



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 6LTW / pdb_00006ltw
Title : Crystal structure of Apo form of I122A/I330A variant of S-adenosylmethionine synthetase from *Cryptosporidium hominis*
Authors : Singh, R.K.; Michailidou, F.; Rentmeister, A.; Kuemmel, D.
Deposited on : 2020-01-23
Resolution : 1.65 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

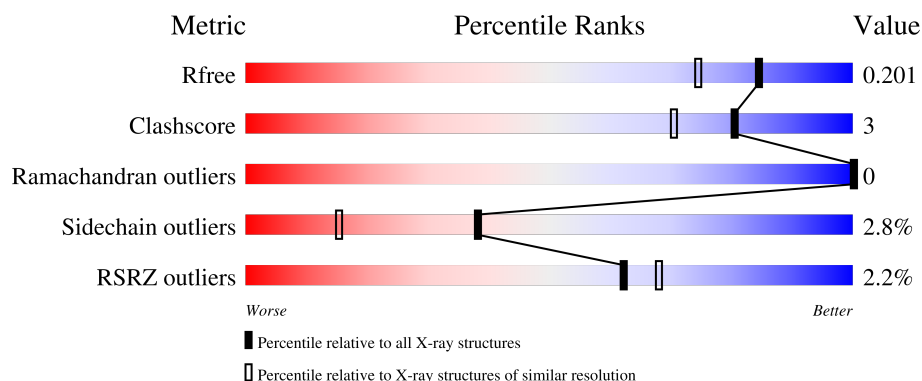
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

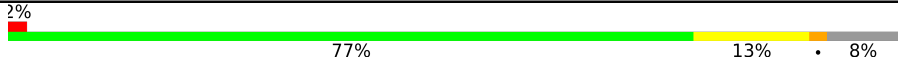
The reported resolution of this entry is 1.65 Å.

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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	414	
1	B	414	

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
3	PO4	A	503	-	X	-	-
3	PO4	B	504	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6547 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	5	0
			2992	1889	514	571	18			
1	B	379	Total	C	N	O	S	0	3	0
			2951	1866	500	566	19			

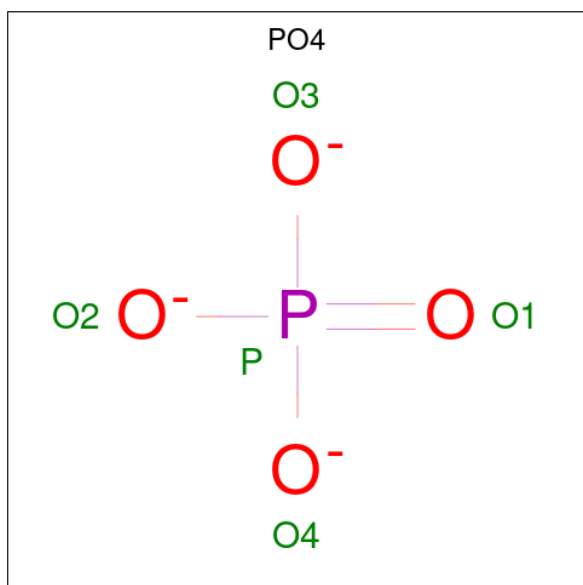
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A0S4TKQ5
A	-6	ALA	-	expression tag	UNP A0A0S4TKQ5
A	-5	HIS	-	expression tag	UNP A0A0S4TKQ5
A	-4	HIS	-	expression tag	UNP A0A0S4TKQ5
A	-3	HIS	-	expression tag	UNP A0A0S4TKQ5
A	-2	HIS	-	expression tag	UNP A0A0S4TKQ5
A	-1	HIS	-	expression tag	UNP A0A0S4TKQ5
A	0	HIS	-	expression tag	UNP A0A0S4TKQ5
A	122	ALA	ILE	variant	UNP A0A0S4TKQ5
A	330	ALA	ILE	variant	UNP A0A0S4TKQ5
B	-7	MET	-	initiating methionine	UNP A0A0S4TKQ5
B	-6	ALA	-	expression tag	UNP A0A0S4TKQ5
B	-5	HIS	-	expression tag	UNP A0A0S4TKQ5
B	-4	HIS	-	expression tag	UNP A0A0S4TKQ5
B	-3	HIS	-	expression tag	UNP A0A0S4TKQ5
B	-2	HIS	-	expression tag	UNP A0A0S4TKQ5
B	-1	HIS	-	expression tag	UNP A0A0S4TKQ5
B	0	HIS	-	expression tag	UNP A0A0S4TKQ5
B	122	ALA	ILE	variant	UNP A0A0S4TKQ5
B	330	ALA	ILE	variant	UNP A0A0S4TKQ5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P) (labeled as "Ligand of Interest" by depositor).



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

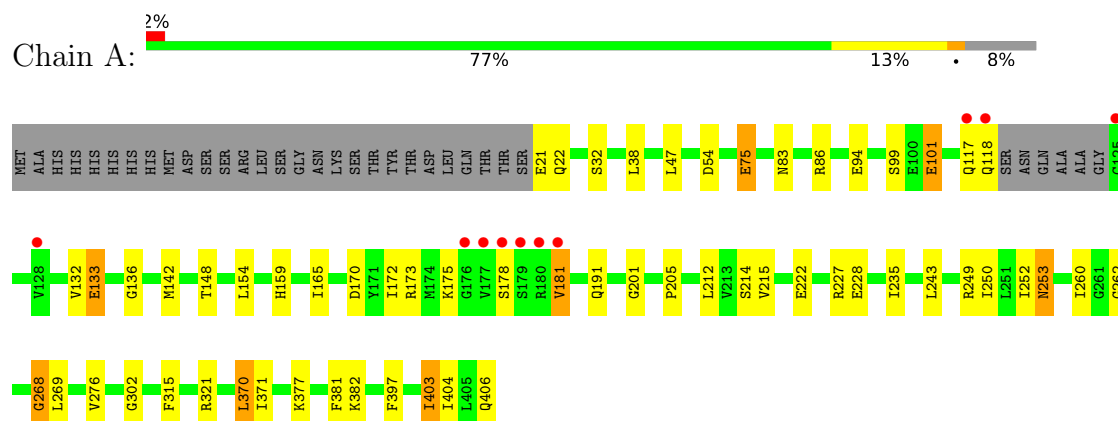
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	305	Total O 305 305	0	0
4	B	275	Total O 275 275	0	0

