



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2021 – 12:14 PM JST

PDB ID : 7C5R
Title : Crystal Structure of C150S mutant Glyceraldehyde-3-phosphate dehydrogenase1 from Escherichia coli complexed with BPG at 2.31 Angstrom resolution
Authors : Zhang, L.; Liu, M.R.; Bao, L.Y.; Yao, Y.C.; Bostrom, I.K.; Wang, Y.D.; Chen, A.Q.; Li, J.X.; Gu, S.H.; Ji, C.N.
Deposited on : 2020-05-20
Resolution : 2.31 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 ⓘ symbol.

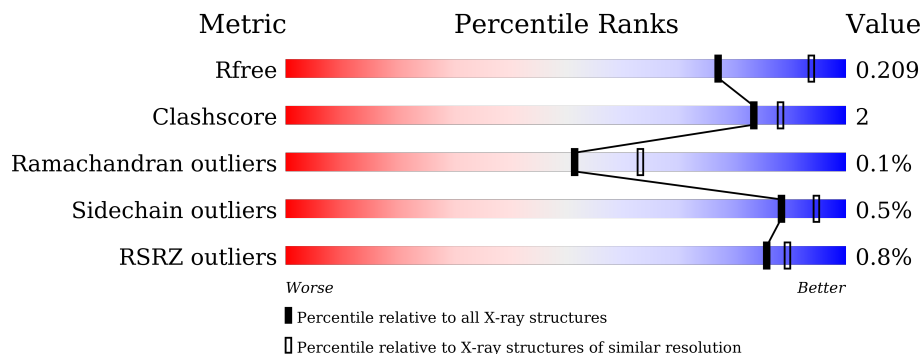
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

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X-RAY DIFFRACTION

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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	O	352	<div><div></div><div>89%</div><div>6%</div><div>5%</div></div>
1	P	352	<div><div></div><div>90%</div><div>5%</div><div>5%</div></div>
1	Q	352	<div><div></div><div>89%</div><div>5%</div><div>5%</div></div>
1	R	352	<div><div></div><div>2%</div><div>89%</div><div>5%</div><div>5%</div></div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	G3H	Q	402[A]	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11336 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	334	Total	C	N	O	S	0	7	0
			2580	1627	434	513	6			
1	P	333	Total	C	N	O	S	0	3	0
			2538	1604	428	500	6			
1	Q	333	Total	C	N	O	S	0	1	0
			2521	1594	425	497	5			
1	R	333	Total	C	N	O	S	0	0	0
			2515	1591	424	494	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-18	HIS	-	expression tag	UNP A0A140NCK4
O	-17	HIS	-	expression tag	UNP A0A140NCK4
O	-16	HIS	-	expression tag	UNP A0A140NCK4
O	-15	HIS	-	expression tag	UNP A0A140NCK4
O	-14	HIS	-	expression tag	UNP A0A140NCK4
O	-13	HIS	-	expression tag	UNP A0A140NCK4
O	-12	SER	-	expression tag	UNP A0A140NCK4
O	-11	SER	-	expression tag	UNP A0A140NCK4
O	-10	GLY	-	expression tag	UNP A0A140NCK4
O	-9	LEU	-	expression tag	UNP A0A140NCK4
O	-8	VAL	-	expression tag	UNP A0A140NCK4
O	-7	PRO	-	expression tag	UNP A0A140NCK4
O	-6	ARG	-	expression tag	UNP A0A140NCK4
O	-5	GLY	-	expression tag	UNP A0A140NCK4
O	-4	SER	-	expression tag	UNP A0A140NCK4
O	-3	HIS	-	expression tag	UNP A0A140NCK4
O	-2	MET	-	expression tag	UNP A0A140NCK4
O	-1	ALA	-	expression tag	UNP A0A140NCK4
O	0	SER	-	expression tag	UNP A0A140NCK4
O	150	SER	CYS	engineered mutation	UNP A0A140NCK4
P	-18	HIS	-	expression tag	UNP A0A140NCK4

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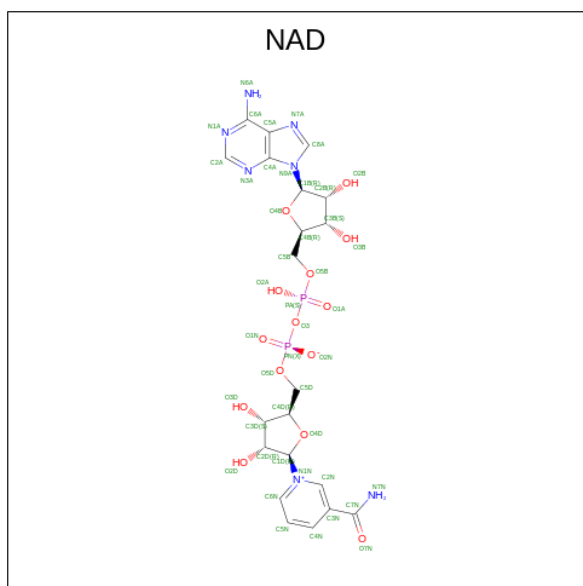
Chain	Residue	Modelled	Actual	Comment	Reference
P	-17	HIS	-	expression tag	UNP A0A140NCK4
P	-16	HIS	-	expression tag	UNP A0A140NCK4
P	-15	HIS	-	expression tag	UNP A0A140NCK4
P	-14	HIS	-	expression tag	UNP A0A140NCK4
P	-13	HIS	-	expression tag	UNP A0A140NCK4
P	-12	SER	-	expression tag	UNP A0A140NCK4
P	-11	SER	-	expression tag	UNP A0A140NCK4
P	-10	GLY	-	expression tag	UNP A0A140NCK4
P	-9	LEU	-	expression tag	UNP A0A140NCK4
P	-8	VAL	-	expression tag	UNP A0A140NCK4
P	-7	PRO	-	expression tag	UNP A0A140NCK4
P	-6	ARG	-	expression tag	UNP A0A140NCK4
P	-5	GLY	-	expression tag	UNP A0A140NCK4
P	-4	SER	-	expression tag	UNP A0A140NCK4
P	-3	HIS	-	expression tag	UNP A0A140NCK4
P	-2	MET	-	expression tag	UNP A0A140NCK4
P	-1	ALA	-	expression tag	UNP A0A140NCK4
P	0	SER	-	expression tag	UNP A0A140NCK4
P	150	SER	CYS	engineered mutation	UNP A0A140NCK4
Q	-18	HIS	-	expression tag	UNP A0A140NCK4
Q	-17	HIS	-	expression tag	UNP A0A140NCK4
Q	-16	HIS	-	expression tag	UNP A0A140NCK4
Q	-15	HIS	-	expression tag	UNP A0A140NCK4
Q	-14	HIS	-	expression tag	UNP A0A140NCK4
Q	-13	HIS	-	expression tag	UNP A0A140NCK4
Q	-12	SER	-	expression tag	UNP A0A140NCK4
Q	-11	SER	-	expression tag	UNP A0A140NCK4
Q	-10	GLY	-	expression tag	UNP A0A140NCK4
Q	-9	LEU	-	expression tag	UNP A0A140NCK4
Q	-8	VAL	-	expression tag	UNP A0A140NCK4
Q	-7	PRO	-	expression tag	UNP A0A140NCK4
Q	-6	ARG	-	expression tag	UNP A0A140NCK4
Q	-5	GLY	-	expression tag	UNP A0A140NCK4
Q	-4	SER	-	expression tag	UNP A0A140NCK4
Q	-3	HIS	-	expression tag	UNP A0A140NCK4
Q	-2	MET	-	expression tag	UNP A0A140NCK4
Q	-1	ALA	-	expression tag	UNP A0A140NCK4
Q	0	SER	-	expression tag	UNP A0A140NCK4
Q	150	SER	CYS	engineered mutation	UNP A0A140NCK4
R	-18	HIS	-	expression tag	UNP A0A140NCK4
R	-17	HIS	-	expression tag	UNP A0A140NCK4
R	-16	HIS	-	expression tag	UNP A0A140NCK4

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-15	HIS	-	expression tag	UNP A0A140NCK4
R	-14	HIS	-	expression tag	UNP A0A140NCK4
R	-13	HIS	-	expression tag	UNP A0A140NCK4
R	-12	SER	-	expression tag	UNP A0A140NCK4
R	-11	SER	-	expression tag	UNP A0A140NCK4
R	-10	GLY	-	expression tag	UNP A0A140NCK4
R	-9	LEU	-	expression tag	UNP A0A140NCK4
R	-8	VAL	-	expression tag	UNP A0A140NCK4
R	-7	PRO	-	expression tag	UNP A0A140NCK4
R	-6	ARG	-	expression tag	UNP A0A140NCK4
R	-5	GLY	-	expression tag	UNP A0A140NCK4
R	-4	SER	-	expression tag	UNP A0A140NCK4
R	-3	HIS	-	expression tag	UNP A0A140NCK4
R	-2	MET	-	expression tag	UNP A0A140NCK4
R	-1	ALA	-	expression tag	UNP A0A140NCK4
R	0	SER	-	expression tag	UNP A0A140NCK4
R	150	SER	CYS	engineered mutation	UNP A0A140NCK4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



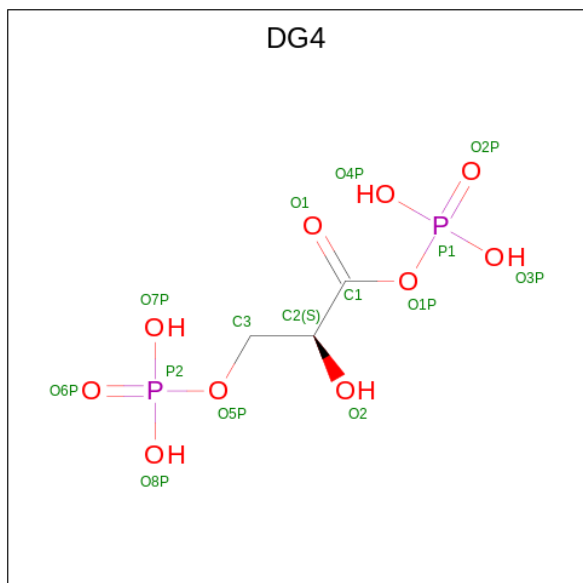
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	P	1	Total	C	N	O	P	0
			44	21	7	14	2	

