



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2026 – 12:12 PM EDT

PDB ID : 9Z01 / pdb_00009z01
Title : Crystal structure of a large RuBisCO from Promethearchaeum syntrophicum
Authors : Pereira, J.H.; Kehl, A.J.; Shih, P.M.; Adams, P.D.
Deposited on : 2025-10-30
Resolution : 1.90 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

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>.

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

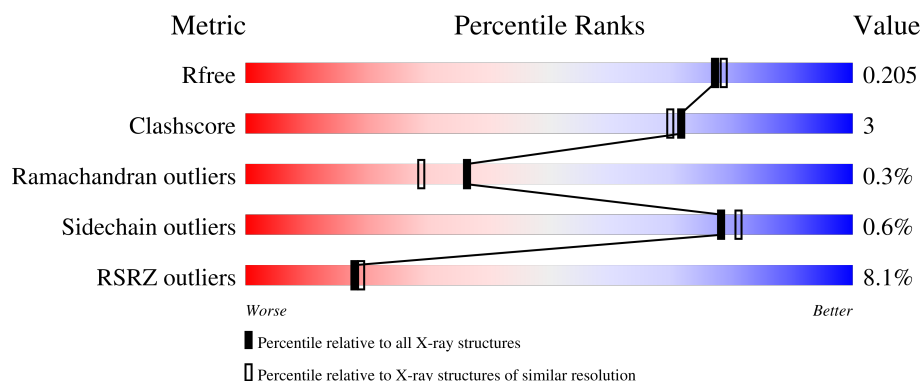
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	559	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	B	559	<div> <div>14%</div> <div>90%</div> <div>9%</div> </div>
1	C	559	<div> <div>5%</div> <div>94%</div> <div>5%</div> </div>
1	D	559	<div> <div>11%</div> <div>91%</div> <div>9%</div> </div>

2 Entry composition [i](#)

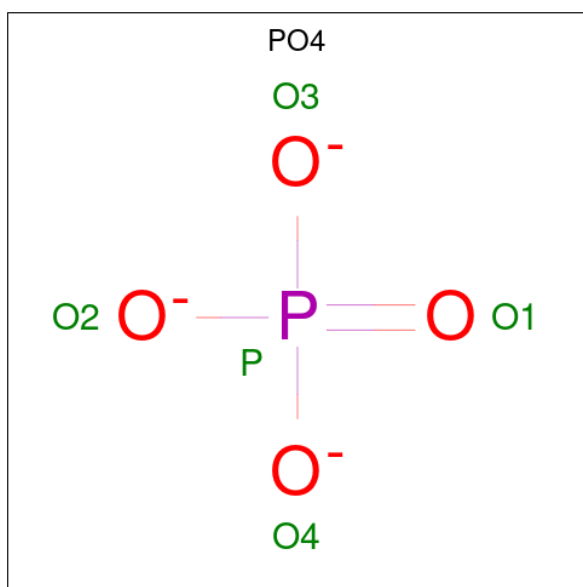
There are 3 unique types of molecules in this entry. The entry contains 36487 atoms, of which 17609 are hydrogens and 0 are deuteriums.

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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	558	Total	C	H	N	O	S	0	0	0
			8759	2775	4398	738	824	24			
1	B	557	Total	C	H	N	O	S	0	0	0
			8751	2770	4397	737	823	24			
1	C	558	Total	C	H	N	O	S	0	0	0
			8768	2775	4407	738	824	24			
1	D	558	Total	C	H	N	O	S	0	0	0
			8769	2775	4407	738	825	24			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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

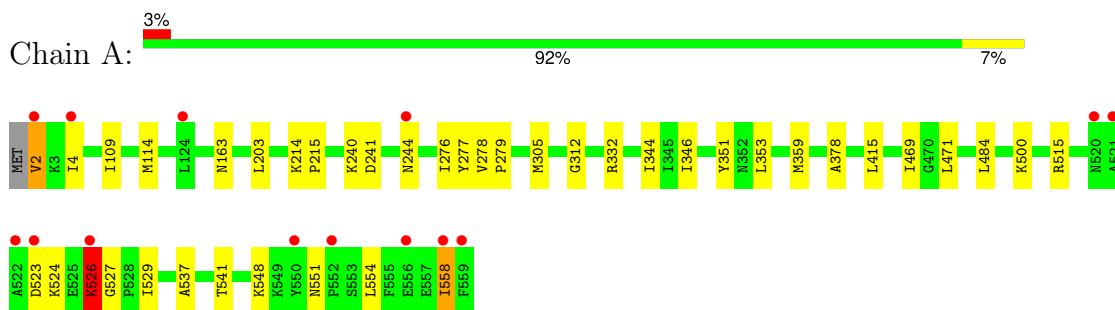
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	460	Total	O	0	0
			460	460		
3	B	327	Total	O	0	0
			327	327		
3	C	316	Total	O	0	0
			316	316		
3	D	297	Total	O	0	0
			297	297		

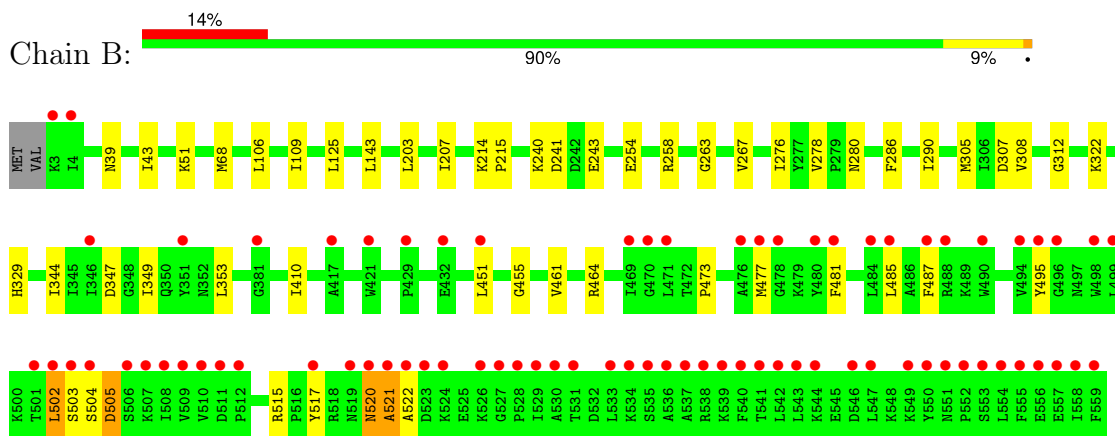
3 Residue-property plots [i](#)

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.

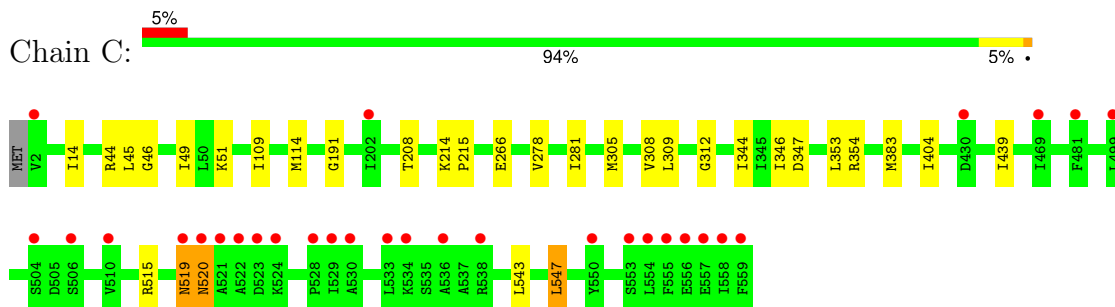
- Molecule 1: Ribulose biphosphate carboxylase



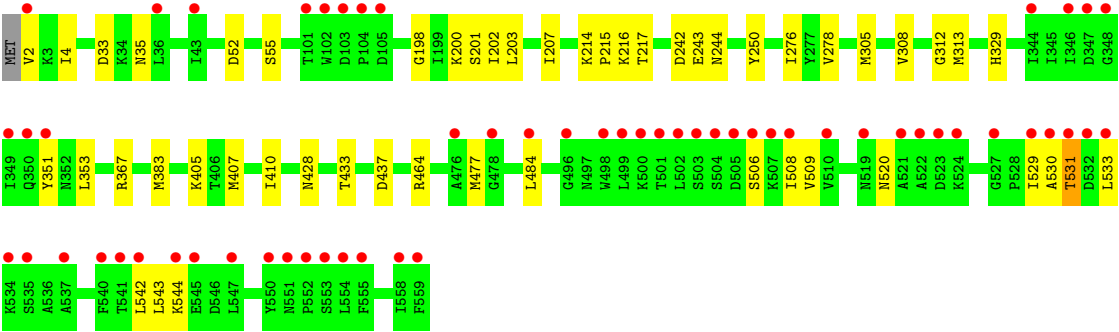
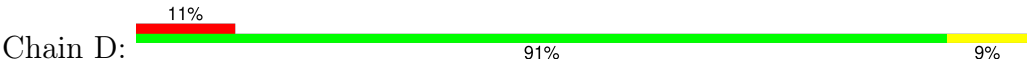
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.55Å 82.70Å 113.30Å 108.17° 97.61° 103.24°	Depositor
Resolution (Å)	46.38 – 1.90 46.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.8 (46.38-1.90) 89.8 (46.38-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.173 , 0.205 0.173 , 0.205	Depositor DCC
R_{free} test set	1809 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36487	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.37	1/4447 (0.0%)	0.44	0/6008
1	B	0.34	0/4440	0.43	2/5998 (0.0%)
1	C	0.29	0/4447	0.39	0/6008
1	D	0.30	0/4448	0.40	0/6008
All	All	0.33	1/17782 (0.0%)	0.41	2/24022 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	ASN	C-O	-5.13	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	502	LEU	N-CA-CB	5.04	119.00	110.49

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	A	4361	4398	4407	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4354	4397	4398	36	0
1	C	4361	4407	4407	22	0
1	D	4362	4407	4407	37	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	460	0	0	4	0
3	B	327	0	0	0	0
3	C	316	0	0	0	0
3	D	297	0	0	0	0
All	All	18878	17609	17619	117	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.