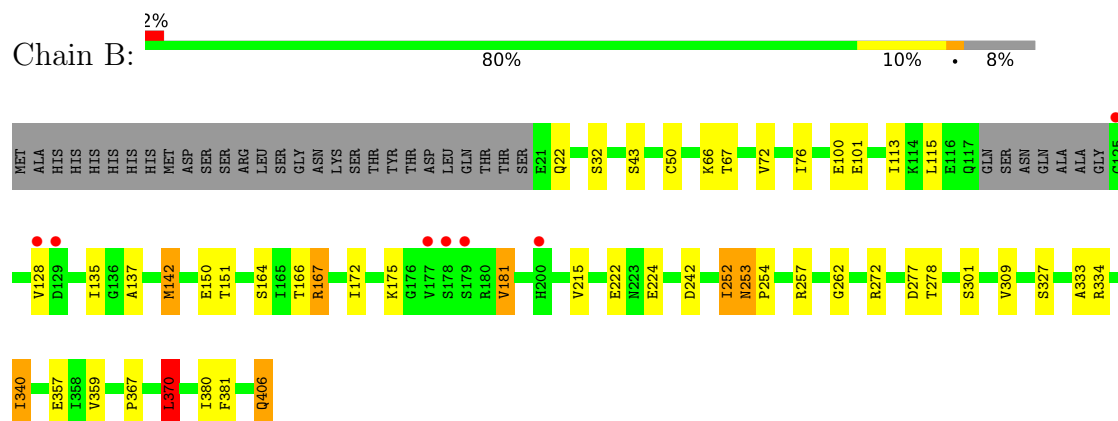
3 Residue-property plots

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

• Molecule 1: S-adenosylmethionine synthase



• Molecule 1: S-adenosylmethionine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.88Å 100.36Å 66.84Å 90.00° 95.86° 90.00°	Depositor
Resolution (Å)	48.08 – 1.65 48.08 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.08-1.65) 99.1 (48.08-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.156 , 0.191 0.169 , 0.201	Depositor DCC
R_{free} test set	4768 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6547	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	1.60	29/3046 (1.0%)	1.35	9/4104 (0.2%)
1	B	1.57	21/3004 (0.7%)	1.34	14/4050 (0.3%)
All	All	1.59	50/6050 (0.8%)	1.34	23/8154 (0.3%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	ARG	N-CA	8.97	1.56	1.46
1	A	253	ASN	C-O	-8.67	1.19	1.23
1	A	371	ILE	N-CA	-7.74	1.37	1.46
1	B	32	SER	CB-OG	-7.34	1.27	1.42
1	A	175	LYS	N-CA	7.22	1.55	1.45
1	A	212	LEU	N-CA	-6.97	1.37	1.46
1	B	135	ILE	CA-C	6.79	1.60	1.52
1	B	224	GLU	C-O	6.69	1.31	1.24
1	A	403	ILE	CB-CG1	-6.45	1.40	1.53
1	A	170	ASP	N-CA	-6.33	1.38	1.46
1	A	228	GLU	N-CA	-6.33	1.38	1.46
1	A	222	GLU	N-CA	-6.31	1.38	1.45
1	B	151	THR	N-CA	-6.27	1.37	1.45
1	A	302	GLY	CA-C	-6.25	1.45	1.52
1	A	260	ILE	C-O	-6.24	1.17	1.24
1	B	334	ARG	CD-NE	6.19	1.54	1.46
1	B	164	SER	N-CA	6.11	1.53	1.46
1	B	43	SER	CA-C	5.93	1.60	1.52
1	B	253	ASN	C-O	-5.93	1.21	1.23
1	B	222	GLU	N-CA	-5.82	1.39	1.45
1	B	50	CYS	C-O	5.80	1.30	1.24
1	B	137	ALA	C-O	-5.78	1.16	1.23
1	B	175	LYS	N-CA	5.77	1.54	1.45
1	B	167	ARG	CZ-NH1	5.76	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	GLY	C-O	5.75	1.30	1.23
1	A	214	SER	N-CA	-5.72	1.39	1.46
1	B	370	LEU	CB-CG	-5.72	1.42	1.53
1	A	276	VAL	N-CA	5.64	1.53	1.46
1	A	191	GLN	CA-C	-5.54	1.45	1.52
1	A	159	HIS	N-CA	5.50	1.53	1.46
1	B	309	VAL	C-O	-5.45	1.18	1.24
1	A	132	VAL	N-CA	5.43	1.52	1.46
1	A	75	GLU	C-O	-5.38	1.17	1.24
1	A	377	LYS	C-O	-5.36	1.16	1.24
1	A	370	LEU	CB-CG	-5.35	1.42	1.53
1	A	253	ASN	N-CA	5.33	1.50	1.46
1	A	397	PHE	N-CA	5.29	1.53	1.46
1	B	254	PRO	C-O	5.28	1.30	1.24
1	A	205	PRO	N-CA	-5.27	1.41	1.47
1	A	173	ARG	C-O	-5.27	1.18	1.24
1	A	32	SER	CB-OG	-5.24	1.31	1.42
1	A	178	SER	C-O	5.13	1.30	1.24
1	A	136	GLY	N-CA	5.07	1.52	1.45
1	A	243	LEU	N-CA	5.07	1.52	1.46
1	B	277	ASP	N-CA	5.07	1.53	1.46
1	B	166	THR	CA-C	5.06	1.59	1.52
1	B	128	VAL	CA-CB	5.04	1.59	1.54
1	B	252	ILE	C-O	5.03	1.29	1.24
1	A	249	ARG	CD-NE	5.02	1.53	1.46
1	A	47	LEU	CA-C	5.02	1.59	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	GLN	CA-C-O	-7.54	107.99	120.80
1	B	278	THR	CA-C-O	-7.23	115.65	119.77
1	B	370	LEU	N-CA-CB	-7.10	99.68	110.12
1	A	235	ILE	N-CA-C	6.47	117.15	110.36
1	A	54	ASP	O-C-N	6.29	125.64	121.23
1	B	224	GLU	CA-C-O	6.15	127.07	120.55
1	B	262	GLY	CA-C-N	6.03	125.91	119.28
1	B	262	GLY	C-N-CA	6.03	125.91	119.28
1	B	301	SER	N-CA-C	6.03	117.85	111.28
1	B	406	GLN	CA-C-O	-5.92	110.74	120.80
1	A	370	LEU	N-CA-CB	-5.76	101.42	110.06
1	A	38	LEU	N-CA-C	-5.64	105.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	GLU	CB-CA-C	5.63	120.13	110.79
1	A	262	GLY	CA-C-N	5.56	125.39	119.28
1	A	262	GLY	C-N-CA	5.56	125.39	119.28
1	B	367	PRO	CA-C-N	-5.49	113.89	119.98
1	B	367	PRO	C-N-CA	-5.49	113.89	119.98
1	B	333	ALA	N-CA-C	5.42	116.99	111.14
1	A	165	ILE	N-CA-C	5.34	115.55	110.42
1	B	381	PHE	N-CA-C	5.31	118.92	112.23
1	B	150	GLU	N-CA-C	5.26	117.76	111.71
1	B	380	ILE	N-CA-C	-5.20	108.06	113.10
1	A	381	PHE	N-CA-C	5.02	118.55	112.23

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	2992	0	3002	18	0
1	B	2951	0	2955	13	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	305	0	0	2	0
4	B	275	0	0	2	0
All	All	6547	0	5957	31	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 (31) 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:B:172:ILE:CG2	1:B:181:VAL:HG11	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HB2	4:B:806:HOH:O	1.89	0.70
1:B:340:ILE:HD11	1:B:359:VAL:HG21	1.85	0.58
1:A:94:GLU:OE1	1:A:382:LYS:NZ	2.37	0.58
1:B:142[A]:MET:HB3	1:B:327[A]:SER:OG	2.06	0.56
1:A:133:GLU:HG3	4:A:639:HOH:O	2.06	0.55
1:A:117:GLN:O	1:A:118:GLN:CB	2.57	0.52
1:A:227[B]:ARG:NH2	1:A:250:ILE:O	2.43	0.51
1:B:66:LYS:HG3	1:B:67:THR:H	1.76	0.51
1:B:72:VAL:HG22	1:B:113:ILE:HD13	1.93	0.50
1:A:117:GLN:O	1:A:118:GLN:HB3	2.12	0.49
1:A:94:GLU:HG3	4:A:722:HOH:O	2.11	0.49
1:B:172:ILE:HG21	1:B:181:VAL:HG11	1.93	0.49
1:B:66:LYS:O	1:B:67:THR:C	2.56	0.48
1:B:167:ARG:HD3	4:B:841:HOH:O	2.14	0.47
1:A:172:ILE:HG23	1:A:181:VAL:HG11	1.96	0.47
1:A:99:SER:HG	1:A:101:GLU:CD	2.23	0.46
1:B:76:ILE:HD12	1:B:115:LEU:HD13	1.96	0.46
1:A:268:GLY:C	1:A:269:LEU:HD12	2.41	0.46
1:A:83:ASN:HD22	1:A:86:ARG:HH21	1.64	0.45
1:B:252:ILE:O	1:B:253:ASN:C	2.59	0.45
1:A:117:GLN:HB3	1:A:118:GLN:HE21	1.82	0.44
1:B:172:ILE:HG22	1:B:181:VAL:HG11	1.94	0.44
1:A:252:ILE:O	1:A:253:ASN:C	2.62	0.43
1:A:201:GLY:O	1:A:321:ARG:HD3	2.19	0.43
1:B:370:LEU:C	1:B:370:LEU:HD23	2.45	0.42
1:A:227[A]:ARG:HG2	1:A:252:ILE:HB	2.01	0.41
1:A:370:LEU:C	1:A:370:LEU:HD23	2.46	0.41
1:A:315:PHE:HE2	1:A:404:ILE:HD11	1.86	0.41
1:A:148:THR:O	1:A:154:LEU:HA	2.21	0.40
1:A:75:GLU:OE2	1:A:118:GLN:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/414 (92%)	371 (97%)	10 (3%)	0	100	100
1	B	378/414 (91%)	367 (97%)	11 (3%)	0	100	100
All	All	759/828 (92%)	738 (97%)	21 (3%)	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	330/354 (93%)	322 (98%)	8 (2%)	43	20
1	B	325/354 (92%)	314 (97%)	11 (3%)	32	10
All	All	655/708 (92%)	636 (97%)	19 (3%)	38	14