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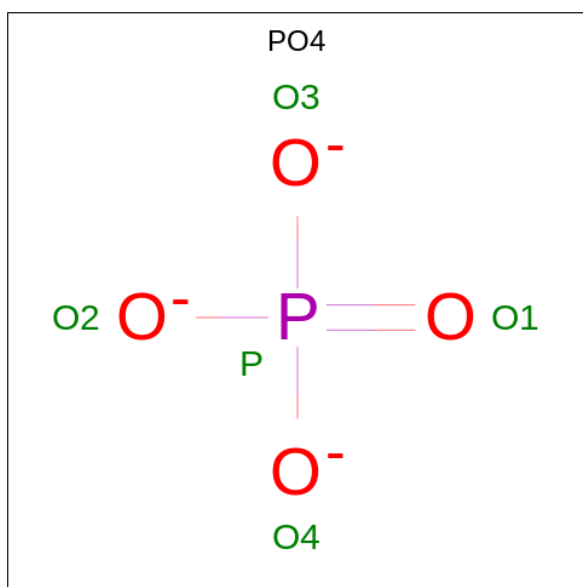
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is phosphono (2S)-2-oxidanyl-3-phosphonooxy-propanoate (three-letter code: DG4) (formula: $C_3H_8O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



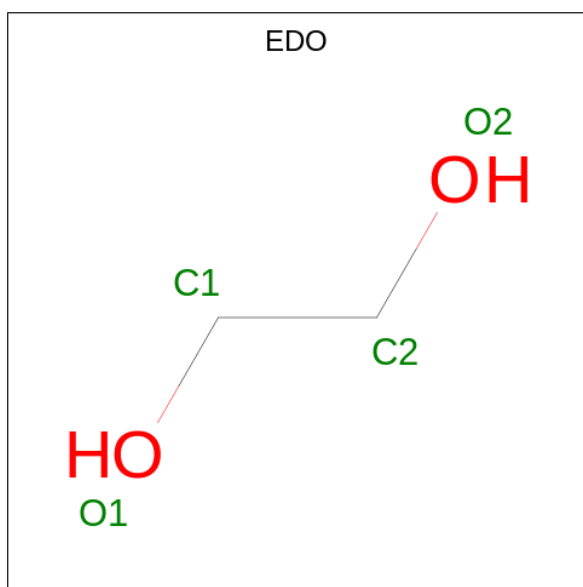
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	O	P	0	0
			15	3	10	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total	O	P	0	0
			5	4	1		
4	O	1	Total	O	P	0	0
			5	4	1		
4	P	1	Total	O	P	0	0
			5	4	1		
4	Q	1	Total	O	P	0	0
			5	4	1		
4	R	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).

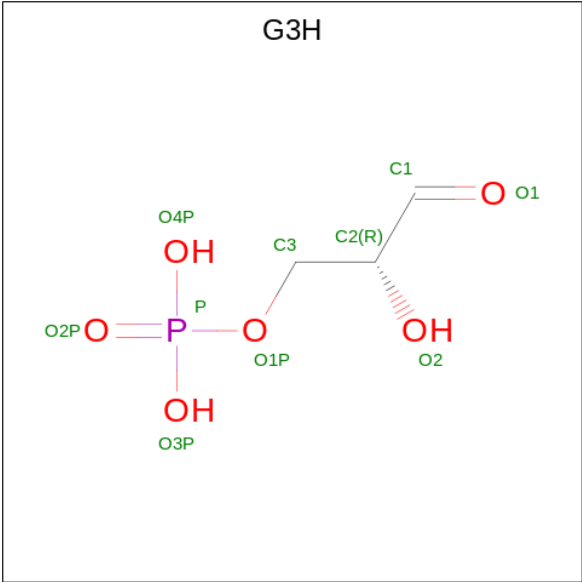


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	O	1	Total	C	O	0	0
			4	2	2		
5	P	1	Total	C	O	0	0
			4	2	2		
5	Q	1	Total	C	O	0	1
			8	4	4		
5	R	1	Total	C	O	0	0
			4	2	2		
5	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	3	Total	Cl	0	0
			3	3		
6	P	1	Total	Cl	0	0
			1	1		
6	Q	3	Total	Cl	0	0
			3	3		
6	R	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: C₃H₇O₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	P	1	Total	C	O	P	0	0
			10	3	6	1		
7	Q	1	Total	C	O	P	0	1
			20	6	12	2		
7	R	1	Total	C	O	P	0	0
			10	3	6	1		


- Molecule 8 is water.

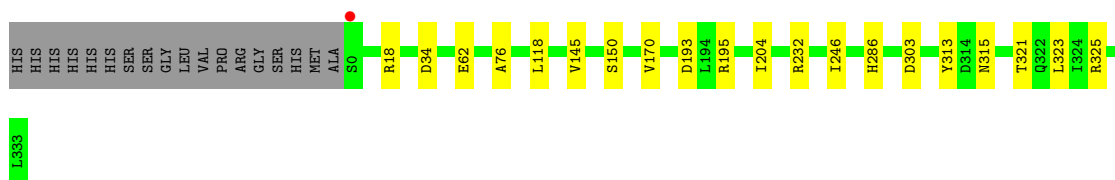
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	O	269	Total	O	0	0
			269	269		
8	P	236	Total	O	0	0
			236	236		
8	Q	229	Total	O	0	0
			229	229		
8	R	160	Total	O	0	0
			160	160		

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.

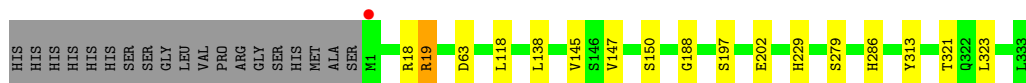
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain O: 




- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain P: 




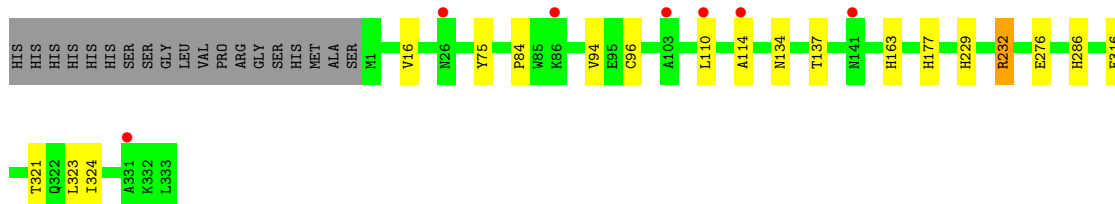
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain Q: 



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain R: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.40Å 89.40Å 340.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 47.94 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.31) 99.9 (47.94-2.31)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.147 , 0.203 0.158 , 0.209	Depositor DCC
R_{free} test set	3076 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11336	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: EDO, NAD, CL, PO4, G3H, DG4

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	O	0.76	0/2622	0.89	8/3558 (0.2%)
1	P	0.77	1/2579 (0.0%)	0.89	2/3500 (0.1%)
1	Q	0.75	0/2562	0.88	5/3477 (0.1%)
1	R	0.77	1/2556 (0.0%)	0.85	1/3468 (0.0%)
All	All	0.76	2/10319 (0.0%)	0.88	16/14003 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	202	GLU	CD-OE2	5.25	1.31	1.25
1	R	316	GLU	CD-OE1	5.24	1.31	1.25

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	19	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	Q	187	ASP	CB-CG-OD1	8.37	125.83	118.30
1	Q	187	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	O	325	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	O	18	ARG	NE-CZ-NH1	6.53	123.56	120.30

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	O	2580	0	2585	11	0
1	P	2538	0	2563	10	0
1	Q	2521	0	2545	14	0
1	R	2515	0	2547	12	0
2	O	44	0	26	1	0
2	P	44	0	26	1	0
2	Q	44	0	26	2	0
2	R	44	0	26	0	0
3	O	15	0	0	1	0
4	O	10	0	0	0	0
4	P	5	0	0	0	0
4	Q	5	0	0	1	0
4	R	5	0	0	1	0
5	O	4	0	6	1	0
5	P	4	0	6	2	0
5	Q	8	0	12	0	0
5	R	8	0	12	0	0
6	O	3	0	0	0	0
6	P	1	0	0	0	0
6	Q	3	0	0	0	0
6	R	1	0	0	0	0
7	P	10	0	5	2	0
7	Q	20	0	10	6	0
7	R	10	0	5	0	0
8	O	269	0	0	2	0
8	P	236	0	0	1	0
8	Q	229	0	0	3	0
8	R	160	0	0	2	0
All	All	11336	0	10400	49	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 2.

The worst 5 of 49 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:O:150:SER:OG	3:O:402:DG4:O4P	1.89	0.90
1:R:134:ASN:O	1:R:137:THR:HG22	1.83	0.79
1:R:137:THR:HG21	8:R:597:HOH:O	1.89	0.73
1:Q:150:SER:OG	7:Q:402[A]:G3H:O1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:118:LEU:HD11	1:P:147:VAL:HG13	1.78	0.64

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	O	339/352 (96%)	327 (96%)	12 (4%)	0	100	100
1	P	334/352 (95%)	324 (97%)	10 (3%)	0	100	100
1	Q	332/352 (94%)	318 (96%)	13 (4%)	1 (0%)	41	50
1	R	331/352 (94%)	314 (95%)	17 (5%)	0	100	100
All	All	1336/1408 (95%)	1283 (96%)	52 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	167	GLY

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	O	281/289 (97%)	280 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	276/289 (96%)	274 (99%)	2 (1%)	84	92
1	Q	273/289 (94%)	272 (100%)	1 (0%)	91	96
1	R	273/289 (94%)	272 (100%)	1 (0%)	91	96
All	All	1103/1156 (95%)	1098 (100%)	5 (0%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	313	TYR
1	P	229	HIS
1	P	313	TYR
1	Q	229	HIS
1	R	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\# Z > 2$
4	PO4	R	403	-	4,4,4	0.69	0	6,6,6	0.88	0
5	EDO	O	405	-	3,3,3	0.40	0	2,2,2	0.45	0
5	EDO	R	404	-	3,3,3	0.34	0	2,2,2	1.03	0
2	NAD	Q	401	-	42,48,48	0.85	2 (4%)	50,73,73	1.46	11 (22%)
4	PO4	Q	403	-	4,4,4	0.75	0	6,6,6	1.09	0
5	EDO	R	405	-	3,3,3	0.59	0	2,2,2	0.21	0
4	PO4	O	404	-	4,4,4	0.88	0	6,6,6	0.41	0
5	EDO	P	404	-	3,3,3	0.52	0	2,2,2	1.05	0
2	NAD	O	401	-	42,48,48	0.87	1 (2%)	50,73,73	1.41	7 (14%)
3	DG4	O	402	-	12,14,14	1.96	1 (8%)	16,21,21	2.37	3 (18%)
2	NAD	R	401	-	42,48,48	0.99	2 (4%)	50,73,73	1.74	8 (16%)
5	EDO	Q	404[A]	-	3,3,3	0.37	0	2,2,2	0.43	0
4	PO4	P	403	-	4,4,4	0.97	0	6,6,6	1.34	1 (16%)
5	EDO	Q	404[B]	-	3,3,3	0.61	0	2,2,2	0.20	0
7	G3H	Q	402[A]	-	8,9,9	0.69	0	10,12,12	1.53	3 (30%)
7	G3H	Q	402[B]	-	8,9,9	0.85	0	10,12,12	1.46	2 (20%)
4	PO4	O	403	-	4,4,4	0.97	0	6,6,6	0.96	0
2	NAD	P	401	-	42,48,48	0.88	1 (2%)	50,73,73	1.47	8 (16%)
7	G3H	R	402	-	8,9,9	1.96	2 (25%)	10,12,12	3.15	5 (50%)
7	G3H	P	402	-	8,9,9	1.43	1 (12%)	10,12,12	1.68	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	Q	404[A]	-	-	1/1/1/1	-
5	EDO	O	405	-	-	1/1/1/1	-
7	G3H	Q	402[B]	-	-	6/7/8/8	-
5	EDO	R	405	-	-	1/1/1/1	-
5	EDO	Q	404[B]	-	-	1/1/1/1	-
5	EDO	R	404	-	-	0/1/1/1	-
2	NAD	P	401	-	-	6/26/62/62	0/5/5/5
7	G3H	R	402	-	-	4/7/8/8	-
5	EDO	P	404	-	-	1/1/1/1	-
7	G3H	Q	402[A]	-	-	5/7/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	O	401	-	-	5/26/62/62	0/5/5/5
3	DG4	O	402	-	-	4/13/15/15	-
2	NAD	R	401	-	-	5/26/62/62	0/5/5/5
7	G3H	P	402	-	-	6/7/8/8	-
2	NAD	Q	401	-	-	5/26/62/62	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	402	DG4	P1-O1P	6.26	1.68	1.59
7	R	402	G3H	O2-C2	3.68	1.50	1.43
7	R	402	G3H	C3-C2	3.31	1.56	1.51
7	P	402	G3H	C3-C2	3.22	1.56	1.51
2	P	401	NAD	C5A-C4A	2.48	1.47	1.40