All (117) 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:D:530:ALA:O	1:D:531:THR:HG22	1.80	0.81
1:C:308:VAL:HG23	1:C:309:LEU:HD12	1.65	0.78
1:C:344:ILE:HD12	1:C:346:ILE:HD11	1.75	0.68
1:D:198:GLY:O	1:D:202:ILE:HD12	1.93	0.68
1:A:312:GLY:HA3	1:C:312:GLY:HA3	1.82	0.62
1:A:344:ILE:HD12	1:A:346:ILE:HD11	1.83	0.59
1:C:51:LYS:O	1:C:51:LYS:HD3	2.02	0.58
1:A:469:ILE:HD11	1:A:471:LEU:HD11	1.86	0.57
1:A:2:VAL:HB	1:C:347:ASP:OD1	2.04	0.57
1:D:533:LEU:H	1:D:533:LEU:HD12	1.68	0.57
1:A:469:ILE:HD11	1:A:471:LEU:CD1	2.35	0.56
1:D:4:ILE:HD11	1:D:351:TYR:CE1	2.40	0.56
1:D:33:ASP:OD1	1:D:35:ASN:OD1	2.24	0.55
1:A:548:LYS:HA	1:A:548:LYS:HE2	1.88	0.55
1:B:520:ASN:O	1:B:521:ALA:HB2	2.07	0.54
1:D:203:LEU:HD11	1:D:276:ILE:HD12	1.90	0.54
1:A:344:ILE:HD13	1:C:353:LEU:HD11	1.90	0.53
1:D:529:ILE:HD12	1:D:529:ILE:O	2.09	0.52
1:A:240:LYS:HE2	1:A:305:MET:HE2	1.91	0.52
1:A:241:ASP:O	1:A:305:MET:HE1	2.09	0.52
1:D:509:VAL:HG22	1:D:530:ALA:HA	1.92	0.52
1:A:4:ILE:CD1	1:A:351:TYR:HE2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:LEU:HD12	1:D:543:LEU:O	2.10	0.52
1:C:191:GLY:HA3	1:C:404:ILE:HG23	1.91	0.51
1:B:349:ILE:HD12	1:B:349:ILE:N	2.26	0.51
1:B:477:MET:HE1	1:B:495:TYR:HA	1.94	0.50
1:A:278:VAL:HG12	1:A:305:MET:HB2	1.94	0.50
1:B:203:LEU:HD11	1:B:276:ILE:HD12	1.93	0.50
1:A:500:LYS:HG2	3:A:708:HOH:O	2.11	0.49
1:B:278:VAL:HG12	1:B:305:MET:HB2	1.94	0.49
1:B:280:ASN:CG	1:B:305:MET:HE2	2.37	0.49
1:B:278:VAL:CG1	1:B:305:MET:HB2	2.42	0.49
1:D:217:THR:HG21	1:D:250:TYR:OH	2.13	0.49
1:A:163:ASN:HB3	1:C:383:MET:HE1	1.95	0.48
1:B:312:GLY:HA3	1:D:312:GLY:HA3	1.94	0.48
1:A:4:ILE:HD11	1:A:351:TYR:HE2	1.79	0.48
1:A:203:LEU:HD11	1:A:276:ILE:HD12	1.96	0.48
1:C:51:LYS:HD3	1:C:51:LYS:C	2.39	0.48
1:C:208:THR:HB	1:C:439:ILE:HG12	1.95	0.48
1:B:473:PRO:O	1:B:477:MET:HG3	2.14	0.48
1:D:52:ASP:OD2	1:D:55:SER:OG	2.32	0.47
1:A:551:ASN:N	3:A:708:HOH:O	2.47	0.47
1:B:263:GLY:O	1:B:267:VAL:HG23	2.14	0.47
1:A:548:LYS:HD3	1:A:548:LYS:C	2.38	0.47
1:D:217:THR:CG2	1:D:250:TYR:OH	2.62	0.47
1:C:281:ILE:HD12	1:C:281:ILE:C	2.39	0.47
1:D:506:SER:O	1:D:533:LEU:HD11	2.15	0.47
1:A:515:ARG:NH1	1:A:527:GLY:N	2.63	0.47
1:A:527:GLY:O	1:A:529:ILE:HD12	2.14	0.47
1:A:554:LEU:O	1:A:558:ILE:HG22	2.15	0.47
1:A:526:LYS:HD2	1:A:527:GLY:H	1.80	0.47
1:B:243:GLU:HA	1:B:305:MET:HE1	1.97	0.47
1:D:329:HIS:CE1	1:D:410:ILE:HD13	2.49	0.47
1:A:378:ALA:HB1	1:A:415:LEU:HD21	1.97	0.46
1:D:308:VAL:HG13	1:D:313:MET:HE1	1.97	0.46
1:D:207:ILE:HB	1:D:464:ARG:HG2	1.98	0.46
1:D:542:LEU:H	1:D:542:LEU:HD12	1.81	0.45
1:A:353:LEU:HD12	1:C:353:LEU:HD12	1.98	0.45
1:B:286:PHE:O	1:B:290:ILE:HG12	2.16	0.45
1:B:305:MET:HE3	1:B:307:ASP:OD1	2.17	0.45
1:B:254:GLU:O	1:B:258:ARG:HG3	2.17	0.45
1:B:39:ASN:O	1:B:43:ILE:HG23	2.16	0.45
1:C:543:LEU:O	1:C:547:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:GLU:HA	1:D:305:MET:HE1	1.99	0.45
1:B:353:LEU:HD12	1:D:353:LEU:HD12	1.99	0.45
1:C:109:ILE:O	1:C:114:MET:HE2	2.17	0.44
1:A:523:ASP:O	1:A:524:LYS:HD2	2.17	0.44
1:D:198:GLY:O	1:D:202:ILE:CD1	2.64	0.44
1:D:477:MET:HG2	1:D:484:LEU:HA	1.99	0.44
1:B:240:LYS:HA	1:B:278:VAL:HB	2.00	0.44
3:A:742:HOH:O	1:D:405:LYS:CE	2.65	0.44
1:A:278:VAL:CG1	1:A:305:MET:HB2	2.48	0.43
1:B:477:MET:HE3	1:B:487:PHE:HB2	2.00	0.43
1:D:313:MET:HA	1:D:313:MET:HE2	2.01	0.43
1:D:383:MET:HG3	2:D:602:PO4:O4	2.18	0.43
1:A:277:TYR:O	1:A:279:PRO:HD3	2.18	0.43
1:B:106:LEU:O	1:B:109:ILE:HG12	2.19	0.43
1:D:508:ILE:O	1:D:530:ALA:O	2.36	0.43
1:B:125:LEU:HD13	1:D:217:THR:HG22	2.01	0.43
1:D:200:LYS:HD2	1:D:437:ASP:OD1	2.18	0.43
1:D:214:LYS:HA	1:D:215:PRO:C	2.43	0.42
1:A:484:LEU:HD23	1:A:484:LEU:C	2.44	0.42
1:D:278:VAL:HG12	1:D:305:MET:HB2	2.02	0.42
1:B:329:HIS:CE1	1:B:410:ILE:HD13	2.55	0.42
1:C:278:VAL:HG12	1:C:305:MET:HB2	2.02	0.42
1:A:214:LYS:HA	1:A:215:PRO:C	2.44	0.42
1:B:451:LEU:HB2	1:B:455:GLY:HA3	2.02	0.42
1:C:46:GLY:HA2	1:C:49:ILE:HD12	2.02	0.42
1:A:109:ILE:O	1:A:114:MET:HE2	2.19	0.42
1:C:14:ILE:HD12	1:C:354:ARG:HD2	2.02	0.42
1:D:367:ARG:HB2	1:D:407:MET:HE2	2.02	0.42
1:B:214:LYS:HA	1:B:215:PRO:C	2.44	0.42
1:B:521:ALA:O	1:B:522:ALA:HB3	2.19	0.42
1:B:207:ILE:HB	1:B:464:ARG:HG2	2.01	0.41
1:B:461:VAL:HG21	1:B:517:TYR:CZ	2.55	0.41
1:C:44:ARG:HG2	1:C:45:LEU:HG	2.01	0.41
1:C:344:ILE:HD12	1:C:346:ILE:CD1	2.47	0.41
1:D:215:PRO:O	1:D:216:LYS:C	2.63	0.41
1:D:543:LEU:O	1:D:544:LYS:C	2.63	0.41
1:B:347:ASP:OD2	1:D:2:VAL:HG13	2.20	0.41
1:C:543:LEU:HD12	1:C:547:LEU:HD22	2.03	0.41
1:B:481:PHE:CZ	1:B:485:LEU:HD11	2.56	0.41
1:B:520:ASN:O	1:B:521:ALA:CB	2.67	0.41
1:C:214:LYS:HA	1:C:215:PRO:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:HG2	1:B:241:ASP:O	2.21	0.41
1:B:461:VAL:HG21	1:B:517:TYR:CE1	2.56	0.41
1:B:51:LYS:N	1:B:51:LYS:HD2	2.36	0.41
1:A:332:ARG:NH1	1:A:359:MET:HG2	2.36	0.41
1:B:344:ILE:HD13	1:D:353:LEU:HD11	2.02	0.41
1:B:515:ARG:HH11	1:B:515:ARG:HG3	1.86	0.40
1:C:519:ASN:O	1:C:520:ASN:C	2.64	0.40
1:D:428:ASN:ND2	1:D:433:THR:HG23	2.37	0.40
1:A:500:LYS:CG	3:A:708:HOH:O	2.69	0.40
1:B:68:MET:HE2	1:B:143:LEU:HD11	2.03	0.40
1:B:290:ILE:HD12	1:B:322:LYS:HD2	2.04	0.40
1:A:537:ALA:O	1:A:541:THR:HA	2.21	0.40
1:D:242:ASP:OD1	1:D:244:ASN:OD1	2.39	0.40

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	556/559 (100%)	532 (96%)	23 (4%)	1 (0%)	43	36
1	B	555/559 (99%)	531 (96%)	21 (4%)	3 (0%)	24	16
1	C	556/559 (100%)	536 (96%)	18 (3%)	2 (0%)	30	22
1	D	556/559 (100%)	532 (96%)	23 (4%)	1 (0%)	43	36
All	All	2223/2236 (99%)	2131 (96%)	85 (4%)	7 (0%)	36	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	ALA
1	A	526	LYS

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Mol	Chain	Res	Type
1	B	520	ASN
1	D	520	ASN
1	B	503	SER
1	C	519	ASN
1	C	520	ASN

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	473/474 (100%)	470 (99%)	3 (1%)	78	81
1	B	472/474 (100%)	468 (99%)	4 (1%)	73	75
1	C	473/474 (100%)	470 (99%)	3 (1%)	78	81
1	D	473/474 (100%)	471 (100%)	2 (0%)	84	87
All	All	1891/1896 (100%)	1879 (99%)	12 (1%)	78	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	526	LYS
1	A	558	ILE
1	B	308	VAL
1	B	502	LEU
1	B	504	SER
1	B	505	ASP
1	C	266	GLU
1	C	515	ARG
1	C	547	LEU
1	D	201	SER
1	D	531	THR

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

Mol	Chain	Res	Type
1	A	13	GLN
1	A	28	ASN
1	A	350	GLN
1	B	13	GLN
1	B	63	ASN
1	C	39	ASN
1	C	352	ASN
1	D	350	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	D	601	-	4,4,4	1.81	1 (25%)	6,6,6	0.59	0
2	PO4	D	602	-	4,4,4	1.49	1 (25%)	6,6,6	0.64	0
2	PO4	A	602	-	4,4,4	1.89	1 (25%)	6,6,6	0.34	0
2	PO4	B	602	-	4,4,4	1.35	1 (25%)	6,6,6	0.74	0
2	PO4	C	602	-	4,4,4	1.75	1 (25%)	6,6,6	0.54	0
2	PO4	B	601	-	4,4,4	1.21	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	C	601	-	4,4,4	1.74	1 (25%)	6,6,6	0.66	0
2	PO4	A	601	-	4,4,4	1.41	1 (25%)	6,6,6	0.88	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	PO4	P-O1	3.59	1.59	1.50
2	D	601	PO4	P-O1	3.45	1.58	1.50
2	C	602	PO4	P-O1	3.06	1.57	1.50
2	C	601	PO4	P-O1	3.02	1.57	1.50
2	D	602	PO4	P-O1	2.73	1.57	1.50
2	A	601	PO4	P-O1	2.63	1.56	1.50
2	B	602	PO4	P-O1	2.19	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