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	22	GLN
1	A	101	GLU
1	A	133	GLU
1	A	142	MET
1	A	181	VAL
1	A	215	VAL
1	A	403	ILE
1	B	22	GLN
1	B	101	GLU
1	B	142[A]	MET
1	B	142[B]	MET
1	B	181	VAL
1	B	215	VAL
1	B	242	ASP

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Mol	Chain	Res	Type
1	B	257	ARG
1	B	340	ILE
1	B	370	LEU
1	B	406	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	118	GLN
1	A	159	HIS
1	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	B	504	2	4,4,4	1.53	1 (25%)	6,6,6	3.41	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	504	2	4,4,4	1.24	1 (25%)	6,6,6	1.41	1 (16%)
3	PO4	A	503	2	4,4,4	1.25	1 (25%)	6,6,6	3.30	4 (66%)
3	PO4	B	503	2	4,4,4	1.62	1 (25%)	6,6,6	1.53	1 (16%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	504	PO4	P-O2	-2.43	1.47	1.54
3	B	503	PO4	P-O1	2.40	1.56	1.50
3	B	504	PO4	P-O2	-2.31	1.47	1.54
3	A	503	PO4	P-O2	-2.24	1.48	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	PO4	O4-P-O1	-5.65	90.98	110.95
3	A	503	PO4	O4-P-O1	-5.44	91.73	110.95
3	B	504	PO4	O2-P-O1	4.92	128.36	110.95
3	A	503	PO4	O3-P-O2	3.45	118.65	107.91
3	A	503	PO4	O4-P-O2	3.38	118.42	107.91
3	A	503	PO4	O3-P-O1	-2.66	101.55	110.95
3	B	504	PO4	O3-P-O2	2.54	115.82	107.91
3	A	504	PO4	O2-P-O1	-2.50	102.11	110.95
3	B	503	PO4	O4-P-O2	-2.40	100.45	107.91
3	B	504	PO4	O4-P-O2	-2.35	100.60	107.91

There are no chirality outliers.

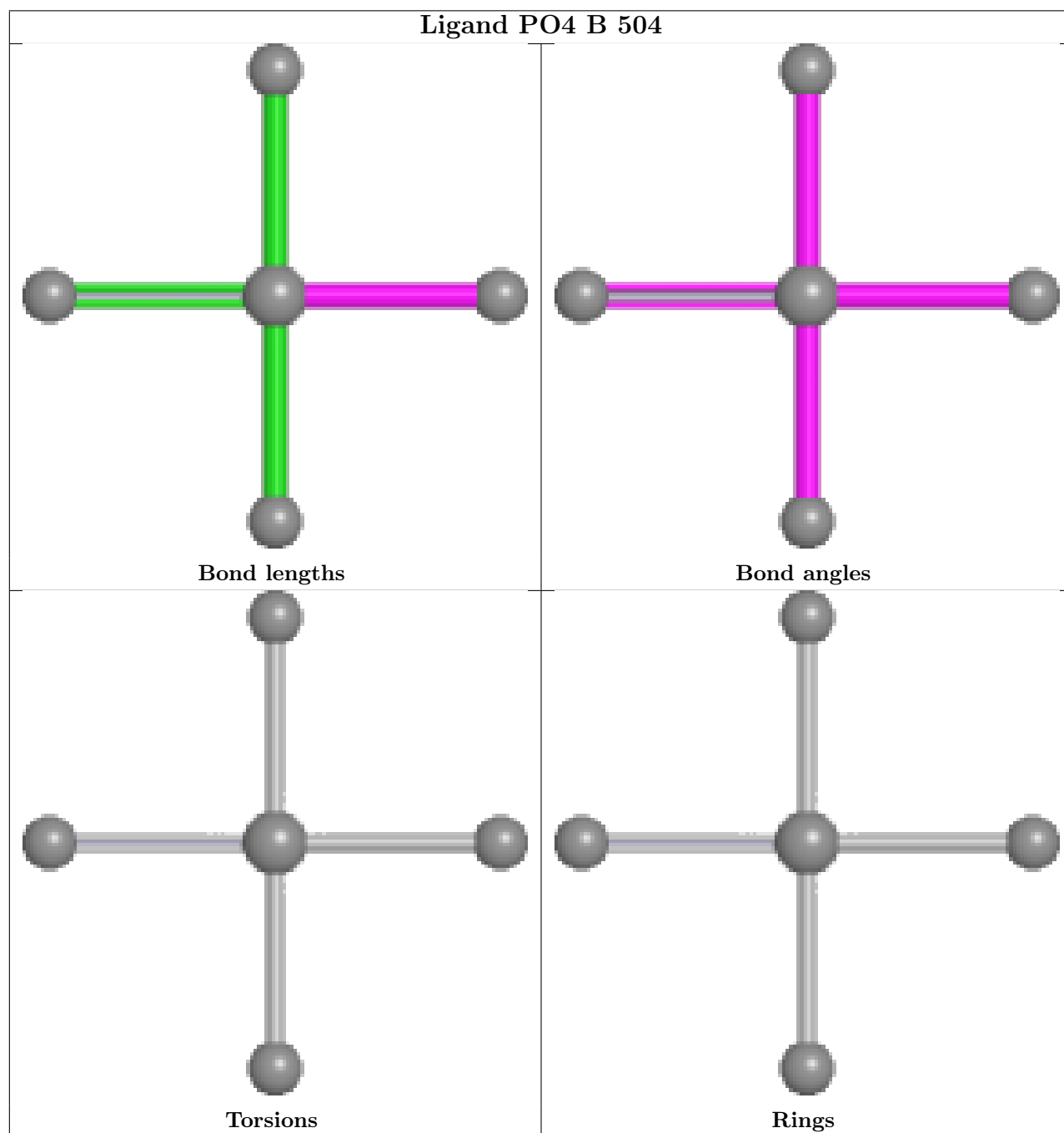
There are no torsion outliers.