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	402	G3H	O1P-C3-C2	7.76	128.91	108.33
2	R	401	NAD	C1B-N9A-C4A	-6.52	115.18	126.64
3	O	402	DG4	O4P-P1-O1P	-5.49	88.53	105.25
3	O	402	DG4	O3P-P1-O1P	5.11	120.82	105.25
2	R	401	NAD	N3A-C2A-N1A	-4.88	121.05	128.68

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	401	NAD	O4D-C1D-N1N-C2N
2	O	401	NAD	O4D-C1D-N1N-C6N
2	O	401	NAD	C2D-C1D-N1N-C2N
2	O	401	NAD	C2D-C1D-N1N-C6N
2	P	401	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

11 monomers are involved in 16 short contacts:

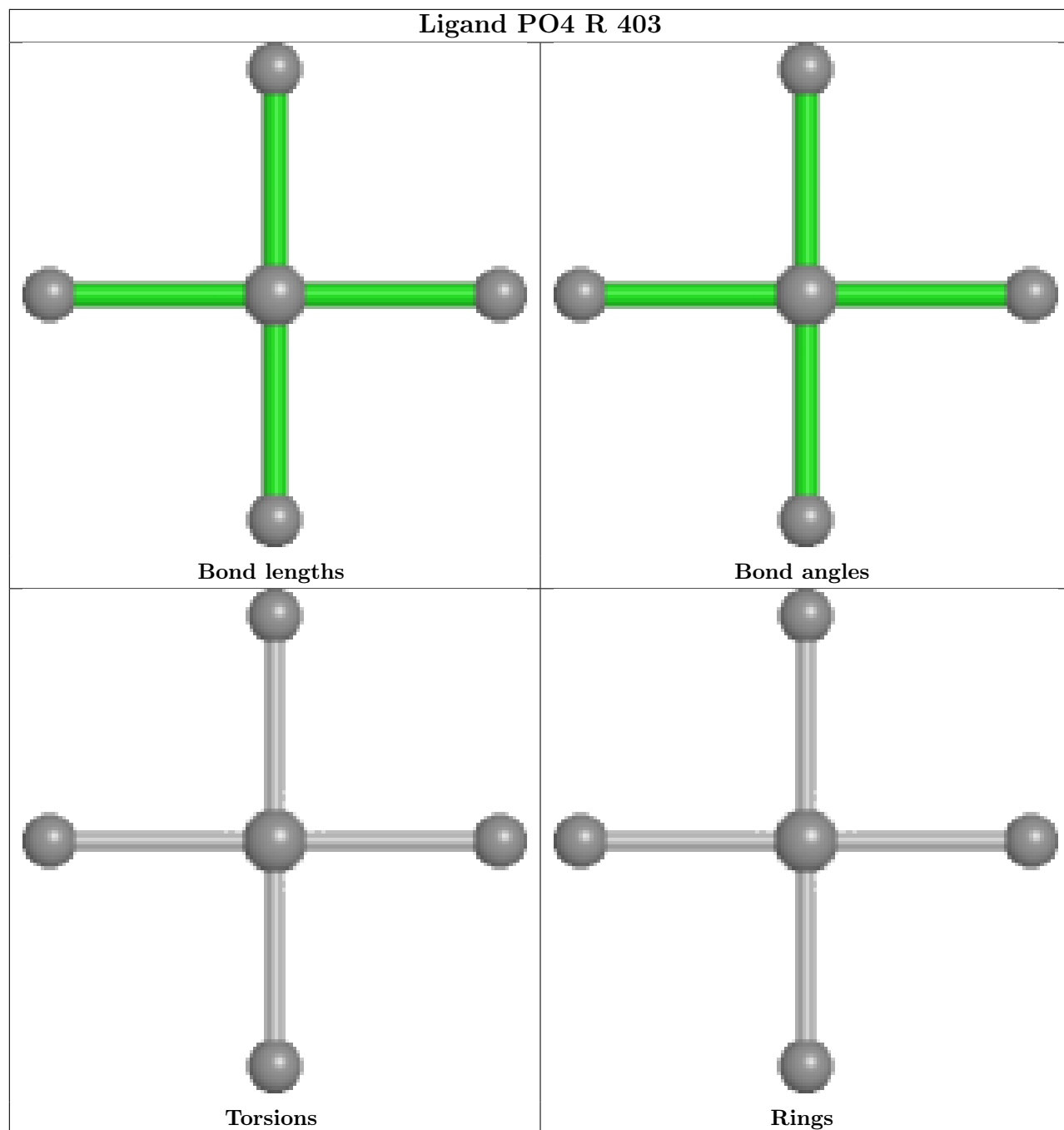
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	403	PO4	1	0
5	O	405	EDO	1	0

