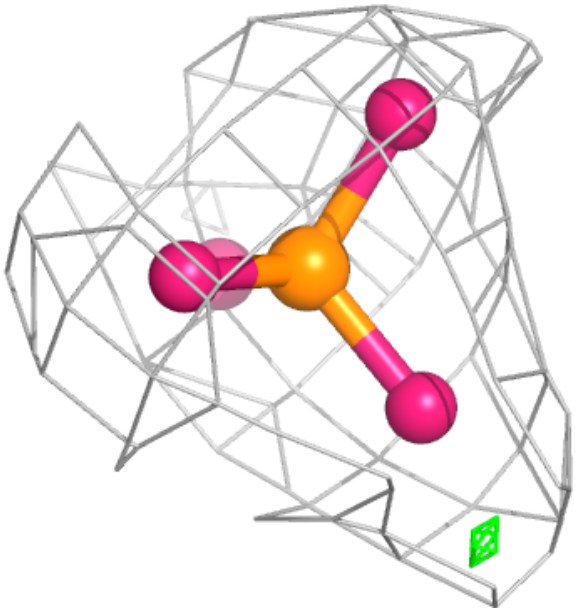
Electron density around PO4 D 801:

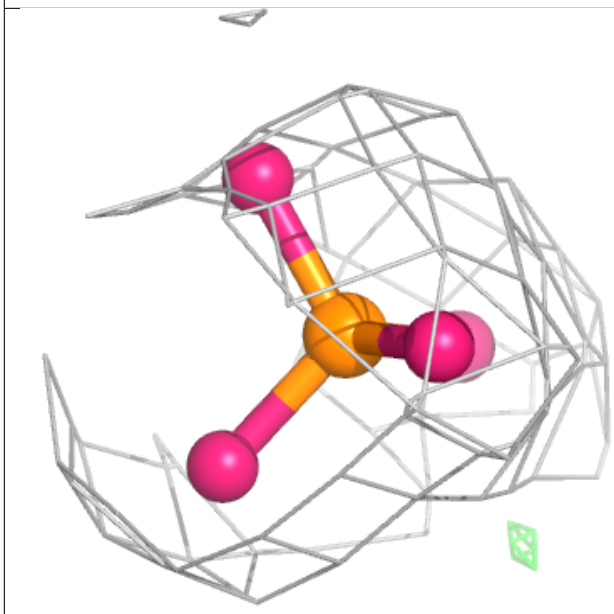
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

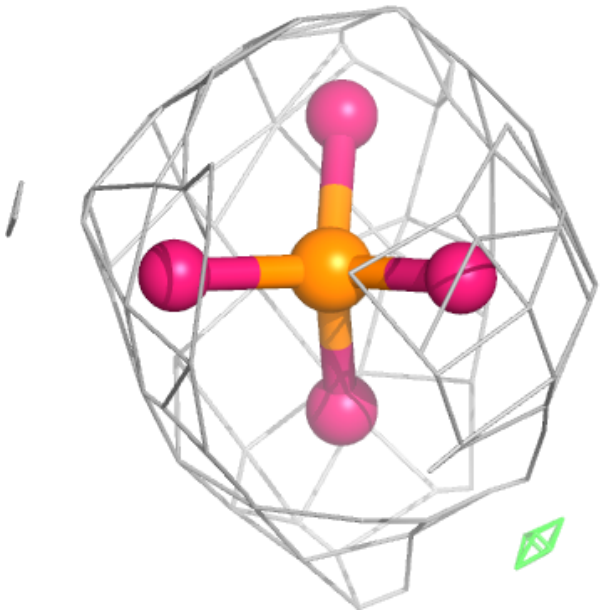


Electron density around PO4 E 801:

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

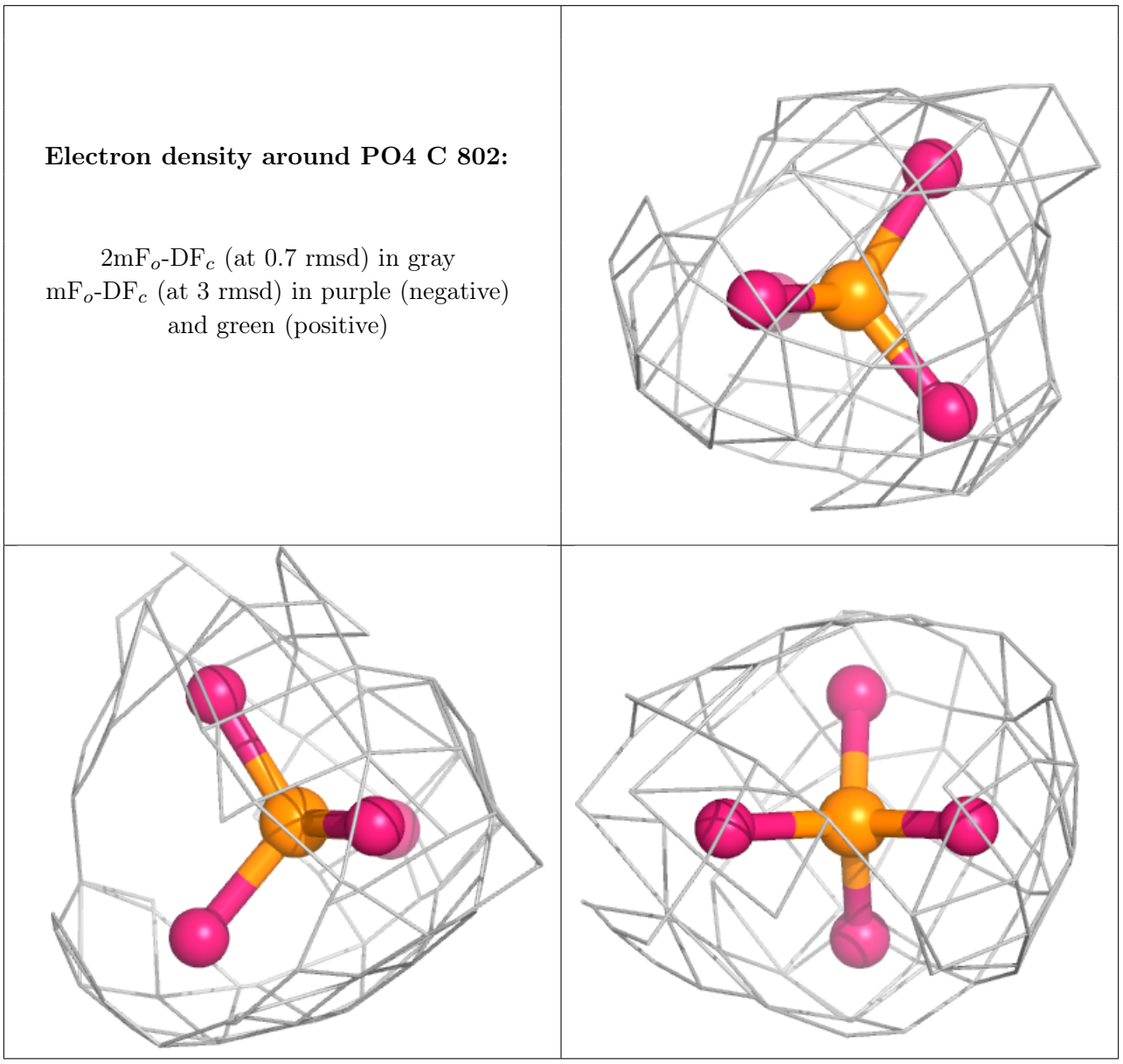






Electron density around PO4 C 802:

$2mF_o$-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

There are no such residues in this entry.