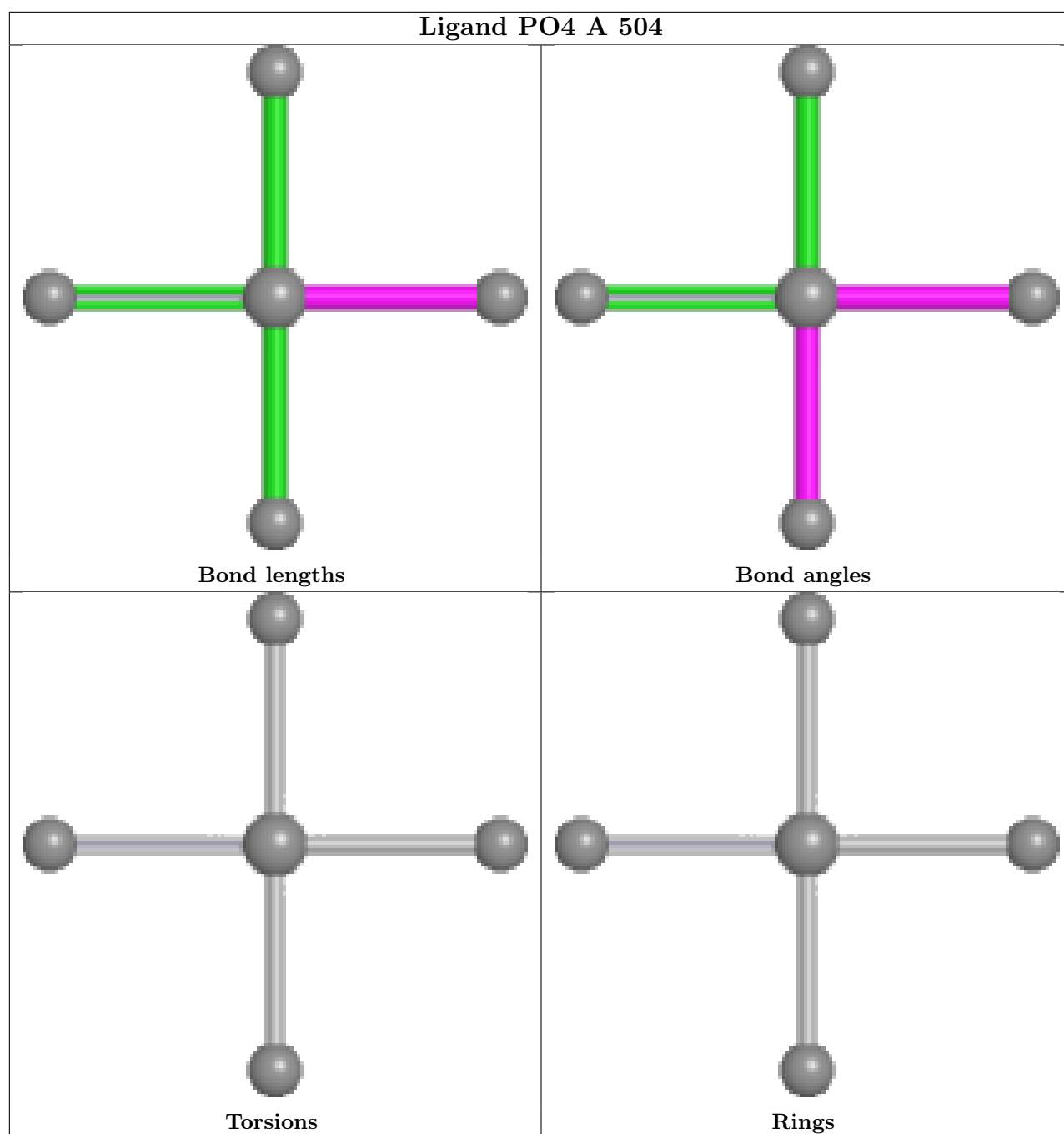
There are no ring outliers.

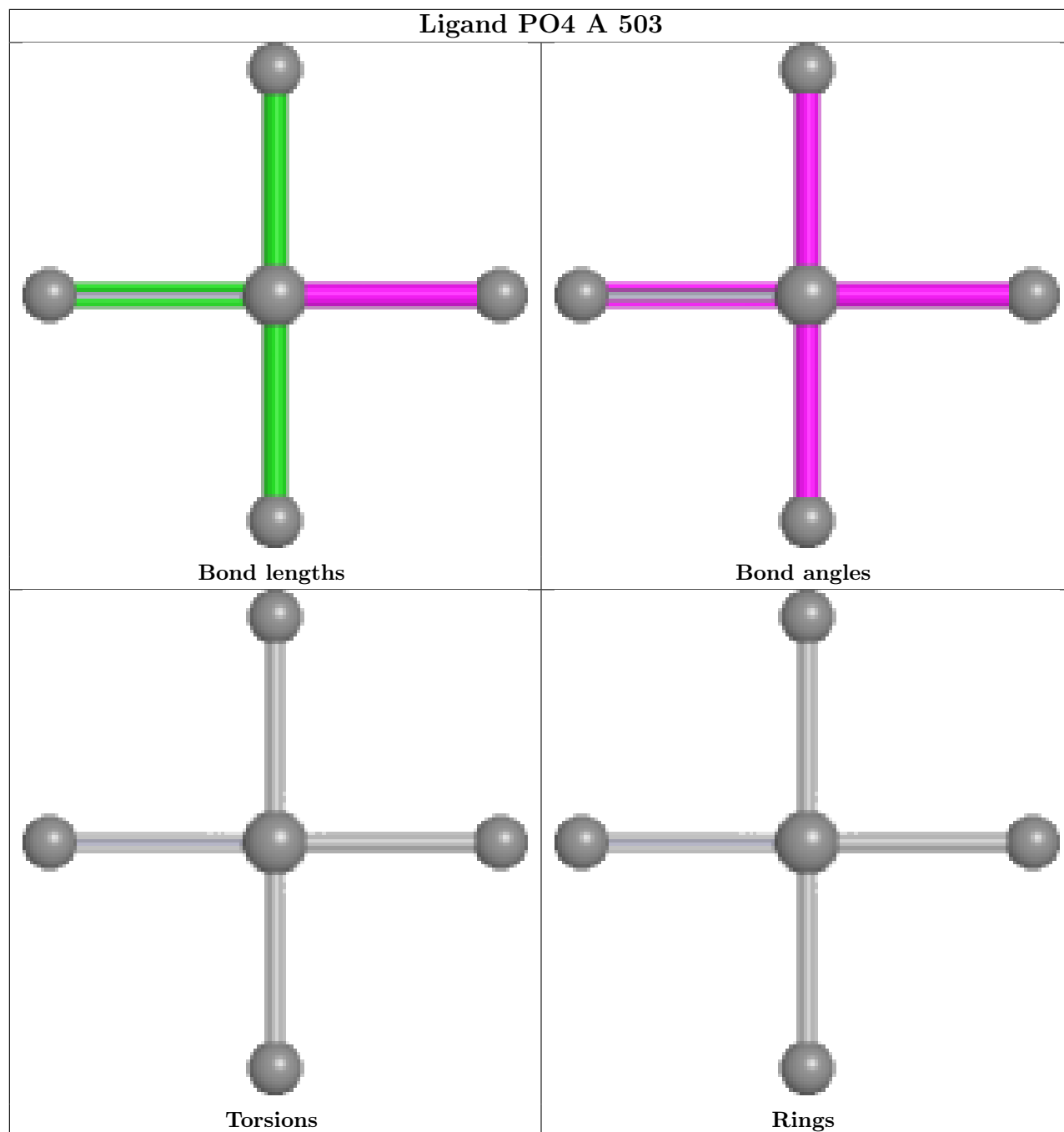
No monomer is involved in short contacts.