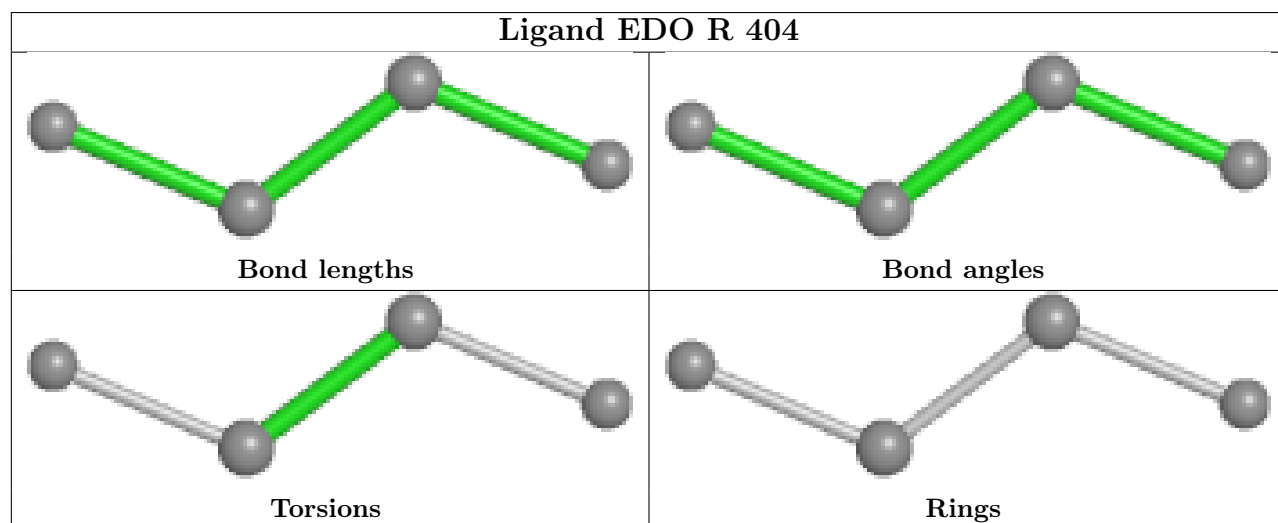
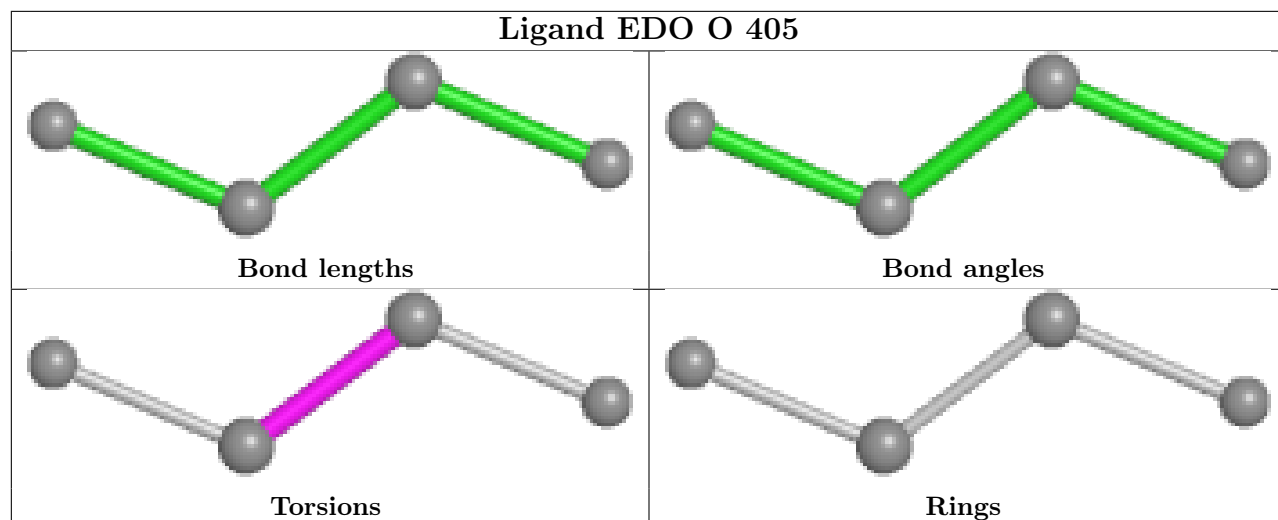
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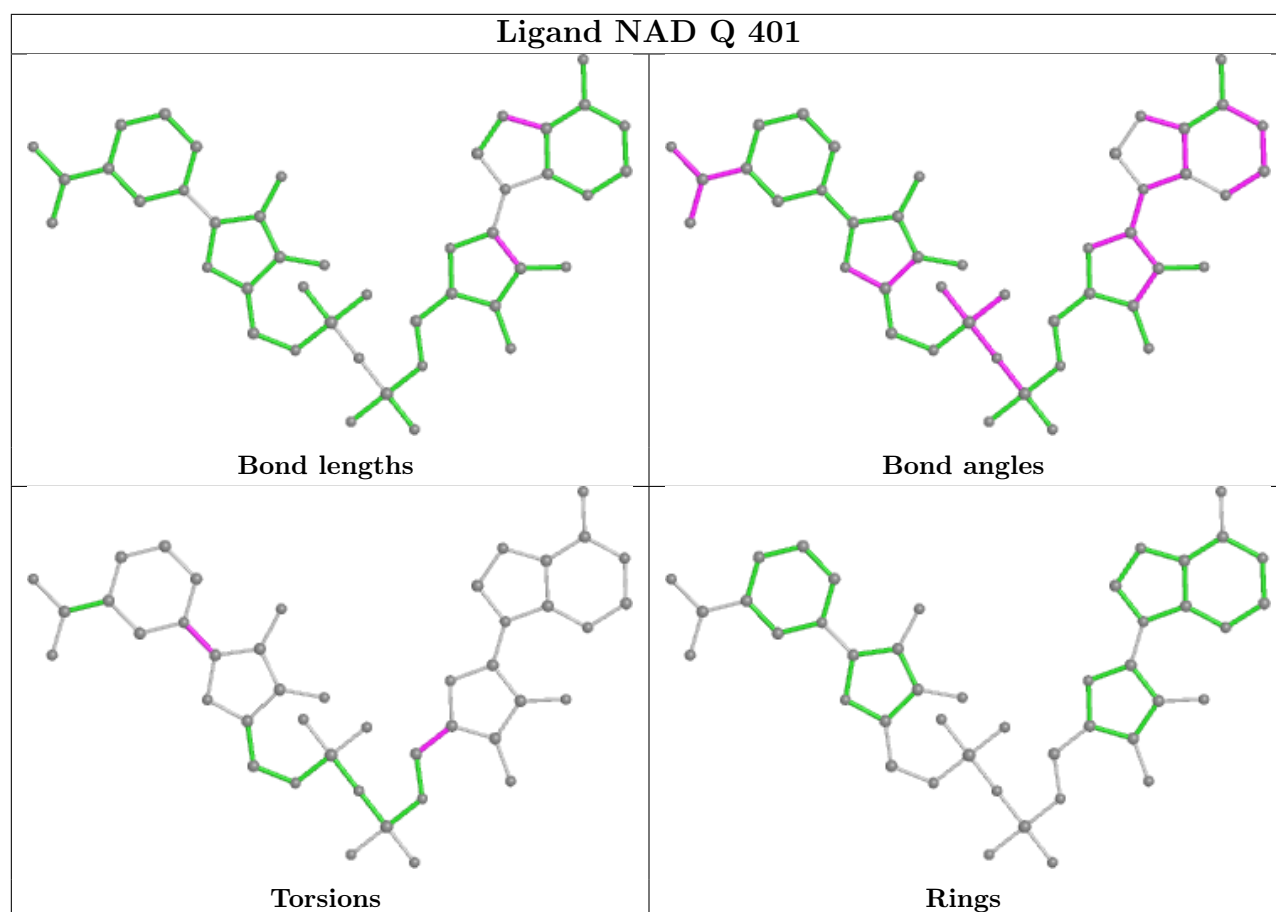
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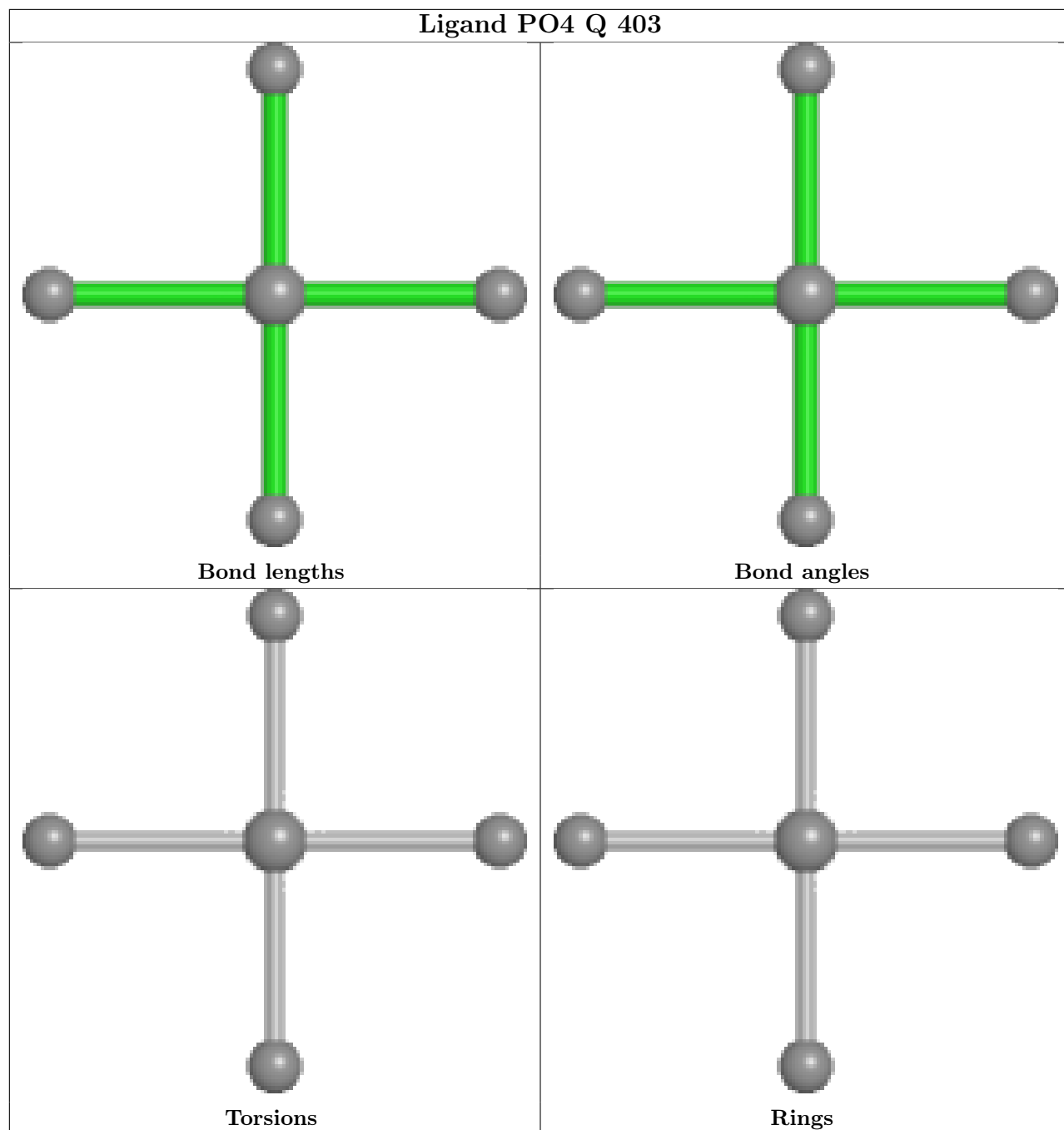
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	401	NAD	2	0
4	Q	403	PO4	1	0
5	P	404	EDO	2	0
2	O	401	NAD	1	0
3	O	402	DG4	1	0
7	Q	402[A]	G3H	4	0
7	Q	402[B]	G3H	2	0
2	P	401	NAD	1	0
7	P	402	G3H	2	0

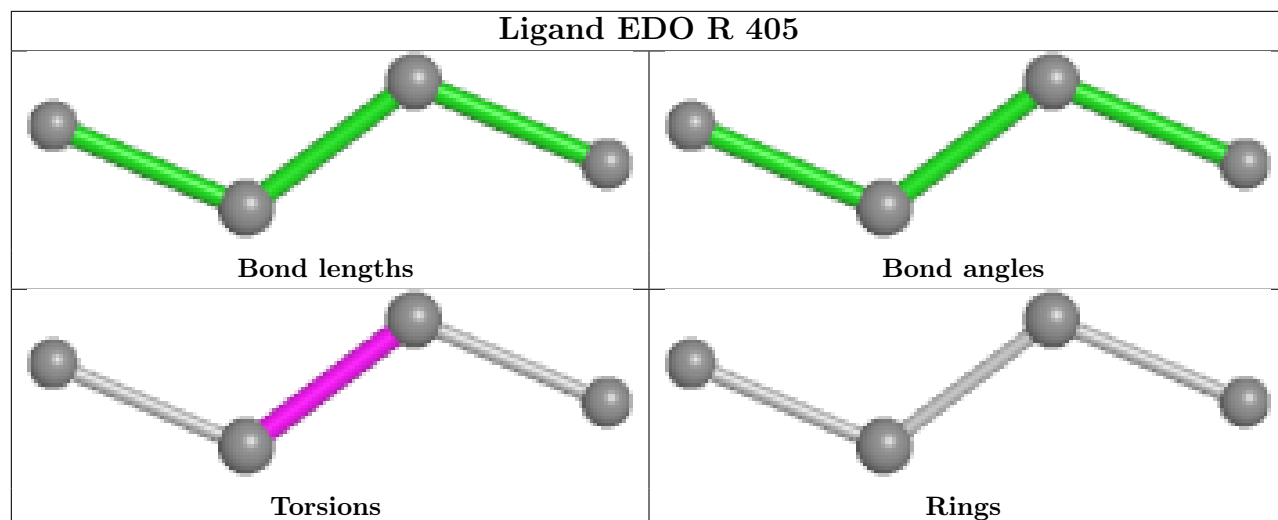
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