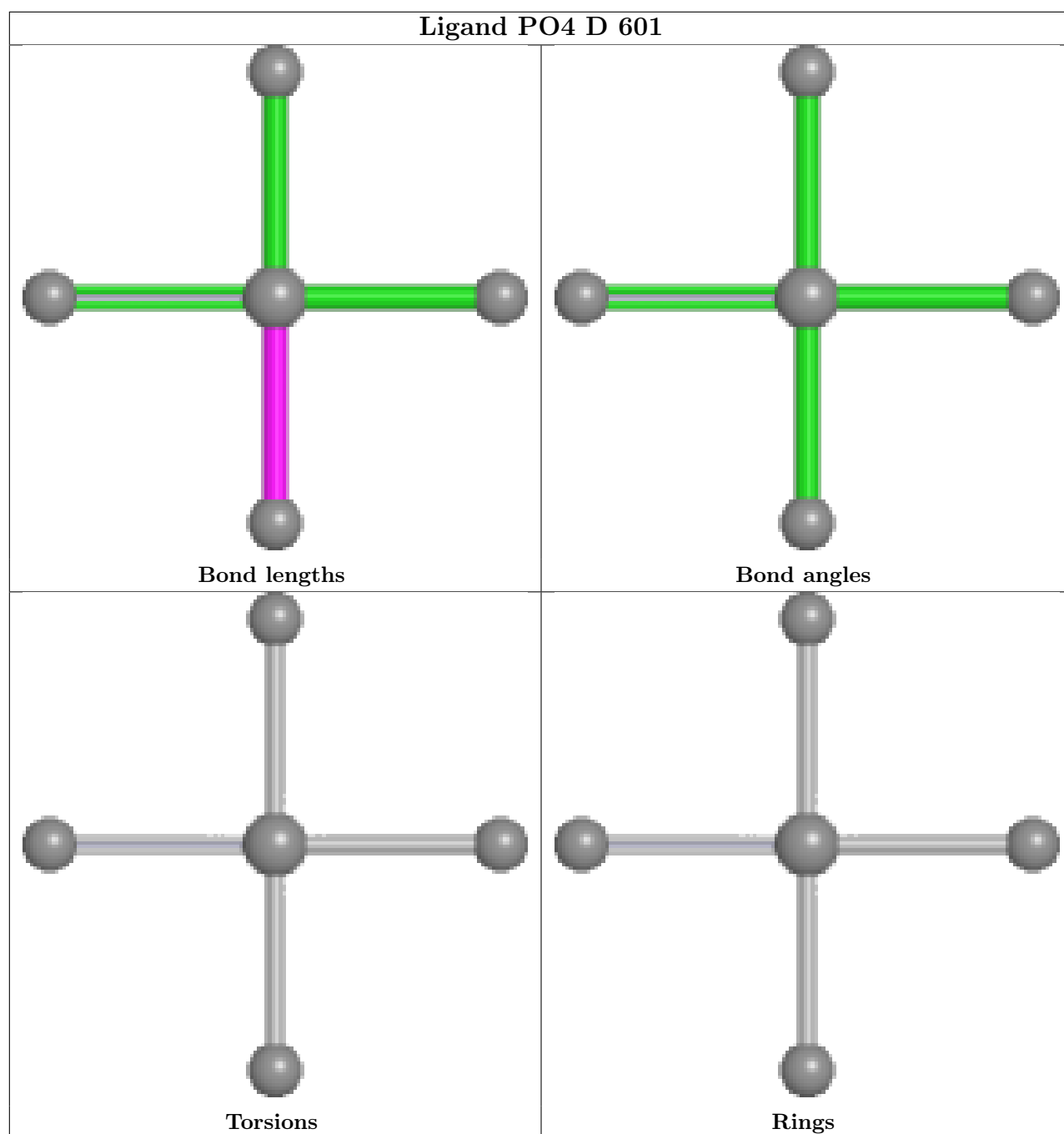
There are no torsion outliers.

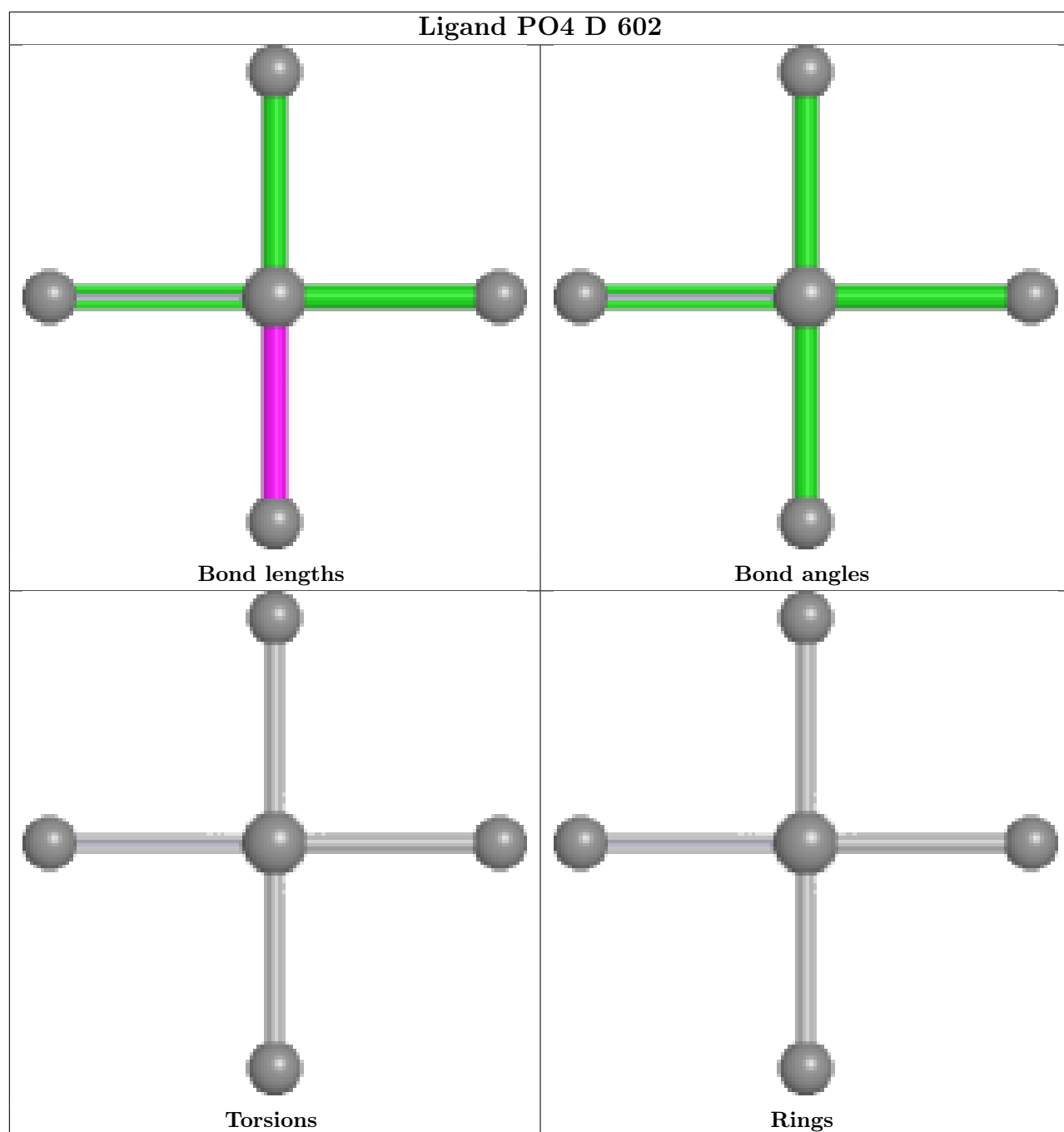
There are no ring outliers.

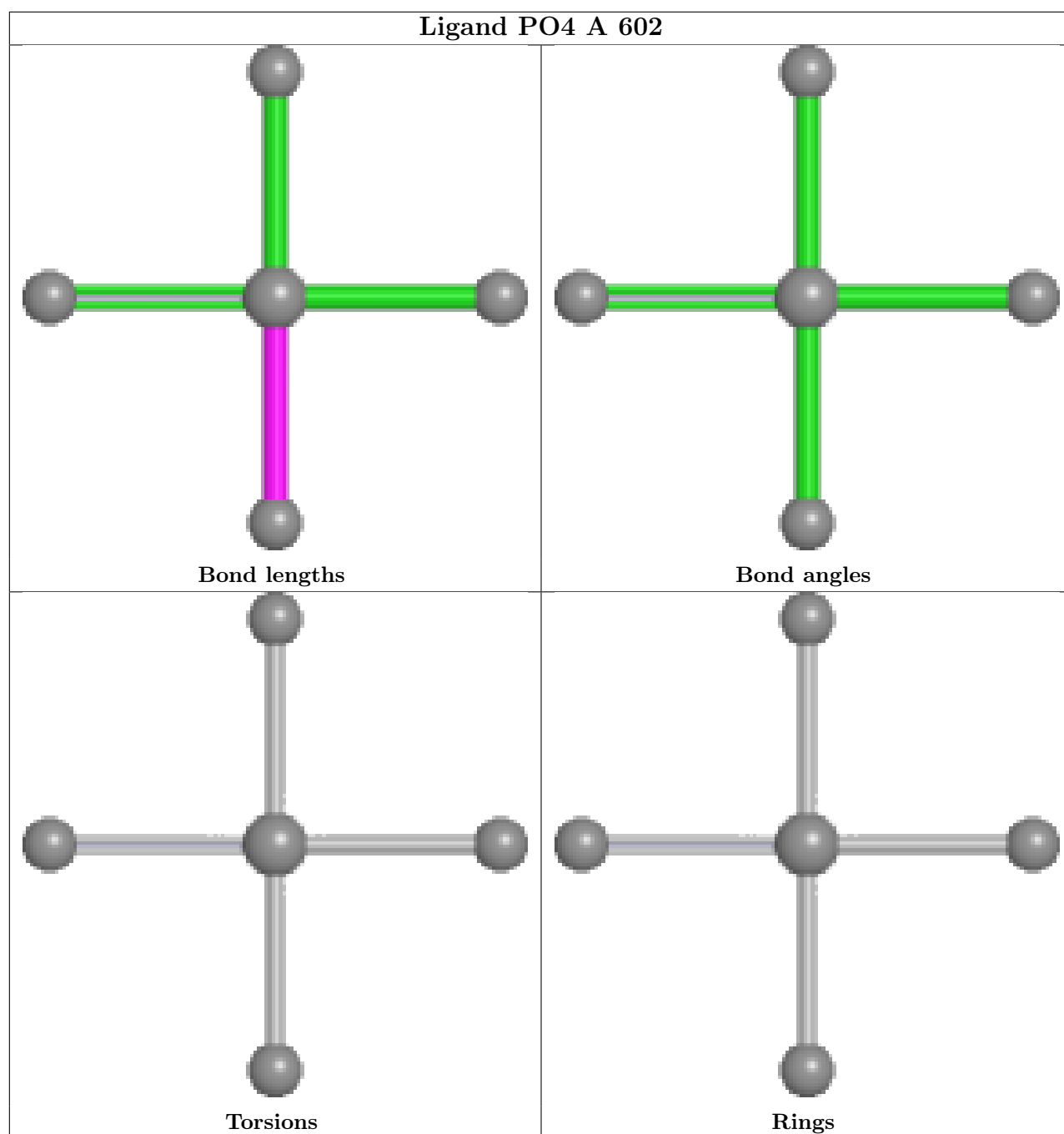
1 monomer is involved in 1 short contact:

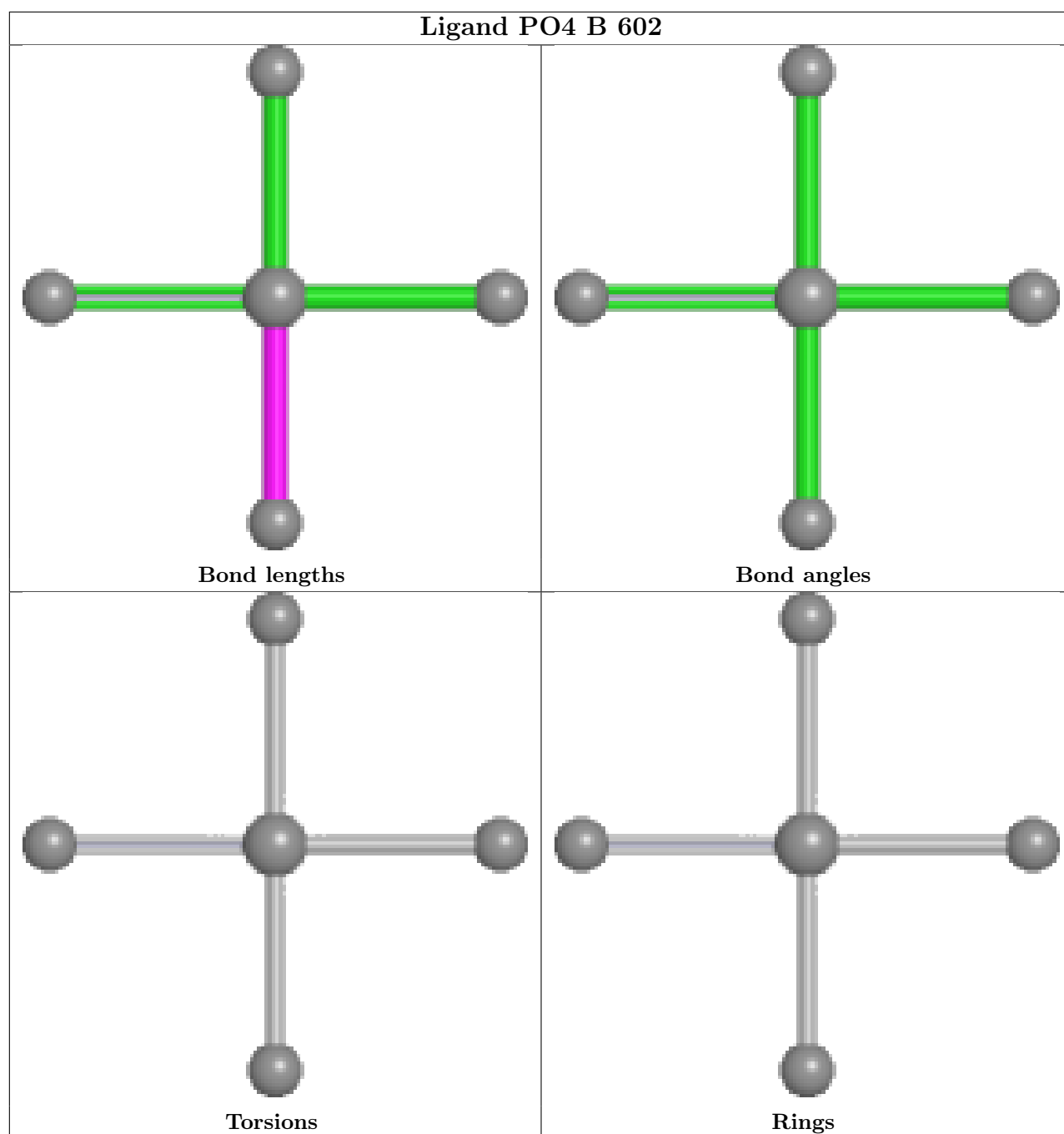
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	602	PO4	1	0

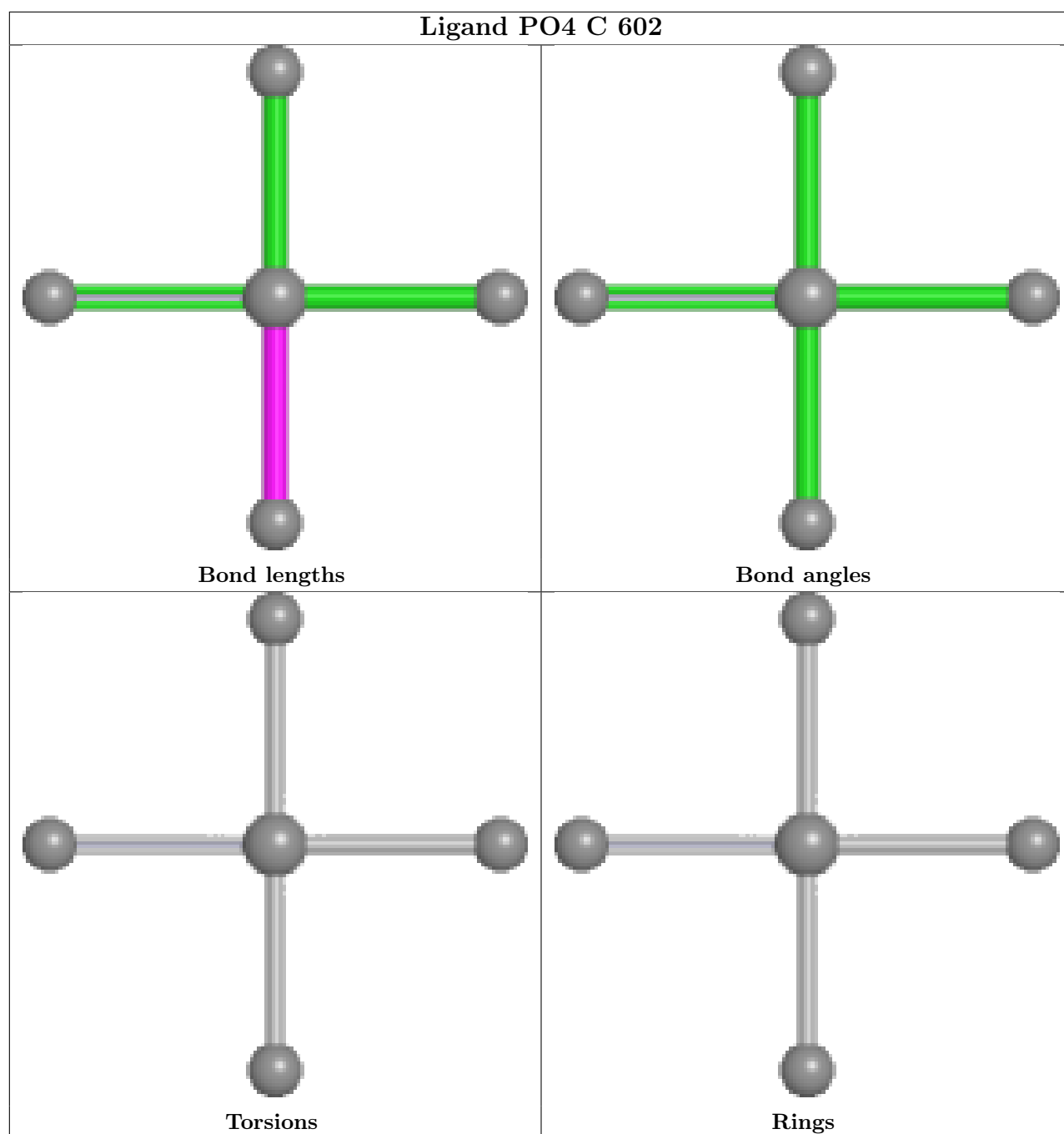
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