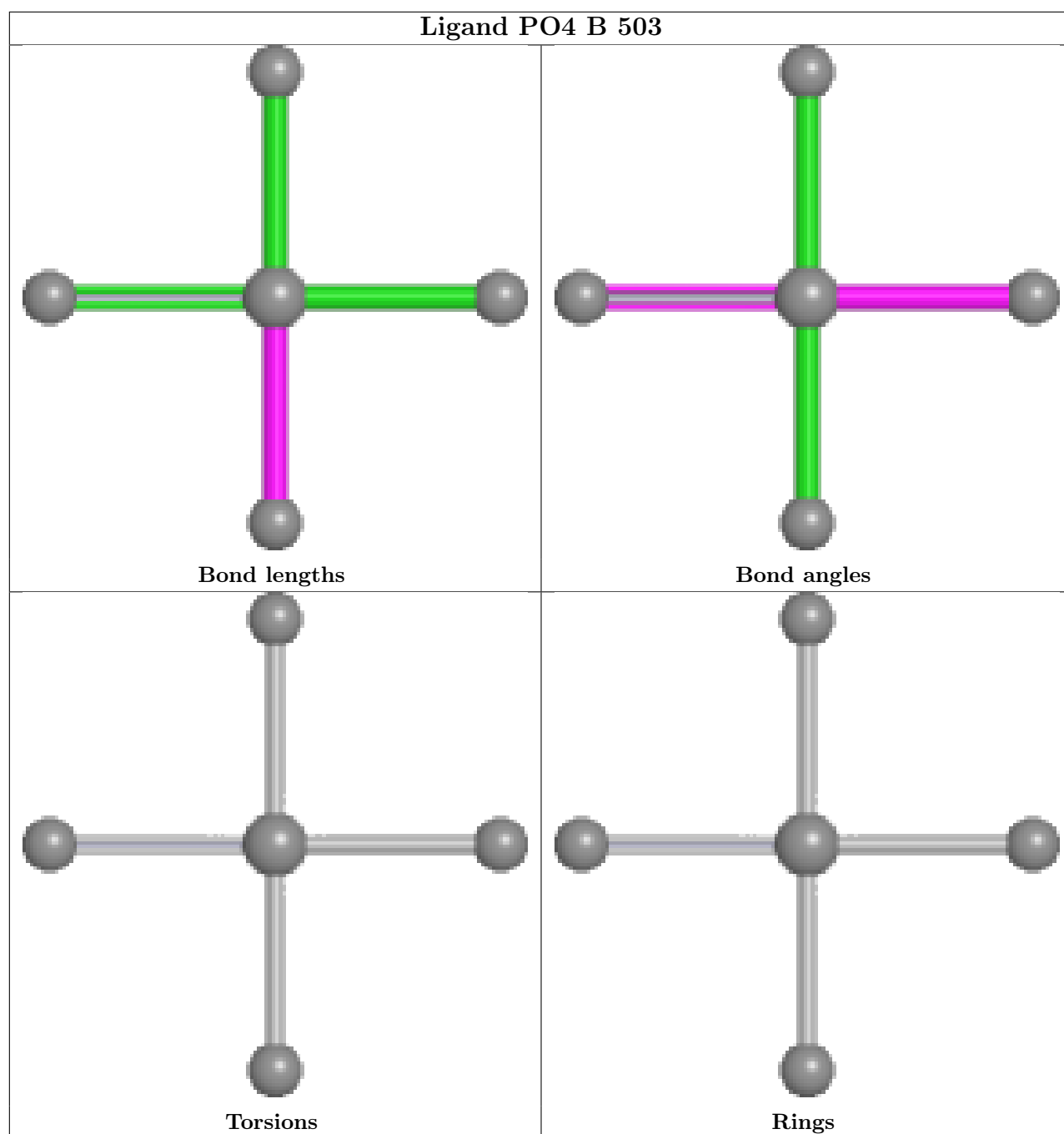
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	380/414 (91%)	-0.17	10 (2%) 57 62	9, 26, 47, 81	5 (1%)
1	B	379/414 (91%)	-0.06	7 (1%) 67 73	10, 28, 50, 68	3 (0%)
All	All	759/828 (91%)	-0.11	17 (2%) 62 68	9, 27, 48, 81	8 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	SER	3.5
1	B	200	HIS	3.2
1	B	178	SER	3.1
1	A	128	VAL	2.7
1	A	180	ARG	2.6
1	A	118	GLN	2.6
1	A	117	GLN	2.5
1	B	125	CYS	2.5
1	B	128	VAL	2.5
1	B	177	VAL	2.5
1	A	125	CYS	2.5
1	A	176	GLY	2.3
1	A	179	SER	2.3
1	B	129	ASP	2.3
1	A	181	VAL	2.1
1	B	179	SER	2.1
1	A	177	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

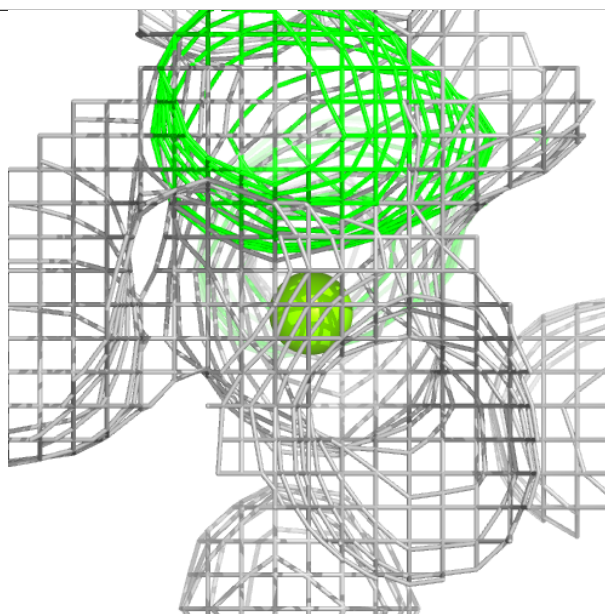
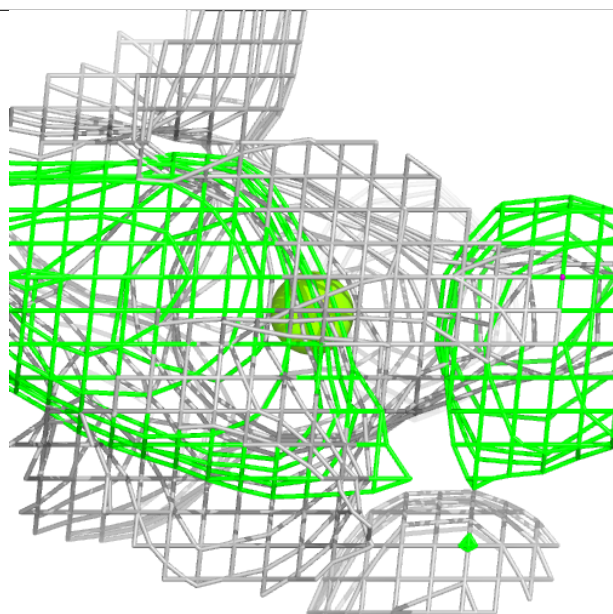
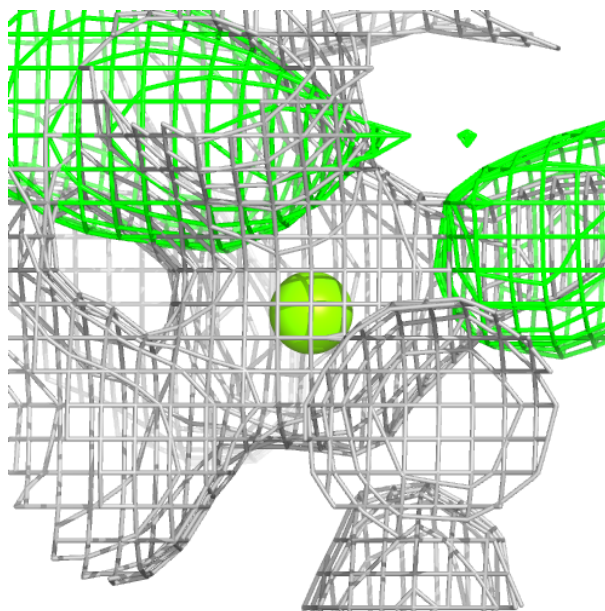
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	502	1/1	0.77	0.14	47,47,47,47	0
2	MG	A	502	1/1	0.84	0.09	39,39,39,39	0
3	PO4	A	503	5/5	0.96	0.09	24,25,30,36	0
3	PO4	B	504	5/5	0.97	0.09	23,25,28,37	0
3	PO4	A	504	5/5	0.98	0.06	21,23,24,27	0
3	PO4	B	503	5/5	0.98	0.05	18,21,24,25	0
2	MG	A	501	1/1	0.98	0.08	20,20,20,20	0
2	MG	B	501	1/1	0.99	0.09	18,18,18,18	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.