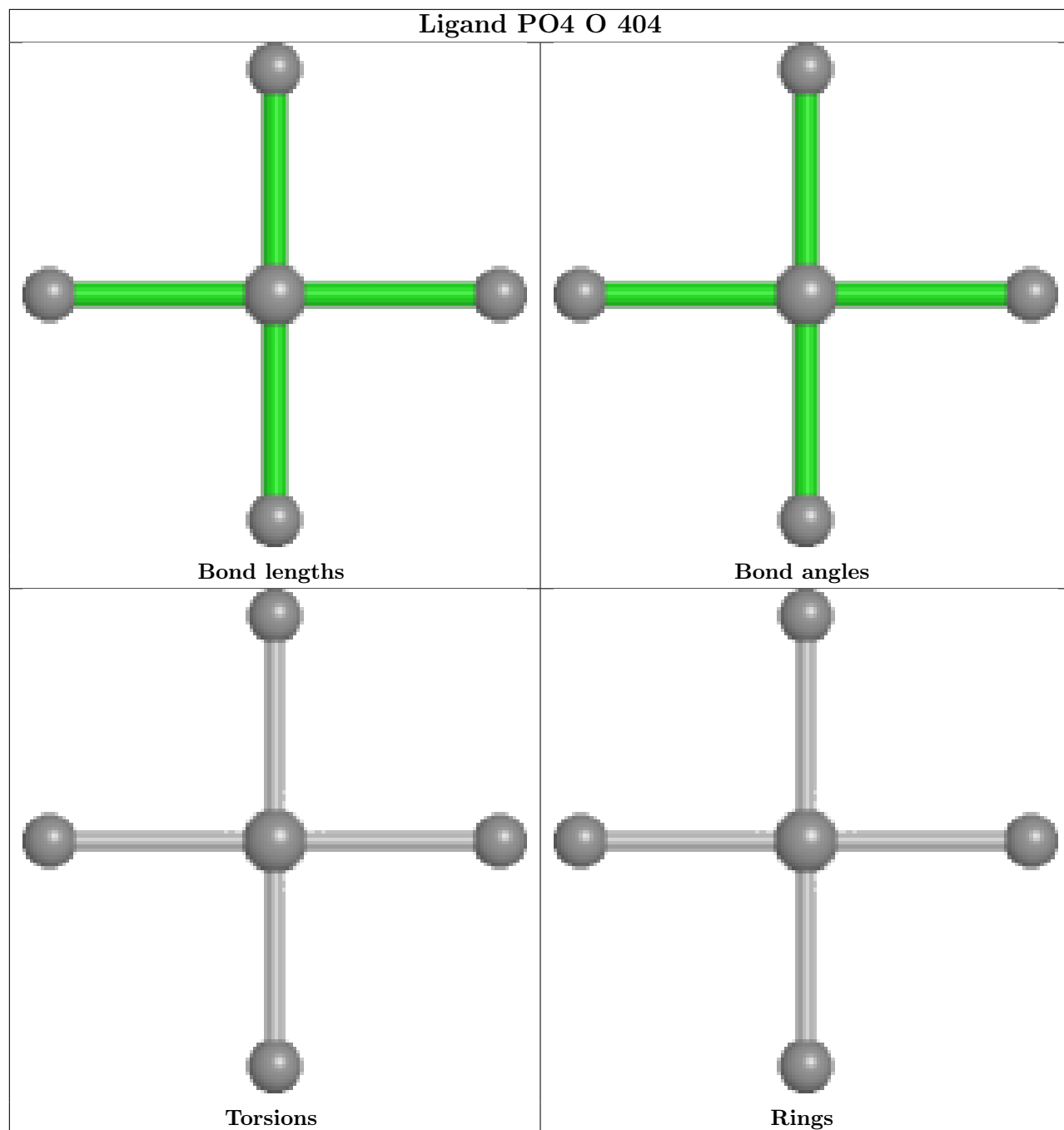


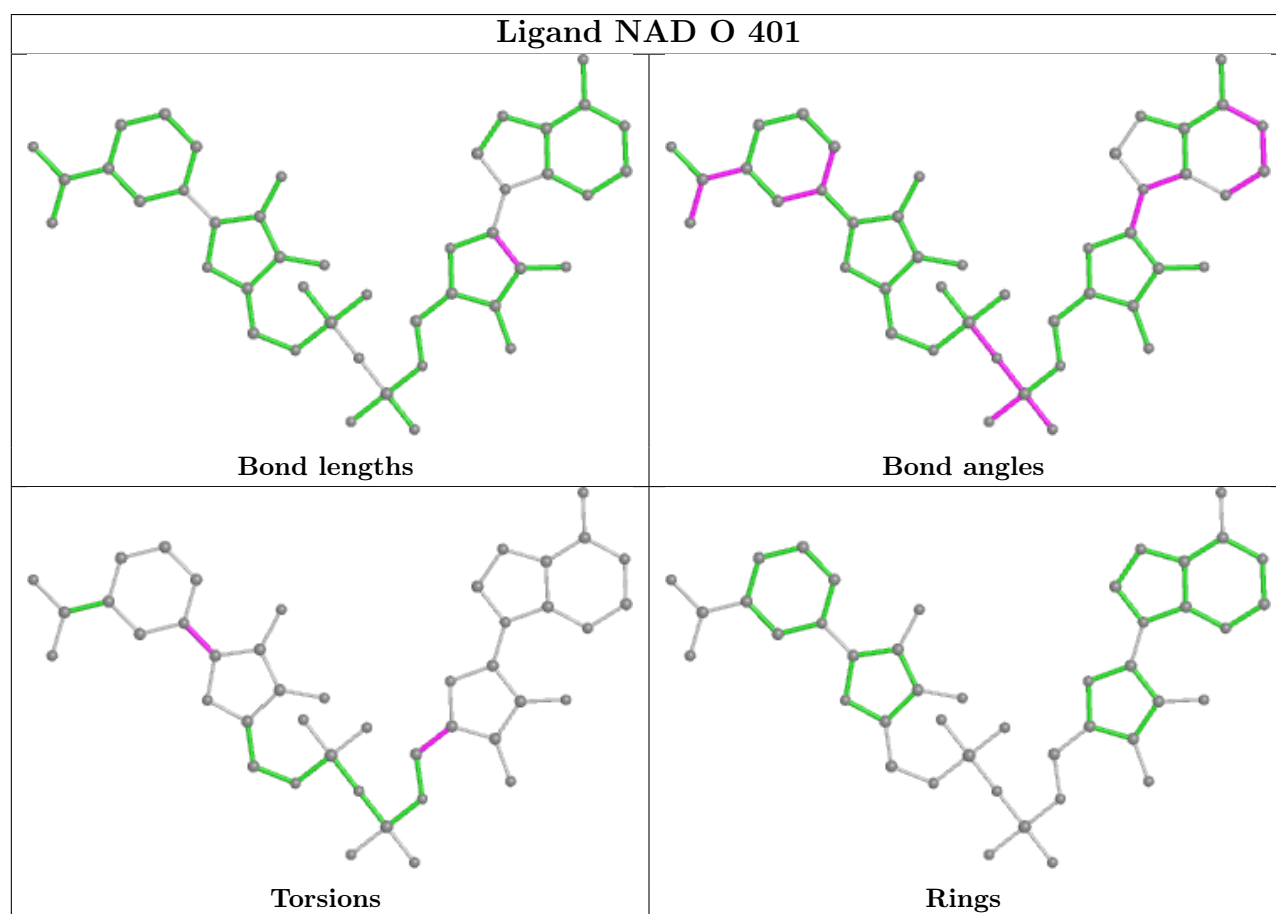
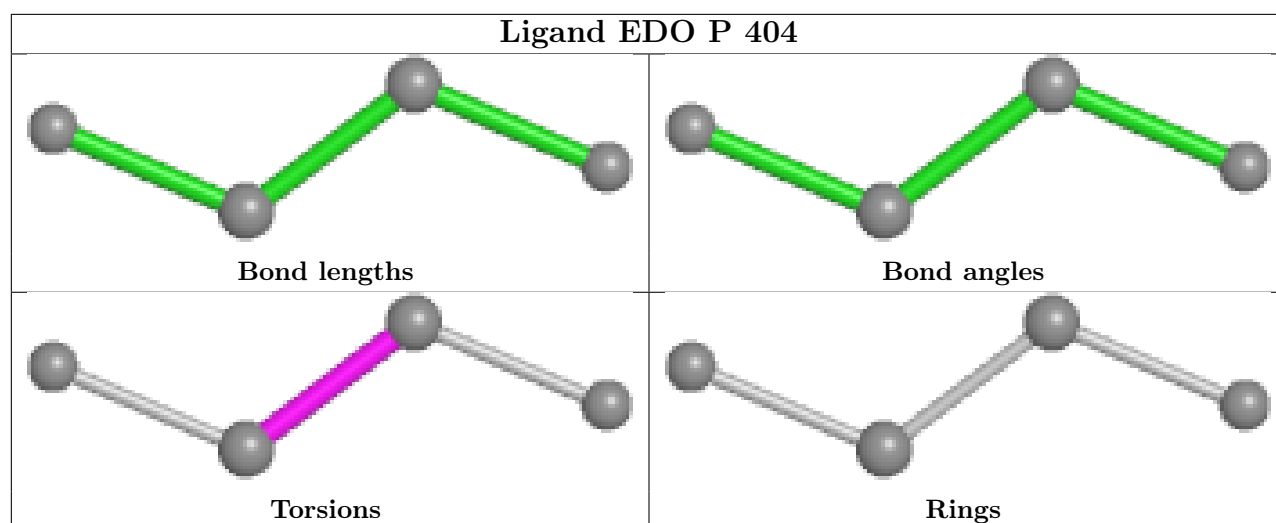