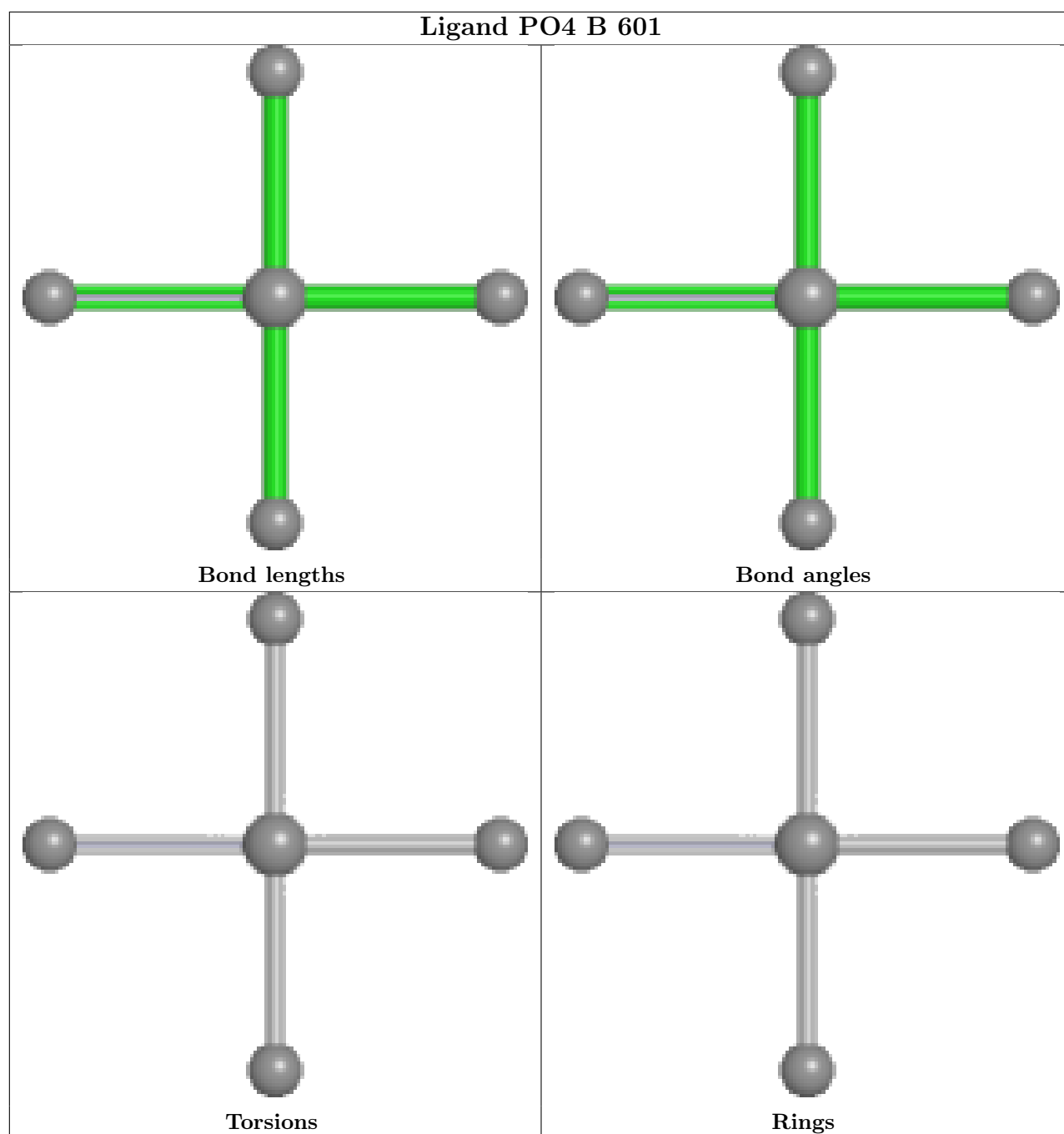


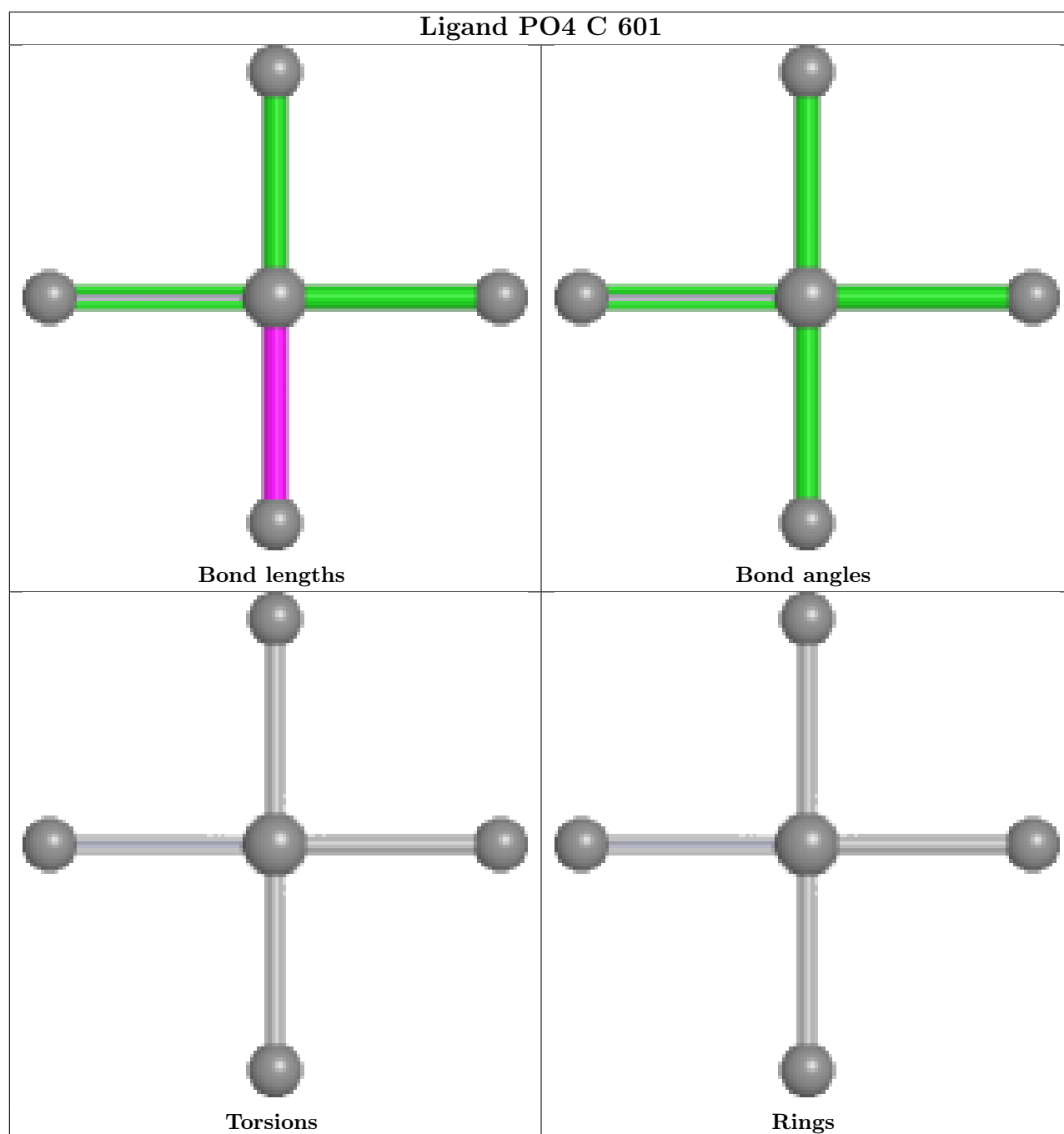


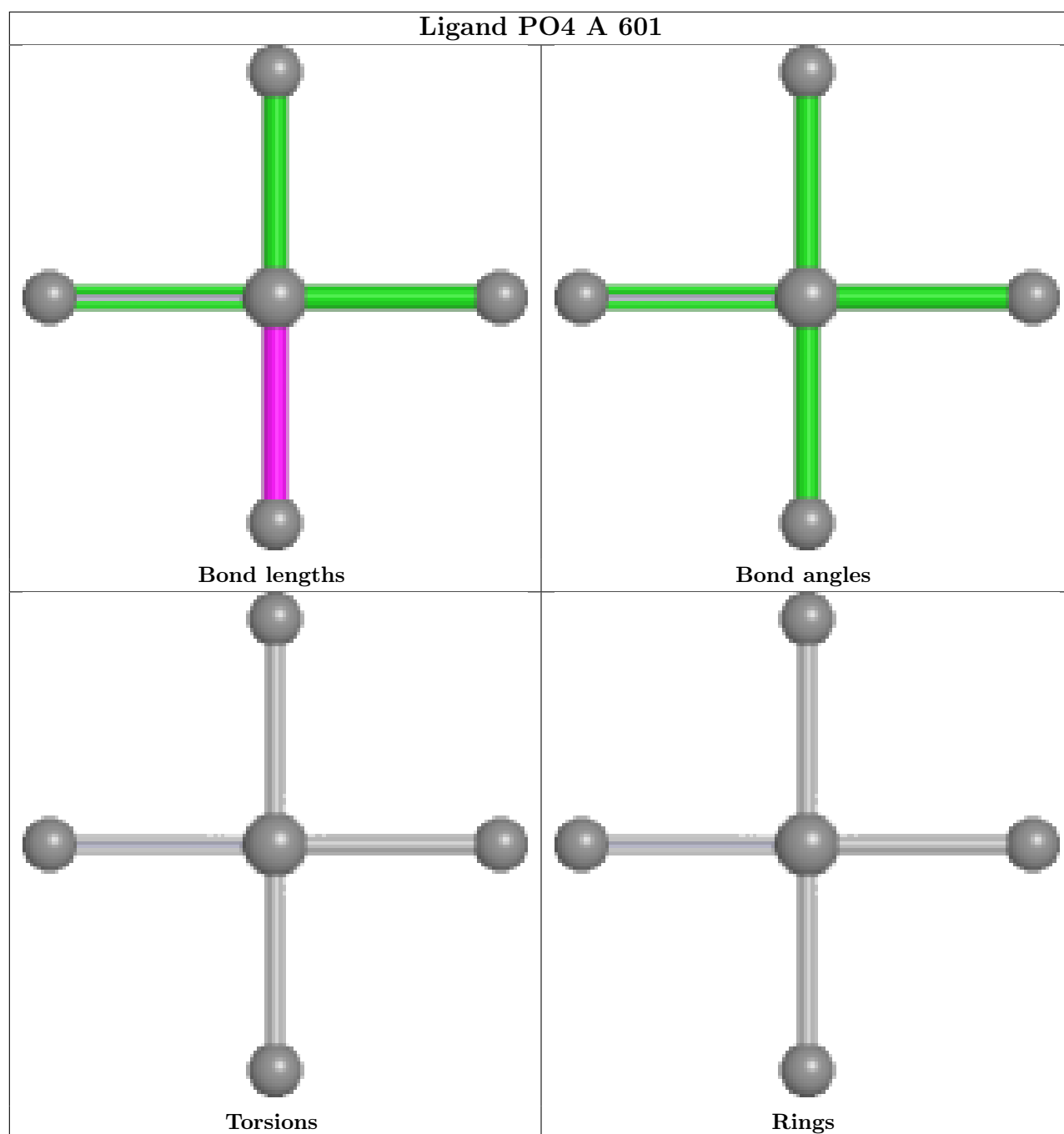












5.7 Other polymers [i](#)

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

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(Å ²)	Q<0.9
1	A	558/559 (99%)	-0.22	14 (2%) 58 62	17, 32, 74, 122	0
1	B	557/559 (99%)	0.39	77 (13%) 6 6	19, 37, 131, 158	0
1	C	558/559 (99%)	0.23	30 (5%) 31 33	18, 42, 98, 188	0
1	D	558/559 (99%)	0.30	59 (10%) 11 12	17, 42, 107, 155	0
All	All	2231/2236 (99%)	0.17	180 (8%) 18 19	17, 38, 106, 188	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	PHE	8.0
1	B	558	ILE	7.8
1	B	543	LEU	7.5
1	C	559	PHE	7.4
1	C	554	LEU	6.8
1	C	558	ILE	6.7
1	A	559	PHE	6.4
1	D	558	ILE	6.1
1	C	555	PHE	5.9
1	B	508	ILE	5.6
1	B	502	LEU	5.4
1	D	559	PHE	5.3
1	B	509	VAL	5.2
1	B	521	ALA	5.1
1	A	2	VAL	5.0
1	D	522	ALA	4.9
1	B	554	LEU	4.8
1	A	521	ALA	4.7
1	B	495	TYR	4.7
1	B	540	PHE	4.6
1	B	529	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	550	TYR	4.5
1	B	544	LYS	4.5
1	B	533	LEU	4.4
1	B	531	THR	4.4
1	B	522	ALA	4.4
1	D	349	ILE	4.3
1	B	541	THR	4.2
1	C	533	LEU	4.2
1	A	558	ILE	4.1
1	D	533	LEU	4.1
1	B	547	LEU	4.1
1	B	555	PHE	4.0
1	B	504	SER	4.0
1	D	554	LEU	4.0
1	B	4	ILE	4.0
1	D	2	VAL	3.9
1	C	522	ALA	3.9
1	A	522	ALA	3.9
1	D	551	ASN	3.8
1	D	542	LEU	3.8
1	C	521	ALA	3.8
1	B	510	VAL	3.8
1	D	506	SER	3.8
1	B	484	LEU	3.8
1	B	552	PRO	3.8
1	B	537	ALA	3.6
1	B	499	LEU	3.6
1	B	530	ALA	3.5
1	D	531	THR	3.5
1	D	499	LEU	3.5
1	D	351	TYR	3.5
1	D	529	ILE	3.4
1	B	496	GLY	3.4
1	B	481	PHE	3.4
1	B	476	ALA	3.3
1	D	346	ILE	3.3
1	B	512	PRO	3.3
1	B	520	ASN	3.3
1	C	553	SER	3.3
1	C	524	LYS	3.3
1	D	502	LEU	3.3
1	C	529	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	498	TRP	3.2
1	B	487	PHE	3.2
1	C	519	ASN	3.1
1	B	542	LEU	3.1
1	B	478	GLY	3.1
1	B	517	TYR	3.1
1	B	501	THR	3.1
1	B	503	SER	3.1
1	D	535	SER	3.1
1	B	523	ASP	3.0
1	D	547	LEU	3.0
1	D	527	GLY	3.0
1	D	552	PRO	3.0
1	D	530	ALA	3.0
1	B	346	ILE	3.0
1	D	102	TRP	3.0
1	D	555	PHE	3.0
1	B	381	GLY	3.0
1	D	521	ALA	3.0
1	B	494	VAL	3.0
1	B	524	LYS	3.0
1	B	553	SER	2.9
1	C	2	VAL	2.9
1	D	478	GLY	2.9
1	B	506	SER	2.9
1	B	527	GLY	2.9
1	D	347	ASP	2.9
1	C	504	SER	2.8
1	B	469	ILE	2.8
1	B	3	LYS	2.8
1	D	508	ILE	2.8
1	C	506	SER	2.8
1	B	471	LEU	2.8