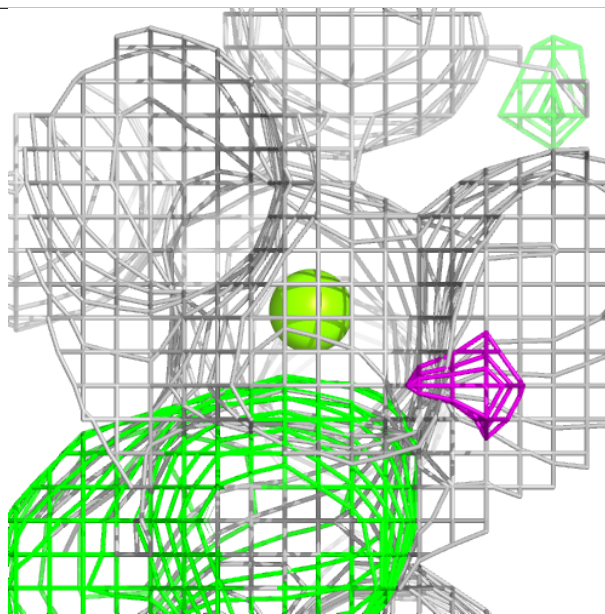
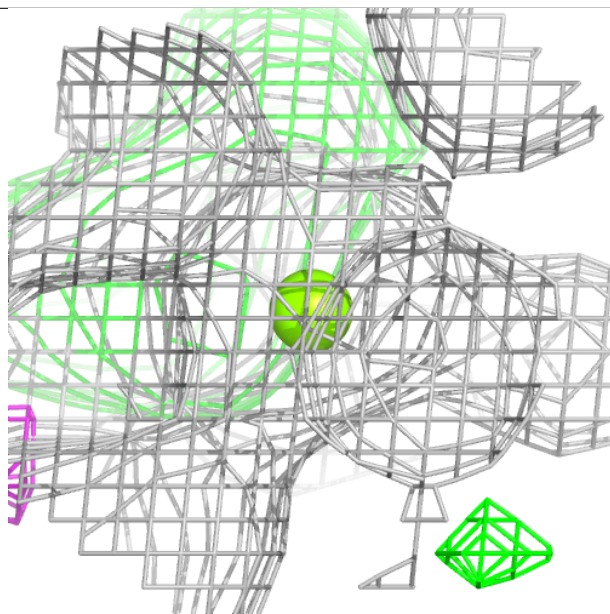
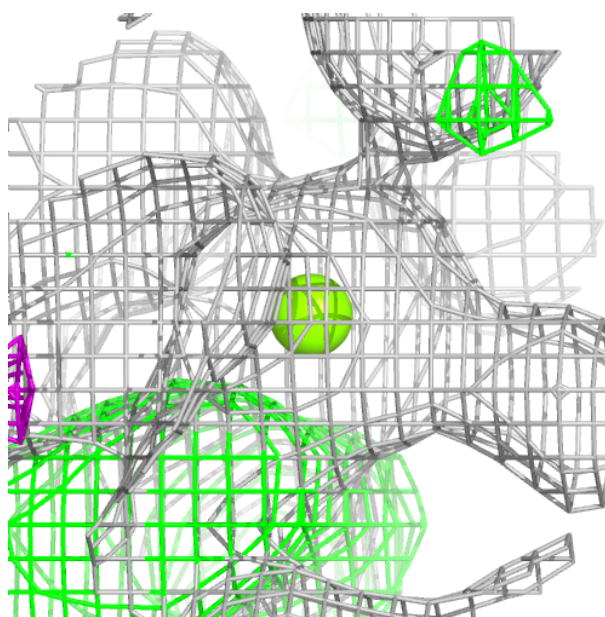
Electron density around MG B 502:

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



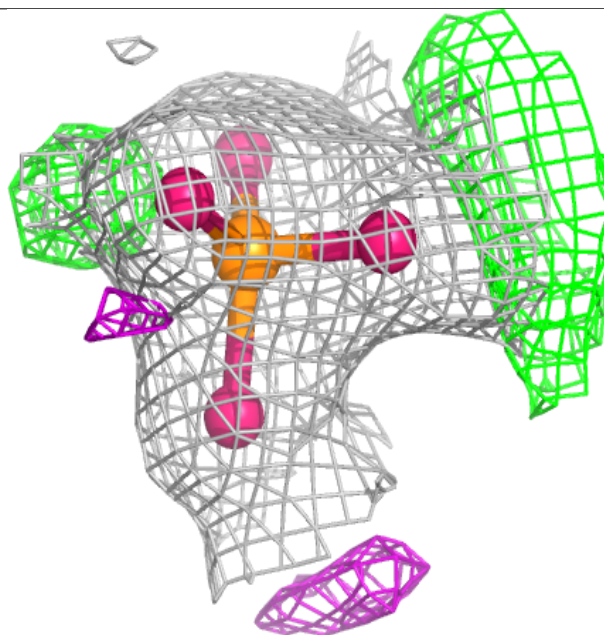
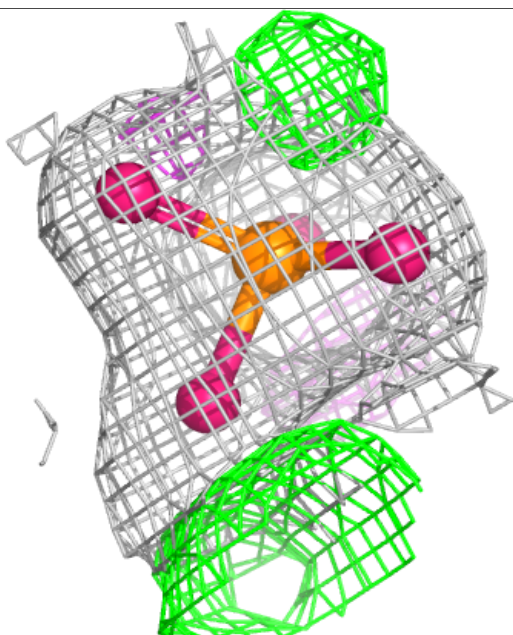
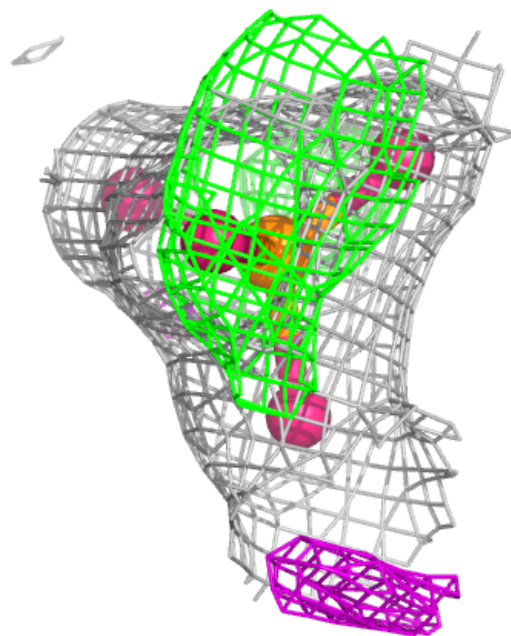
Electron density around MG A 502:

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



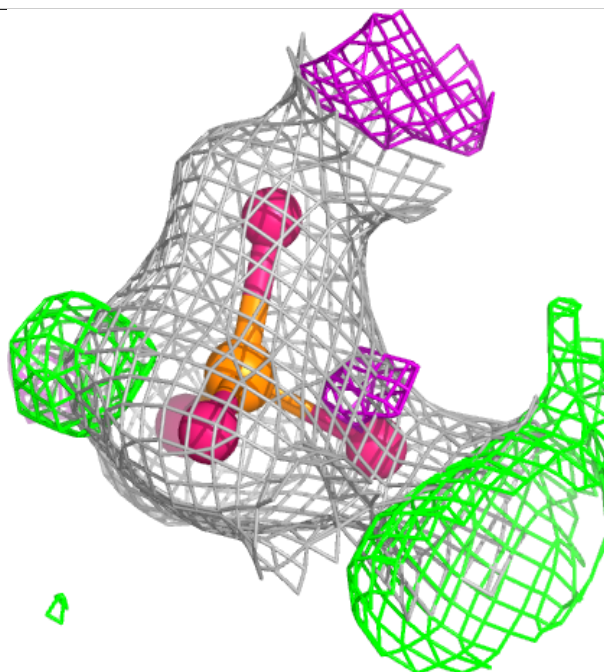
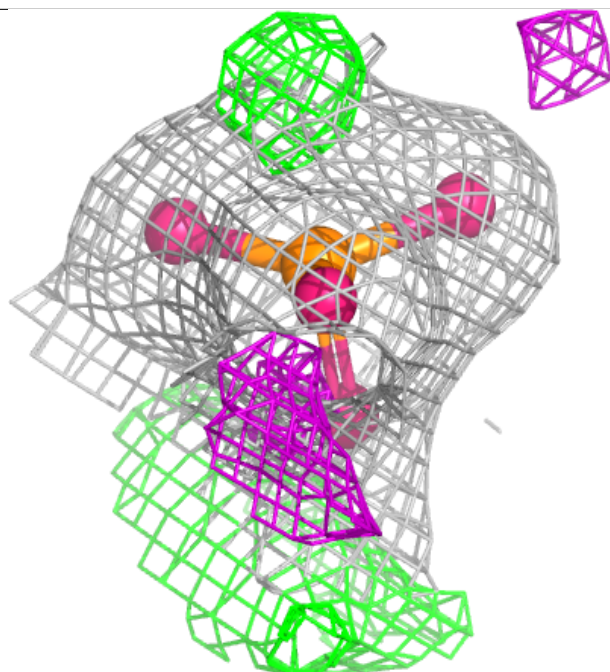
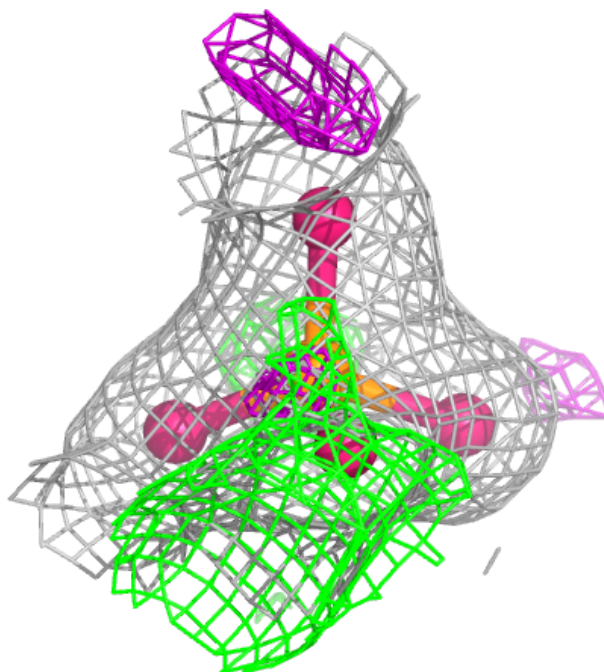
Electron density around PO4 A 503:

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



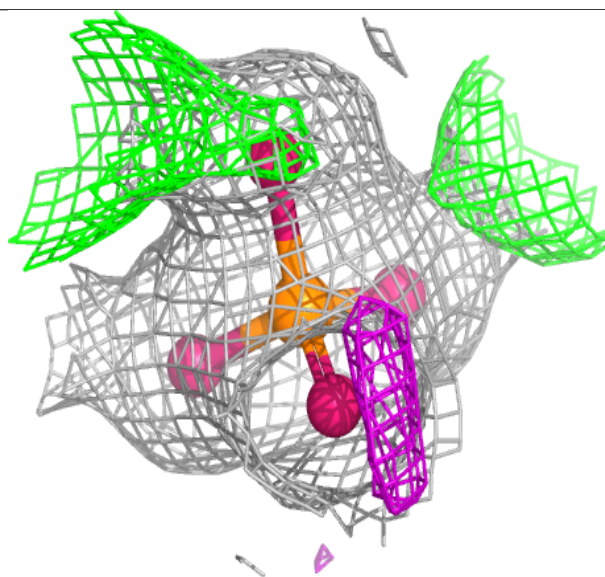
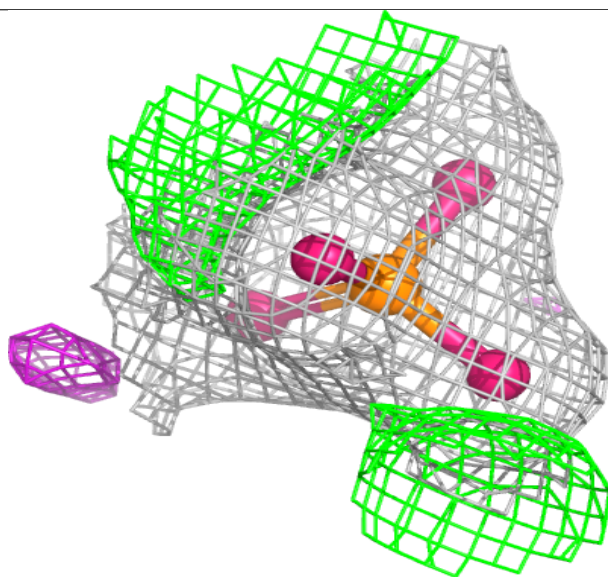
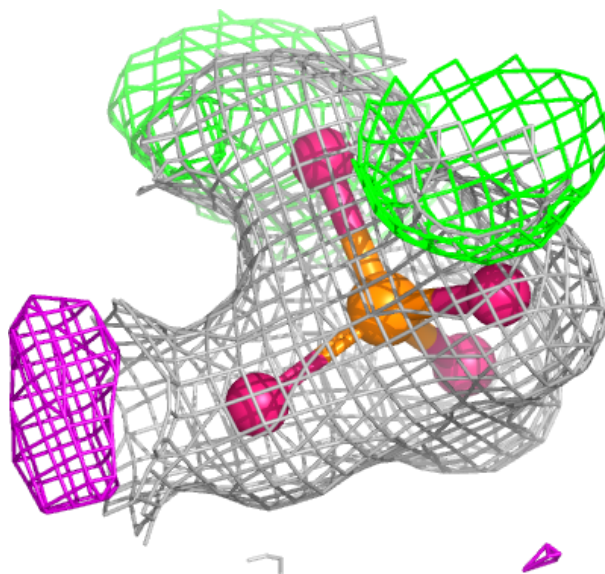
Electron density around PO4 B 504:

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



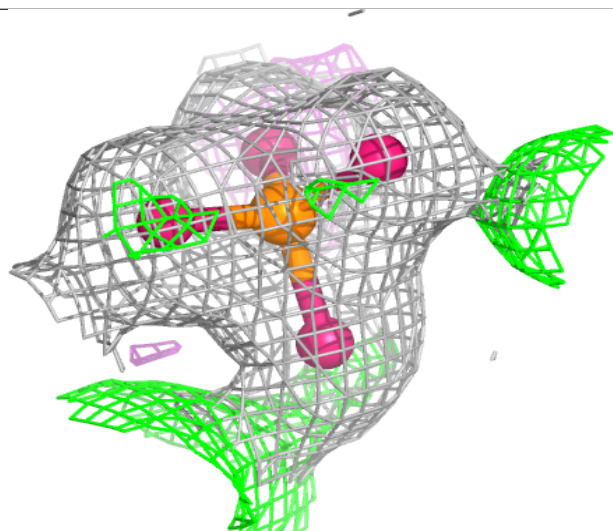
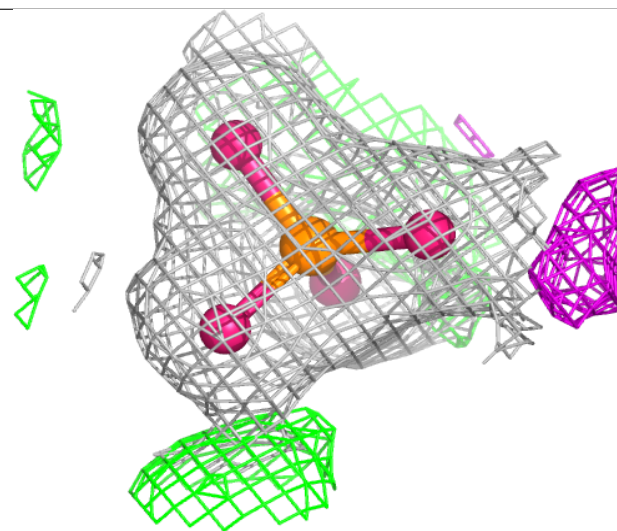
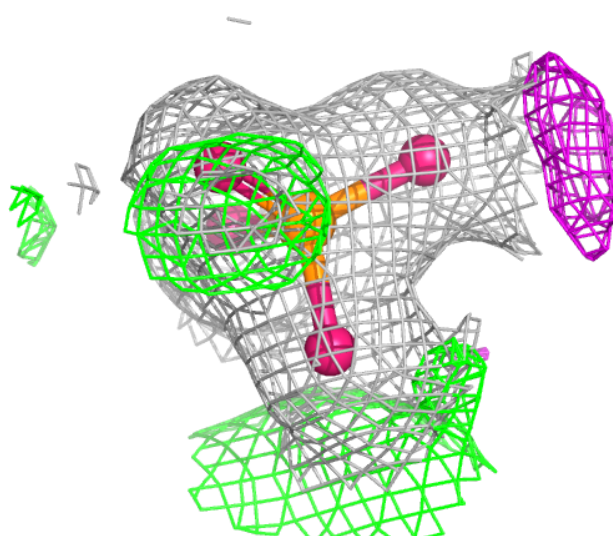
Electron density around PO4 A 504:

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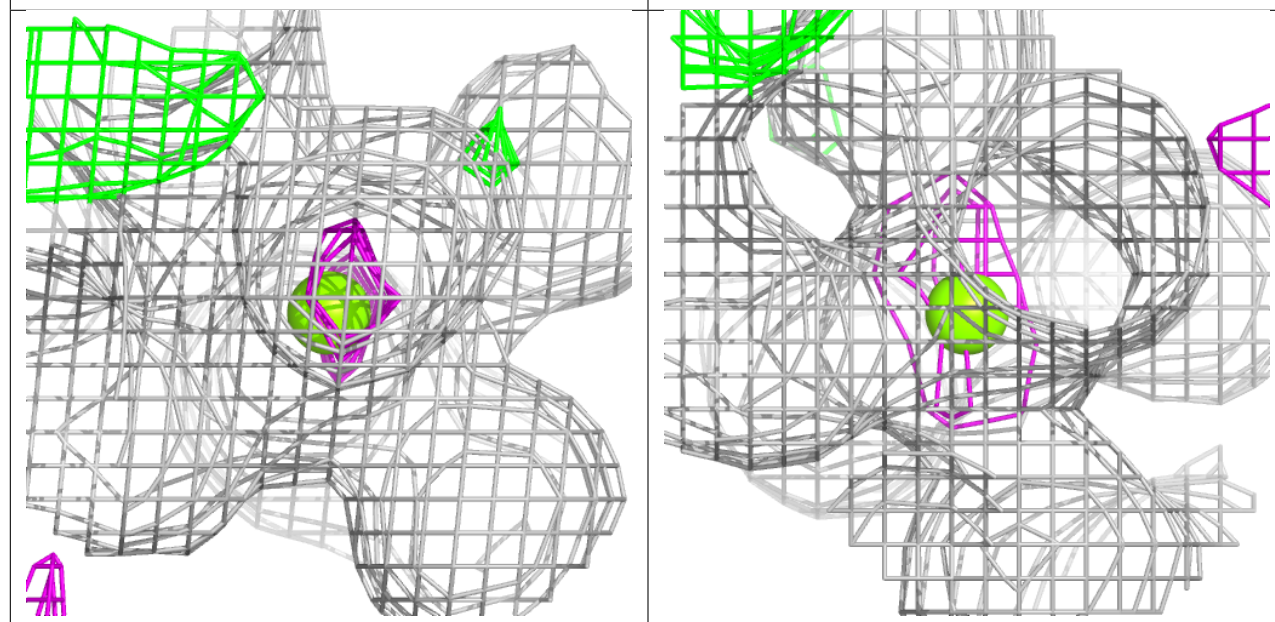
Electron density around PO4 B 503:

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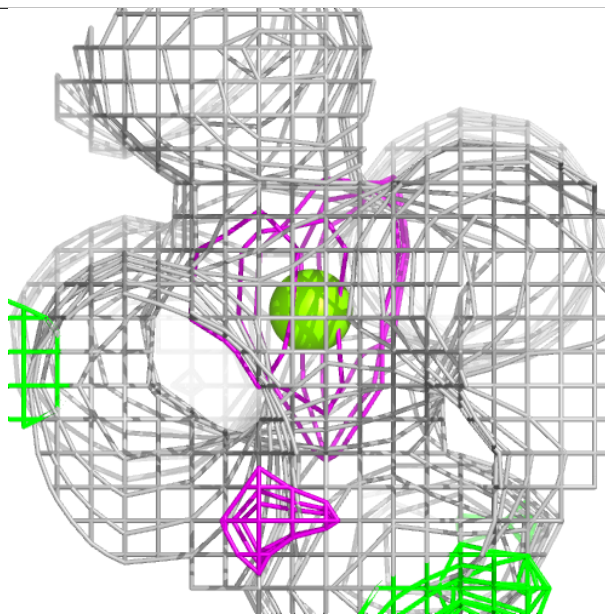
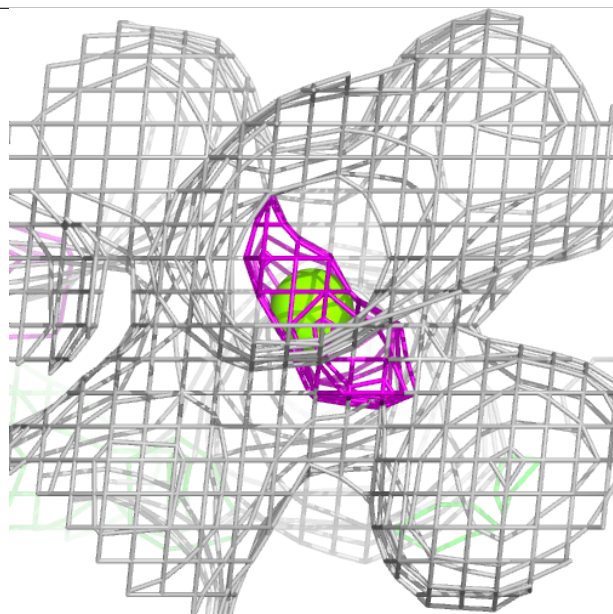
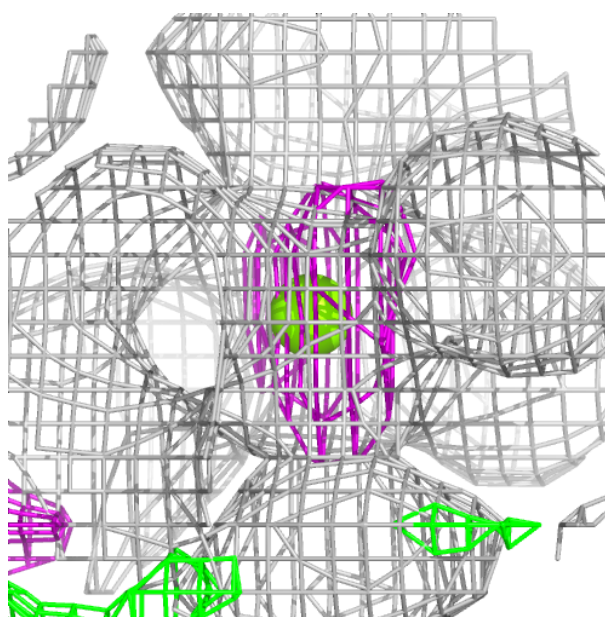
Electron density around MG A 501:

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



Electron density around MG B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.