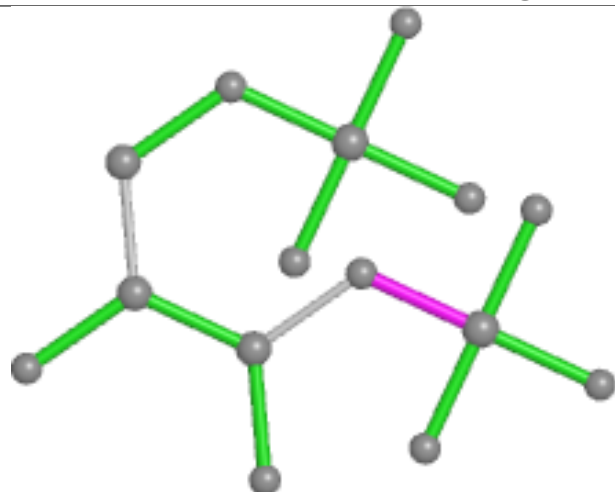




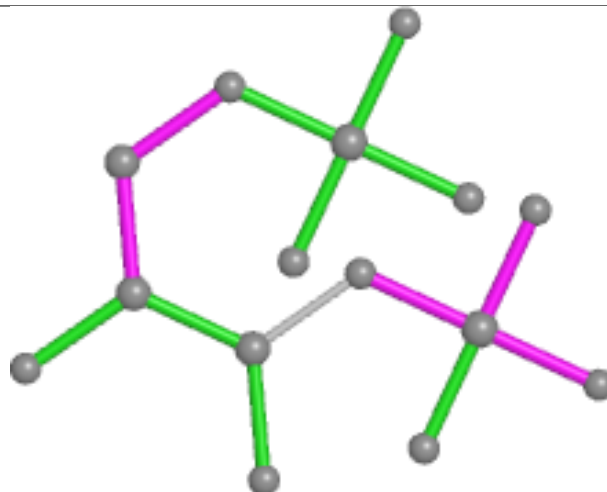




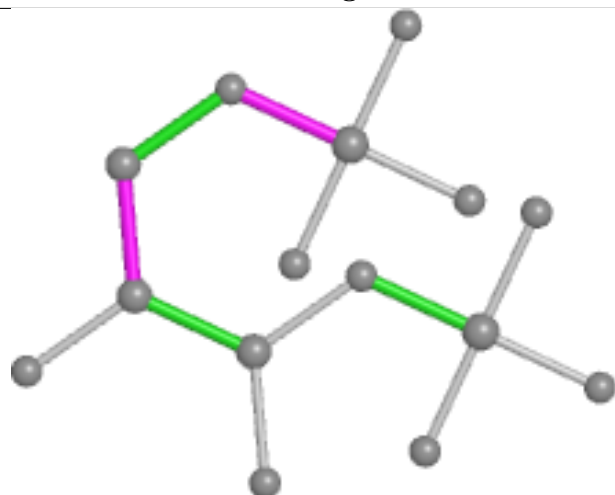
Ligand DG4 O 402



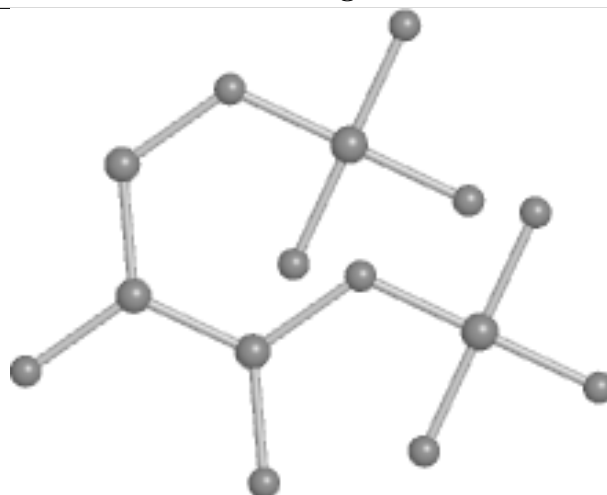
Bond lengths



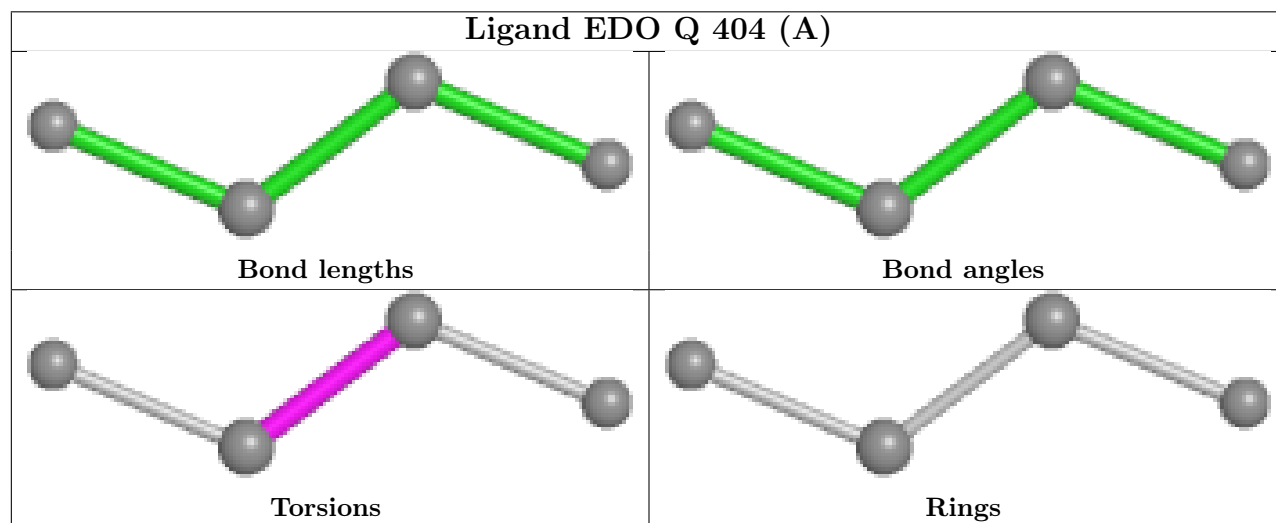
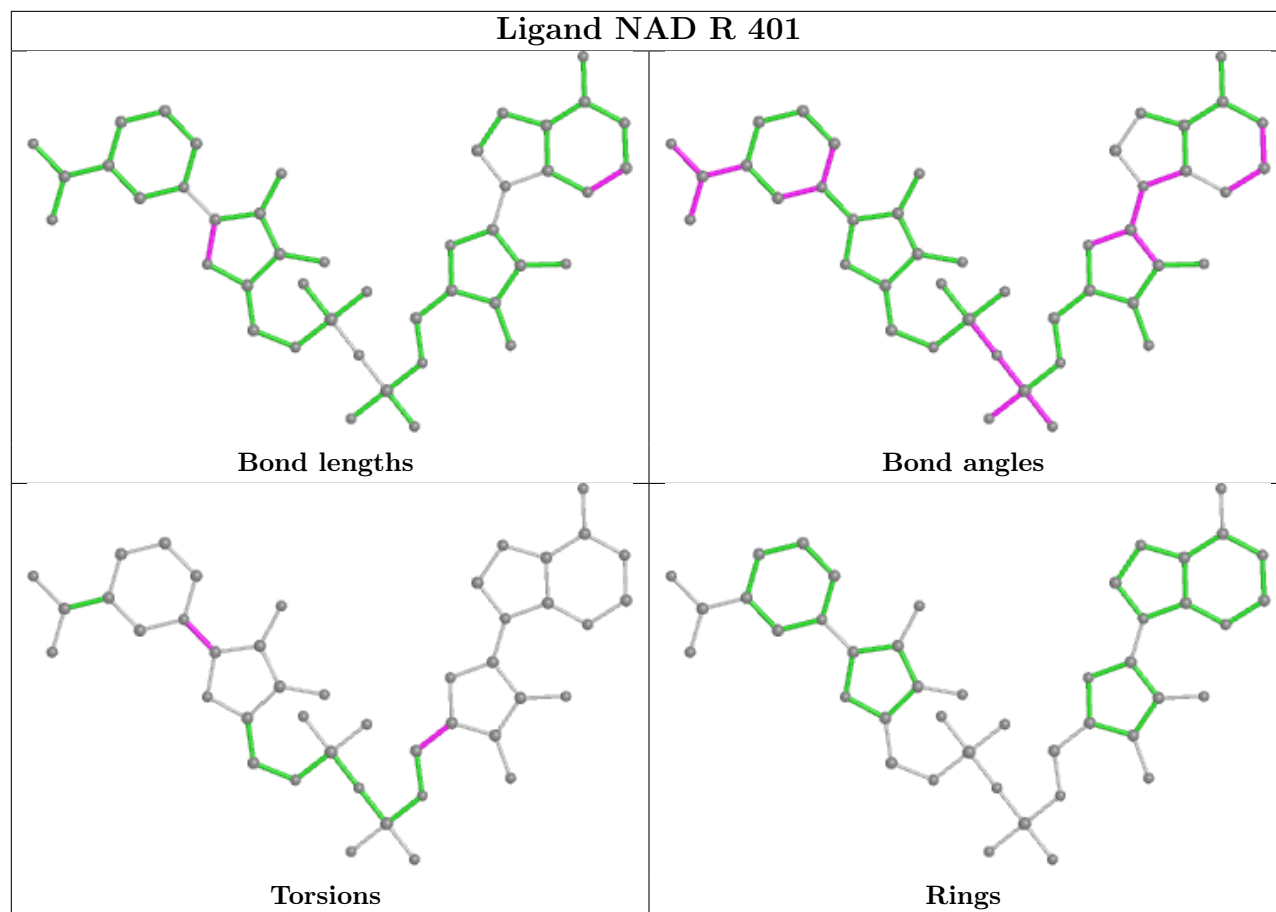
Bond angles