1	D	36	LEU	2.8
1	D	541	THR	2.8
1	C	510	VAL	2.8
1	B	536	ALA	2.7
1	D	519	ASN	2.7
1	D	537	ALA	2.7
1	B	539	LYS	2.7
1	D	540	PHE	2.7
1	B	451	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	526	LYS	2.7
1	B	417	ALA	2.6
1	B	546	ASP	2.6
1	B	538	ARG	2.6
1	B	507	LYS	2.6
1	D	104	PRO	2.6
1	C	557	GLU	2.6
1	B	351	TYR	2.6
1	B	549	LYS	2.6
1	A	520	ASN	2.6
1	D	532	ASP	2.6
1	C	520	ASN	2.6
1	A	4	ILE	2.5
1	D	498	TRP	2.5
1	D	510	VAL	2.5
1	B	485	LEU	2.4
1	B	557	GLU	2.4
1	C	536	ALA	2.4
1	D	105	ASP	2.4
1	B	480	TYR	2.4
1	C	499	LEU	2.4
1	D	503	SER	2.4
1	D	550	TYR	2.4
1	D	544	LYS	2.4
1	B	490	TRP	2.4
1	C	550	TYR	2.4
1	A	550	TYR	2.3
1	D	545	GLU	2.3
1	C	530	ALA	2.3
1	C	528	PRO	2.3
1	B	511	ASP	2.3
1	C	430	ASP	2.3
1	B	432	GLU	2.3
1	D	350	GLN	2.3
1	D	484	LEU	2.3
1	B	519	ASN	2.3
1	B	551	ASN	2.3
1	D	534	LYS	2.3
1	D	505	ASP	2.3
1	B	528	PRO	2.3
1	B	535	SER	2.3
1	A	523	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	556	GLU	2.3
1	C	556	GLU	2.2
1	D	103	ASP	2.2
1	B	488	ARG	2.2
1	B	556	GLU	2.2
1	A	244	ASN	2.2
1	B	534	LYS	2.2
1	D	524	LYS	2.2
1	C	534	LYS	2.2
1	D	523	ASP	2.2
1	D	504	SER	2.2
1	C	481	PHE	2.1
1	D	101	THR	2.1
1	D	507	LYS	2.1
1	B	477	MET	2.1
1	D	501	THR	2.1
1	D	496	GLY	2.1
1	A	526	LYS	2.1
1	B	429	PRO	2.1
1	C	202	ILE	2.0
1	D	553	SER	2.0
1	A	124	LEU	2.0
1	B	421	TRP	2.0
1	D	476	ALA	2.0
1	C	523	ASP	2.0
1	C	538	ARG	2.0
1	D	500	LYS	2.0
1	C	469	ILE	2.0
1	D	43	ILE	2.0
1	D	344	ILE	2.0
1	B	470	GLY	2.0
1	D	348	GLY	2.0
1	A	552	PRO	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 oligosaccharides in this entry.

6.4 Ligands

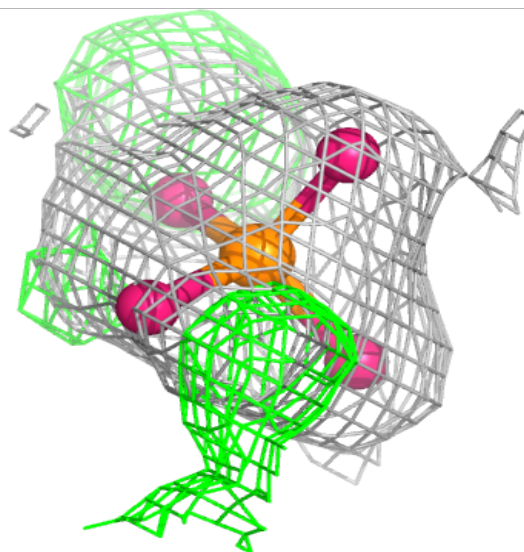
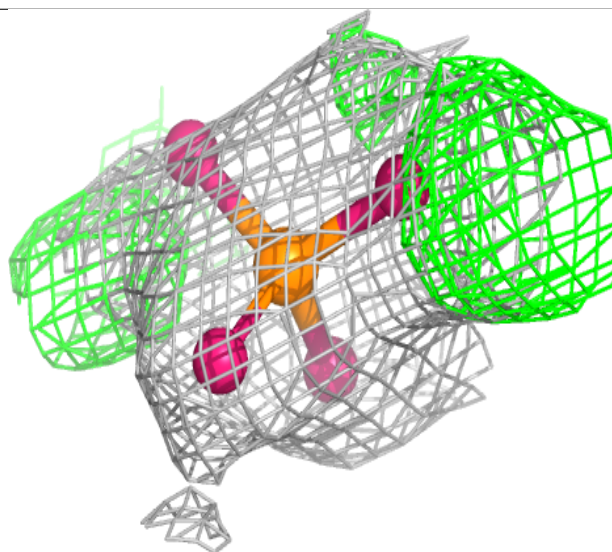
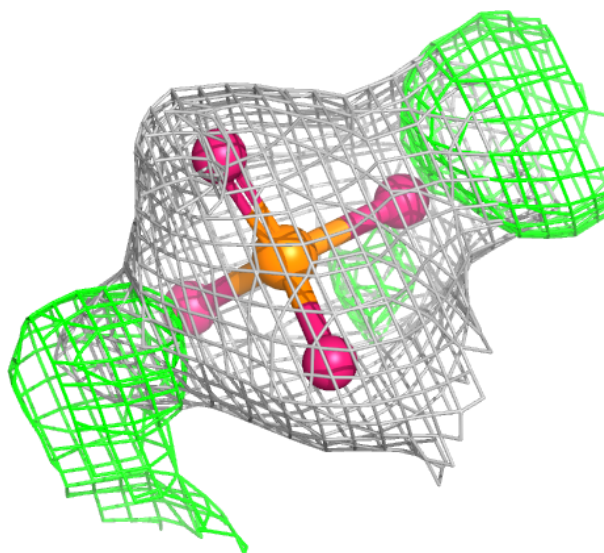
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	D	601	5/5	0.87	0.14	36,38,47,57	0
2	PO4	B	601	5/5	0.89	0.13	46,52,56,60	0
2	PO4	D	602	5/5	0.92	0.14	37,39,48,53	0
2	PO4	C	601	5/5	0.96	0.07	29,34,39,40	0
2	PO4	B	602	5/5	0.97	0.07	31,37,39,39	0
2	PO4	A	602	5/5	0.97	0.07	22,26,28,28	0
2	PO4	C	602	5/5	0.98	0.08	33,34,38,42	0
2	PO4	A	601	5/5	0.99	0.04	22,23,23,24	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.

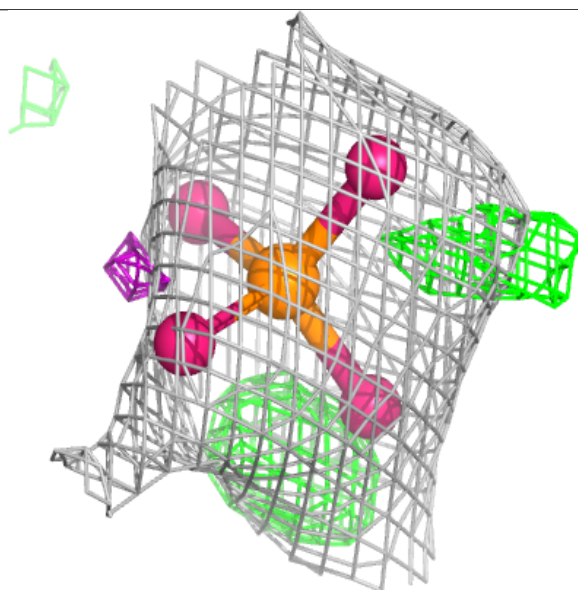
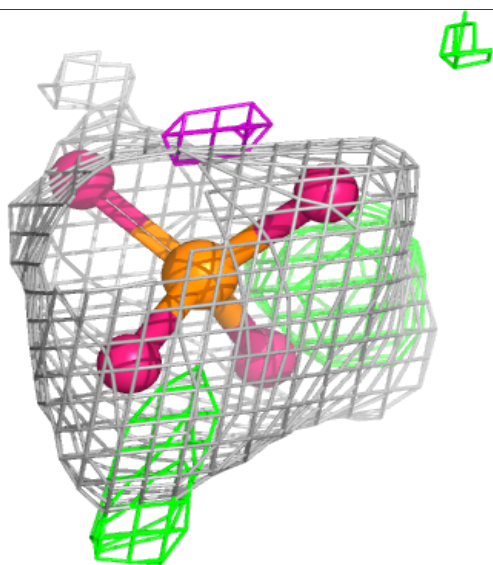
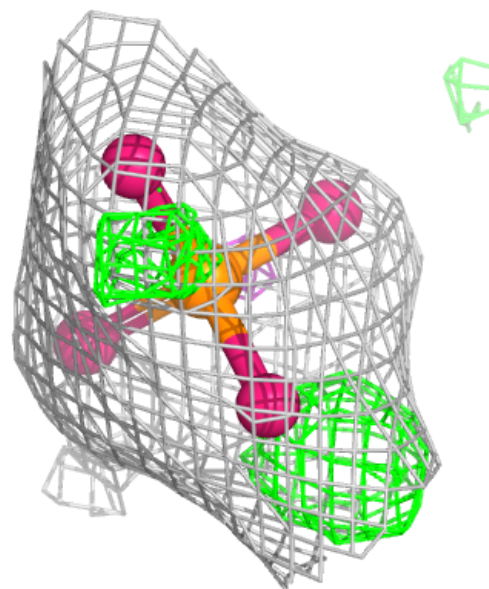
Electron density around PO4 D 601:

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



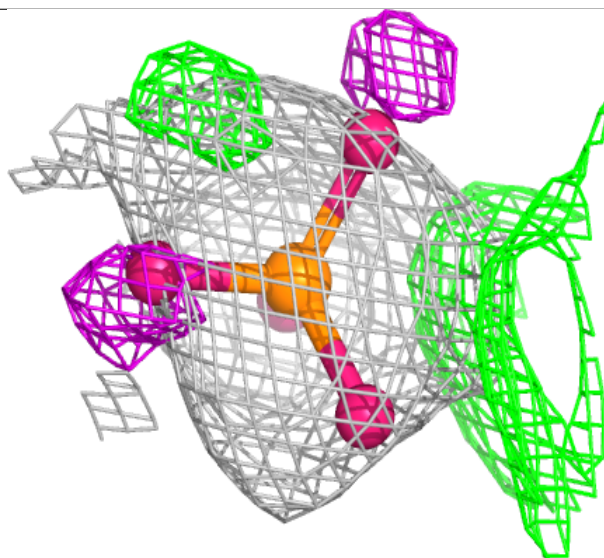
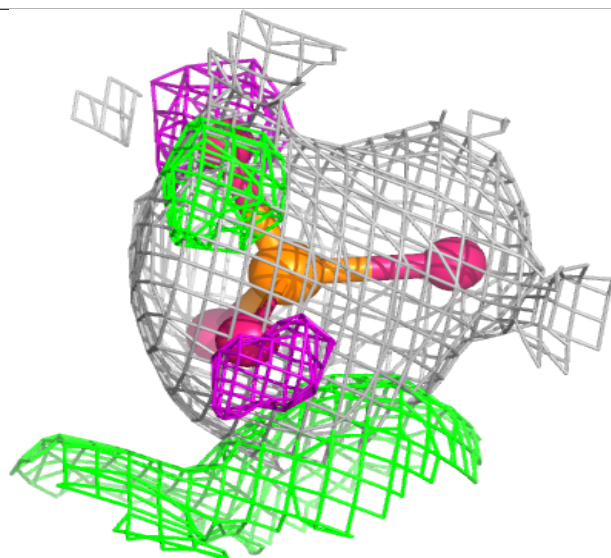
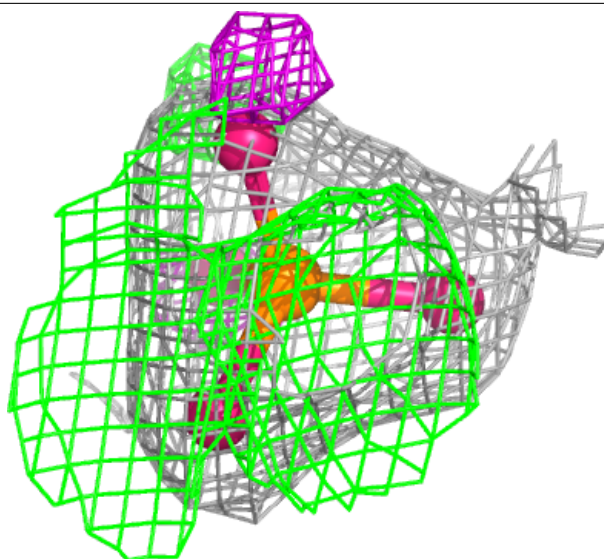
Electron density around PO4 B 601:

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



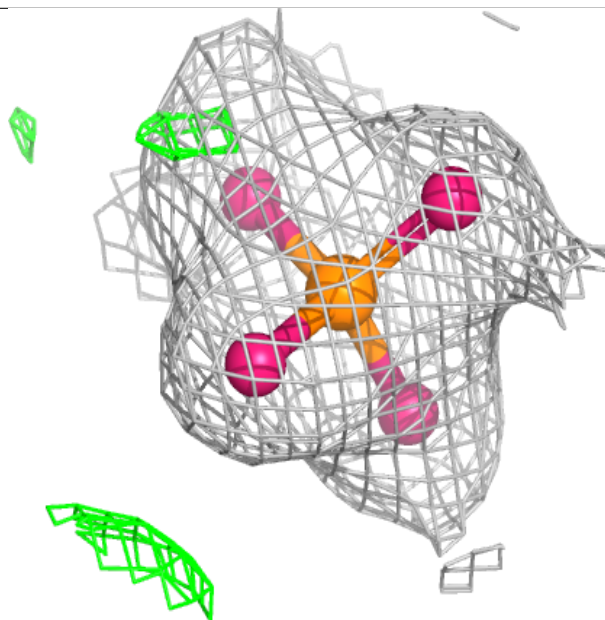
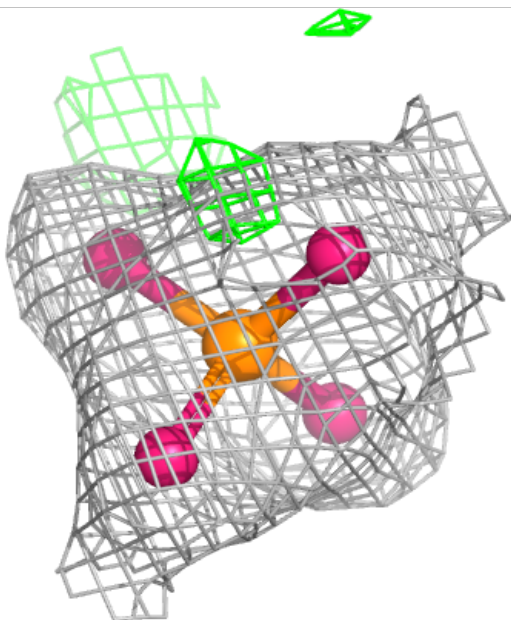
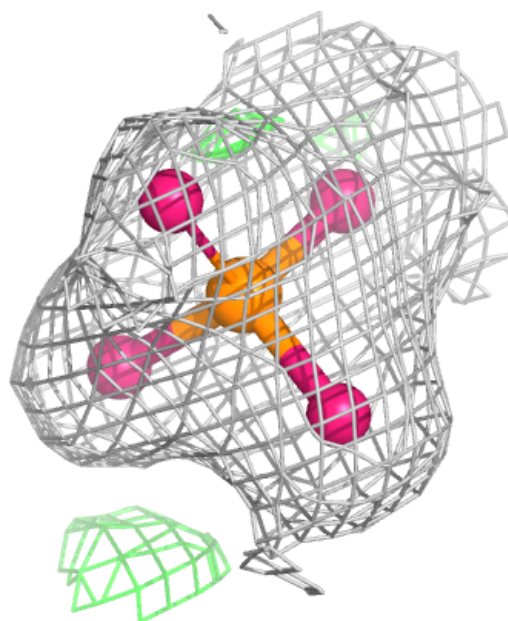
Electron density around PO4 D 602:

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



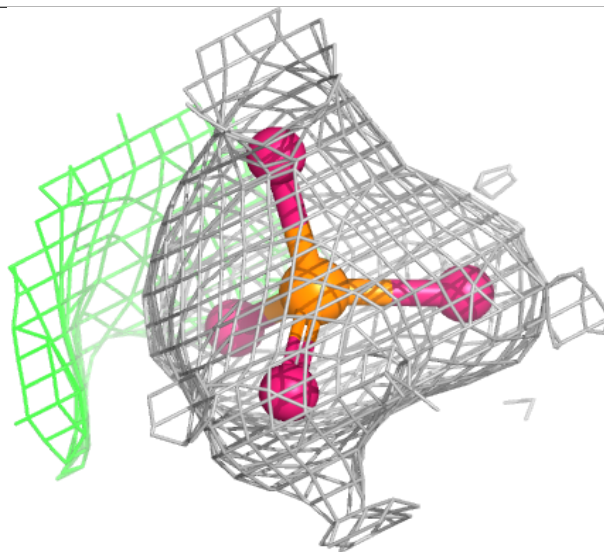
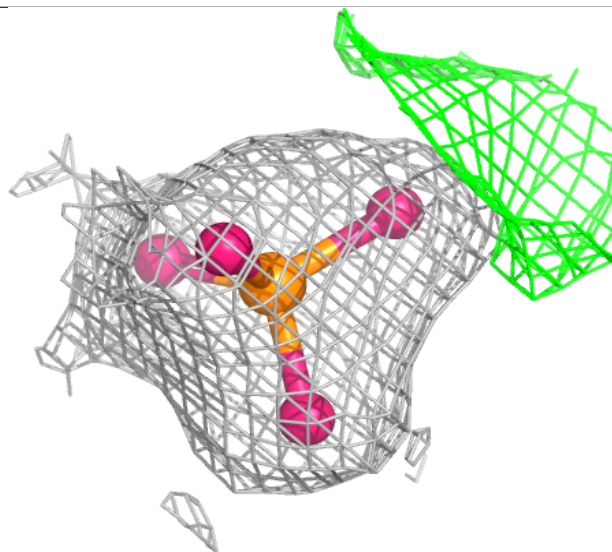
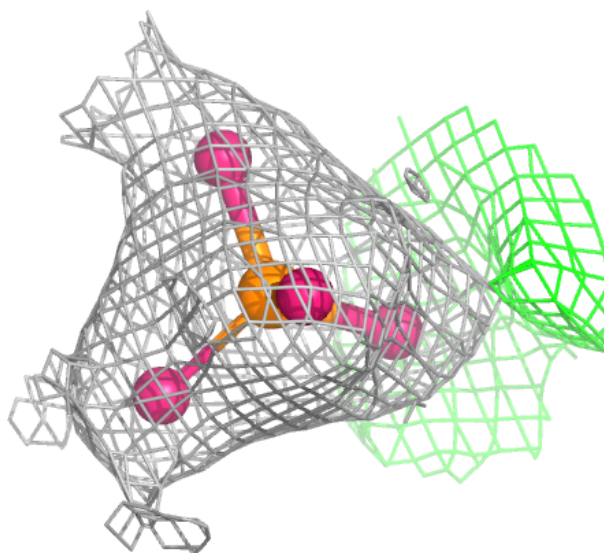
Electron density around PO4 C 601:

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



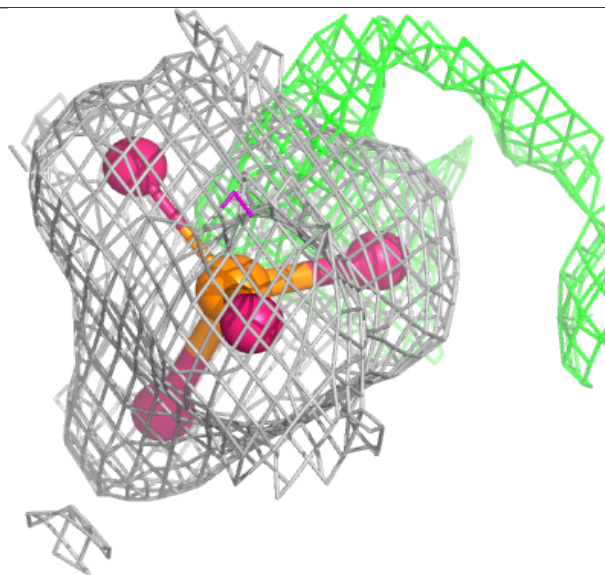
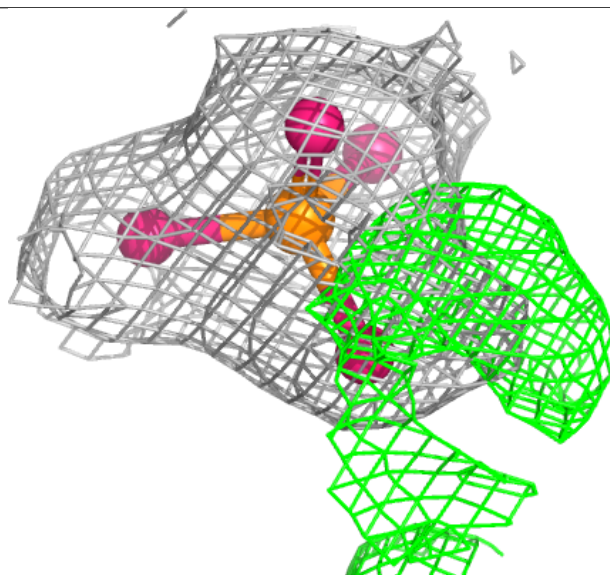
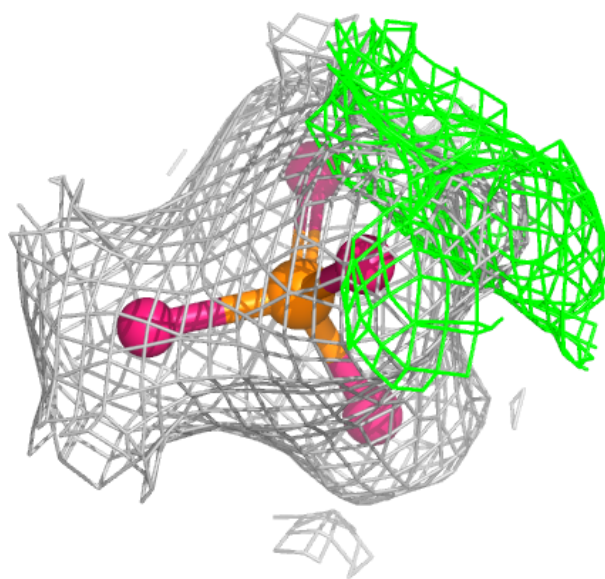
Electron density around PO4 B 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



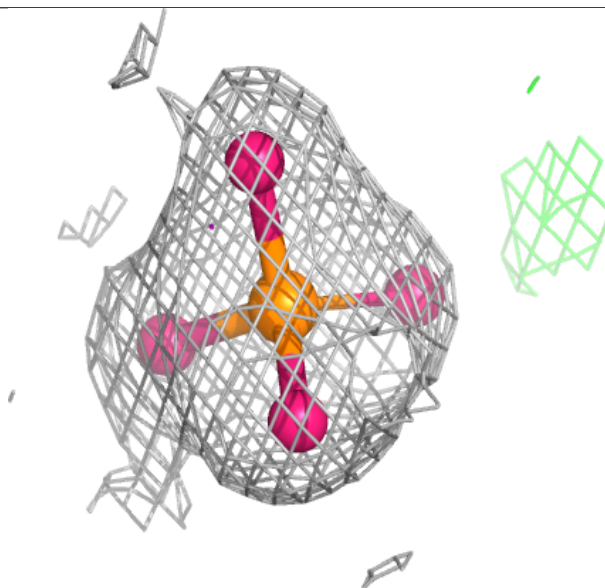
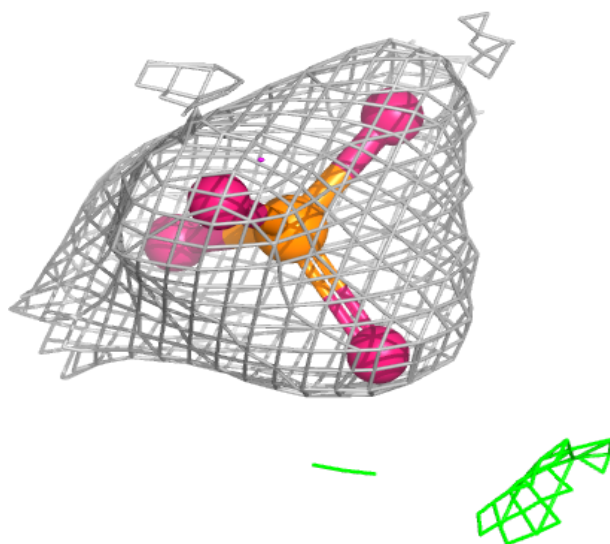
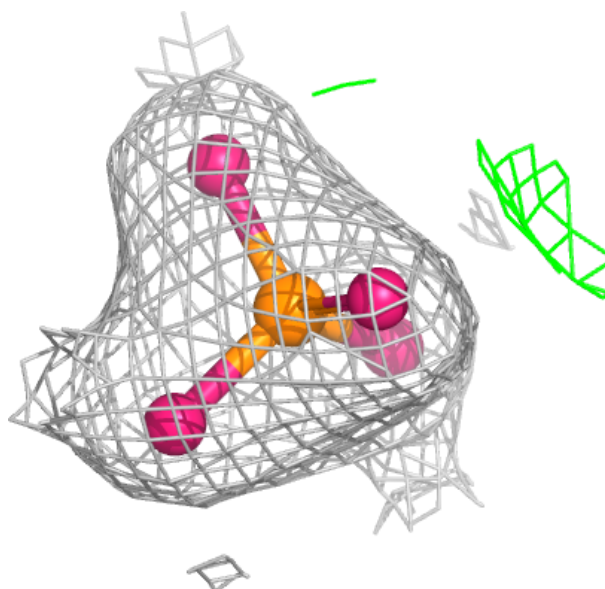
Electron density around PO4 A 602:

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



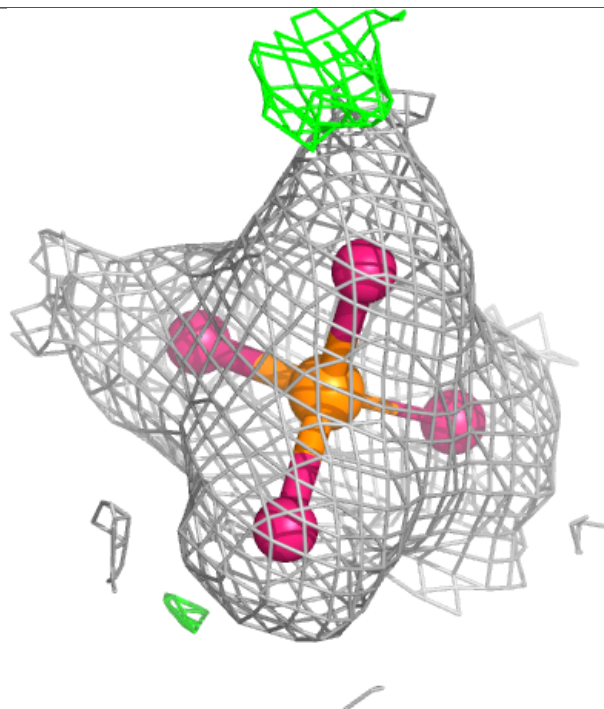
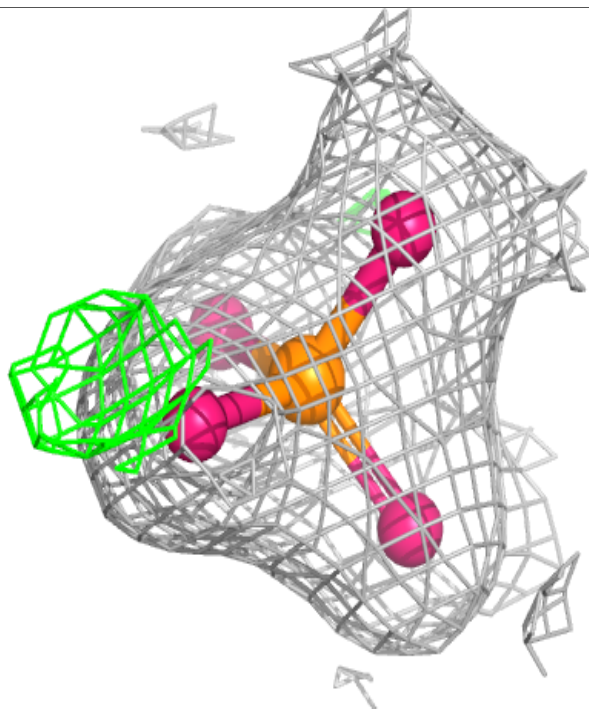
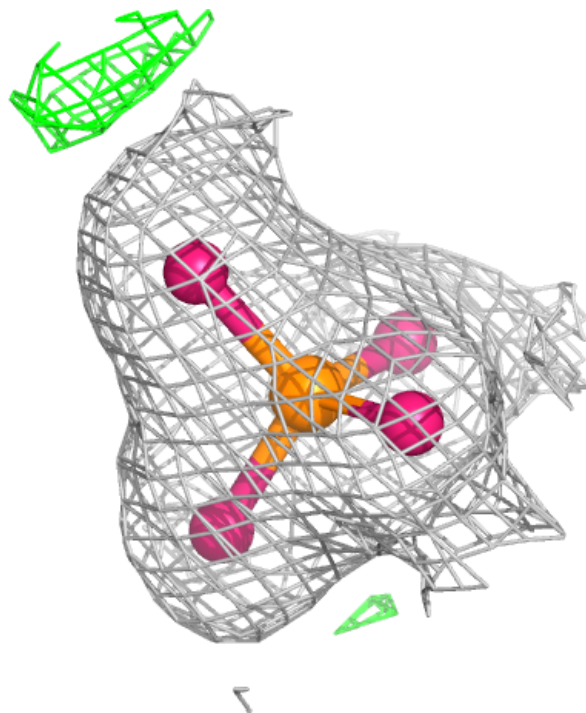
Electron density around PO4 C 602:

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



Electron density around PO4 A 601:

$2mF_o-DF_c$ (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.