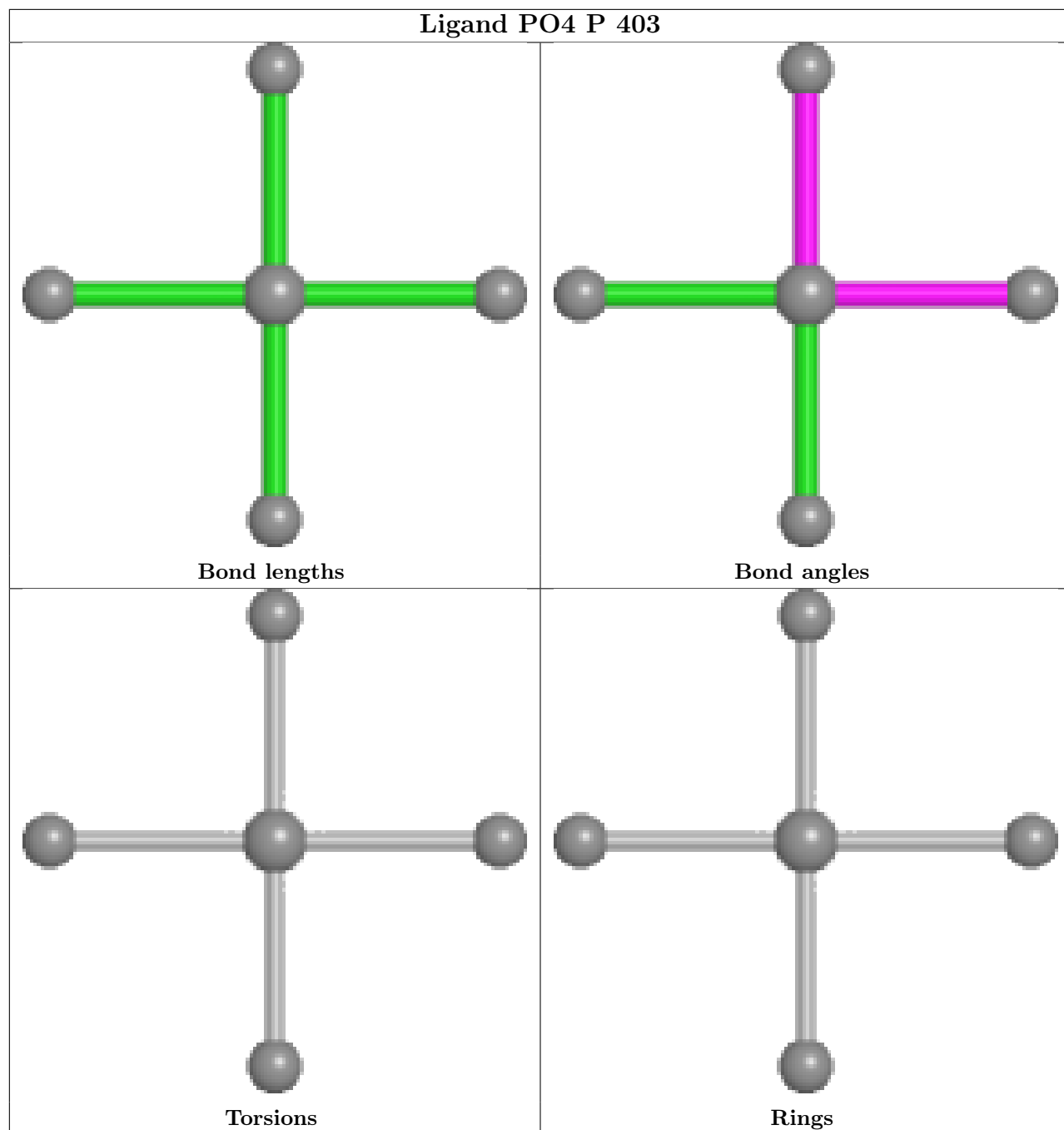


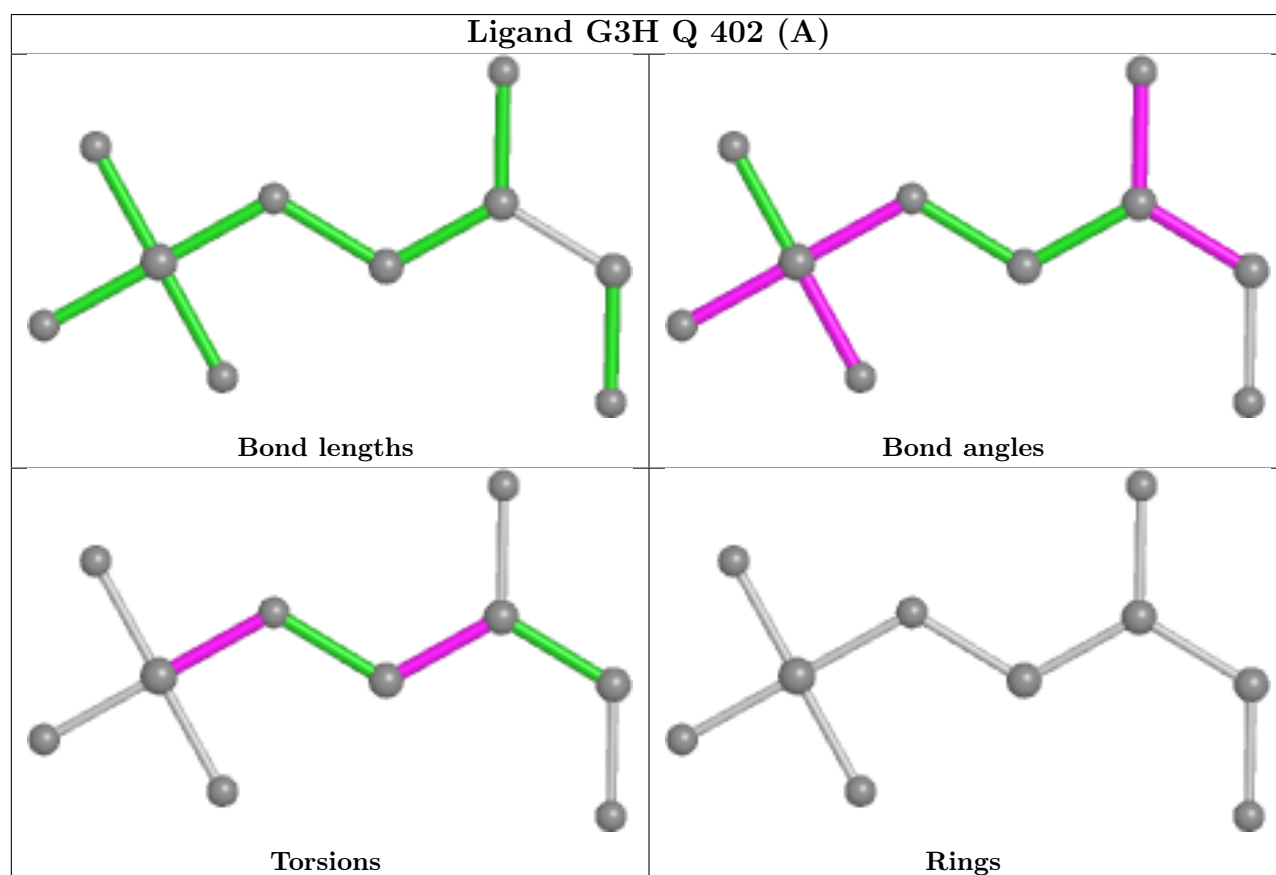
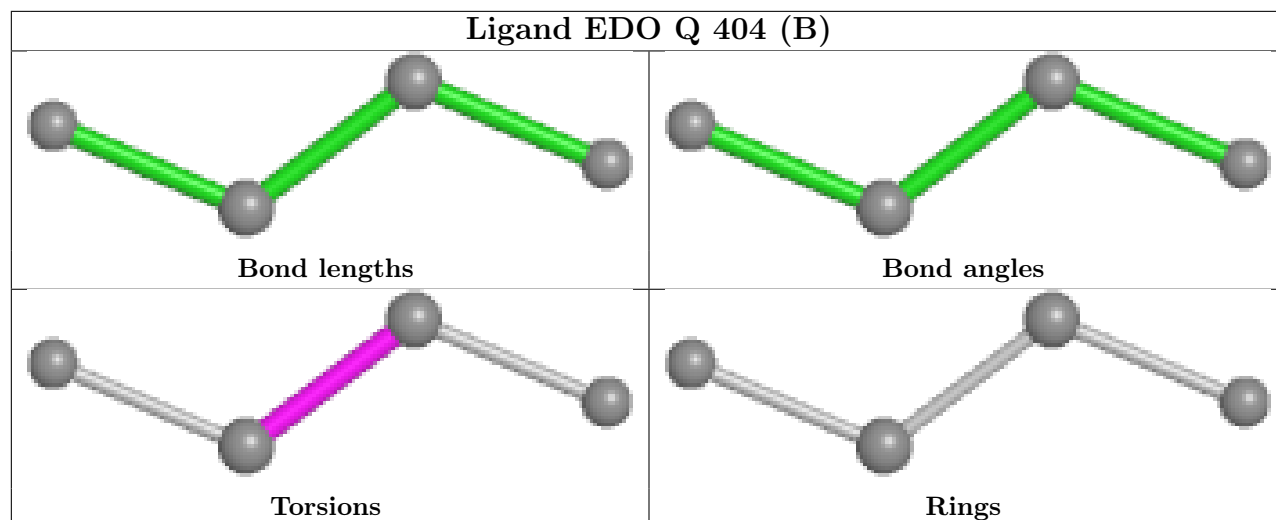
Torsions

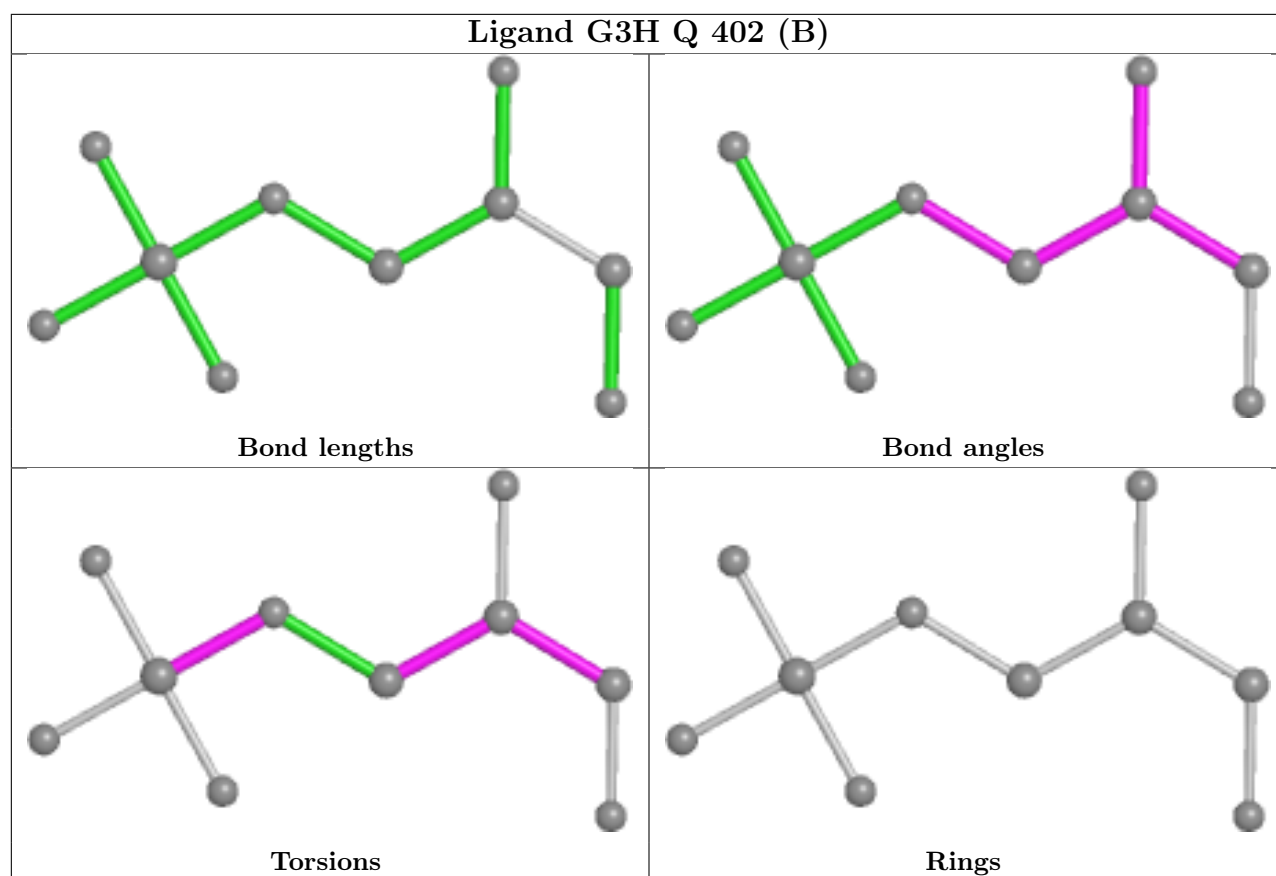


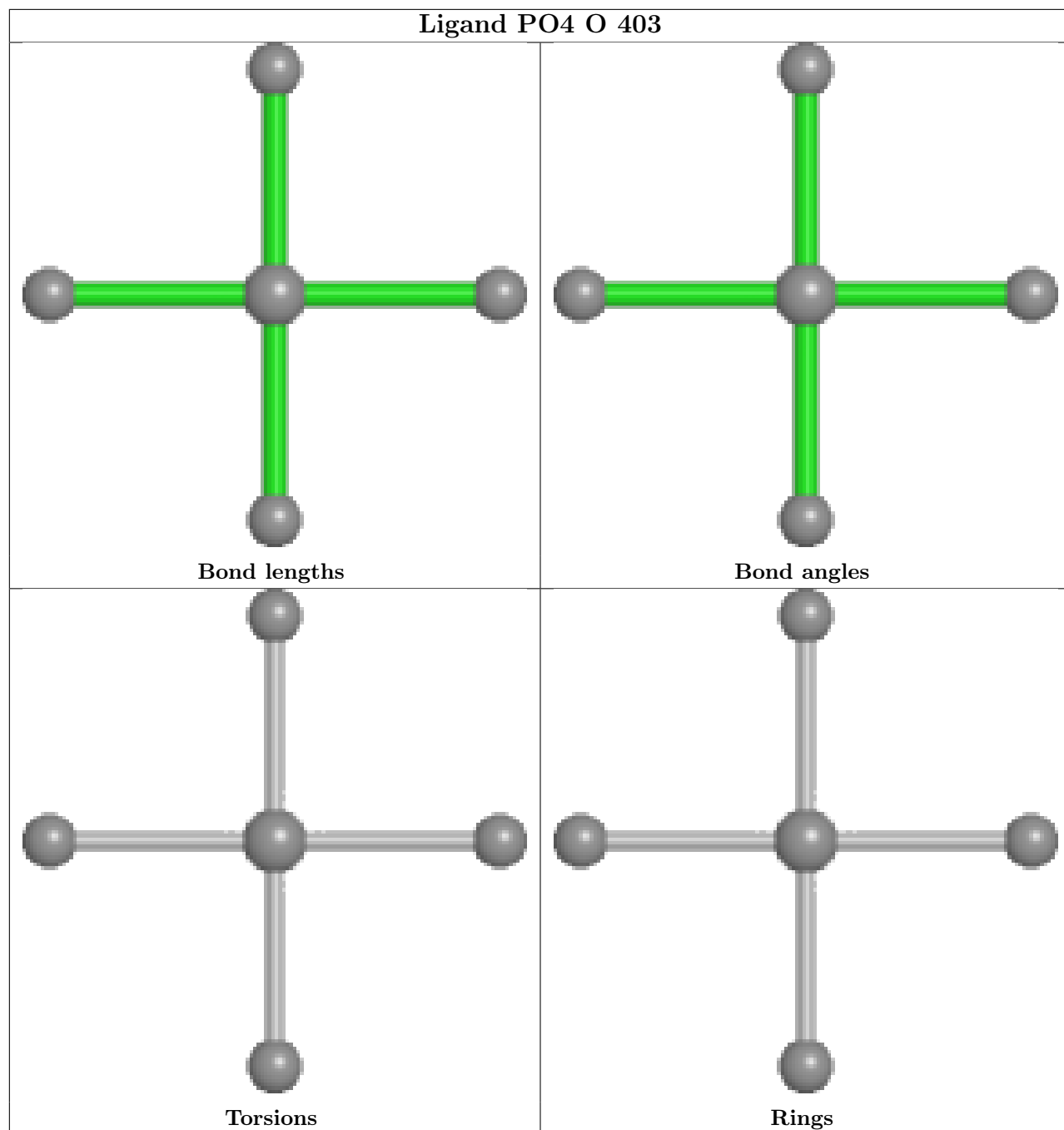
Rings

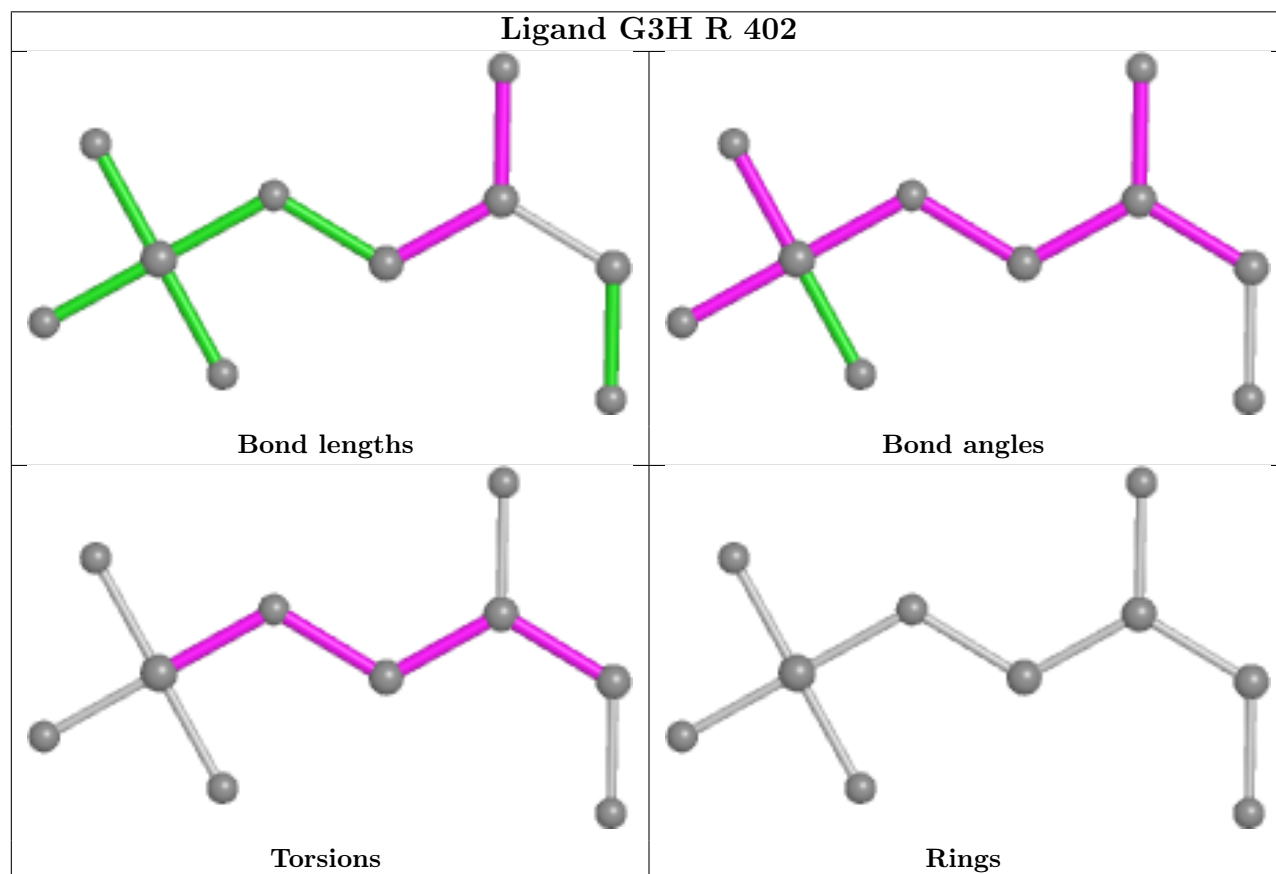
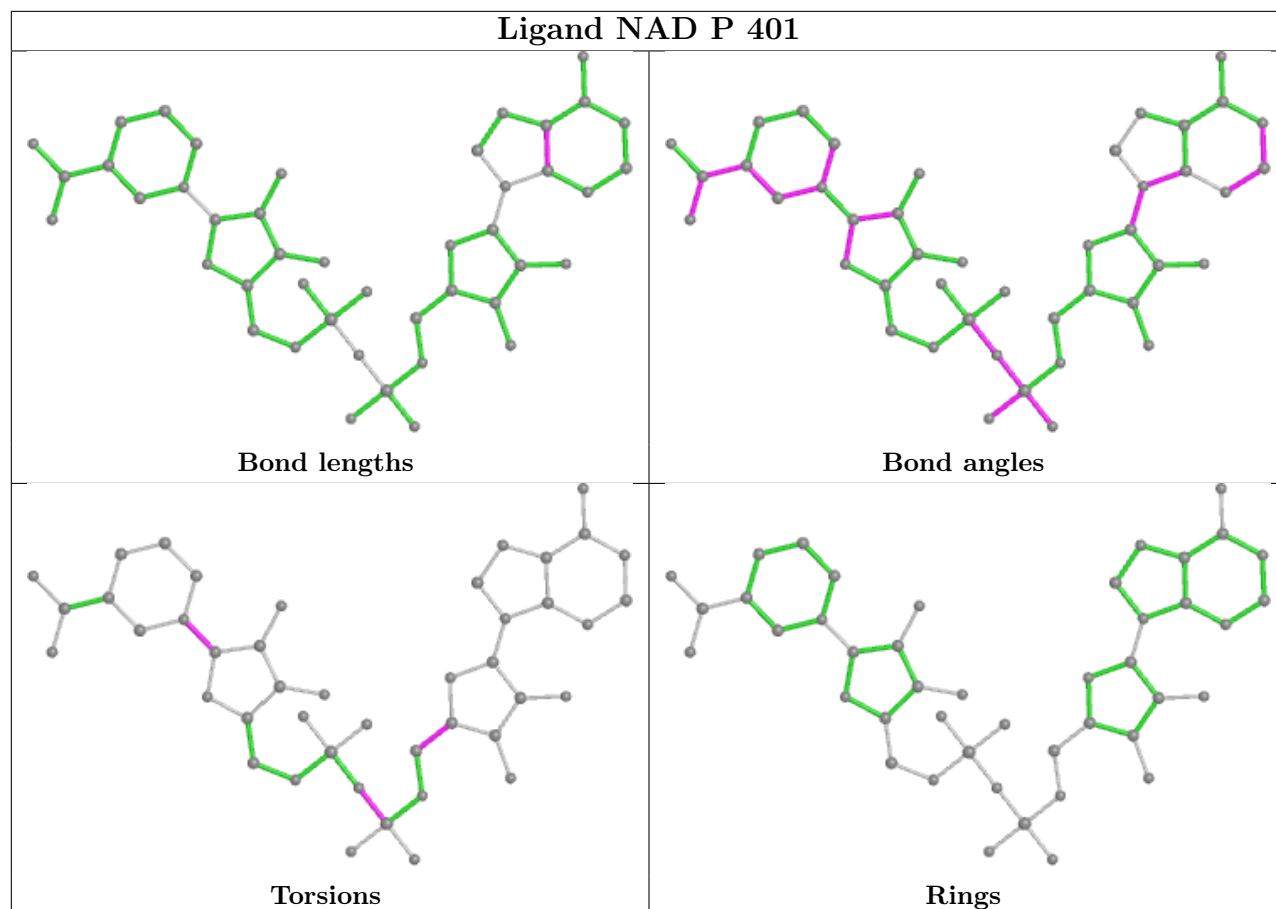


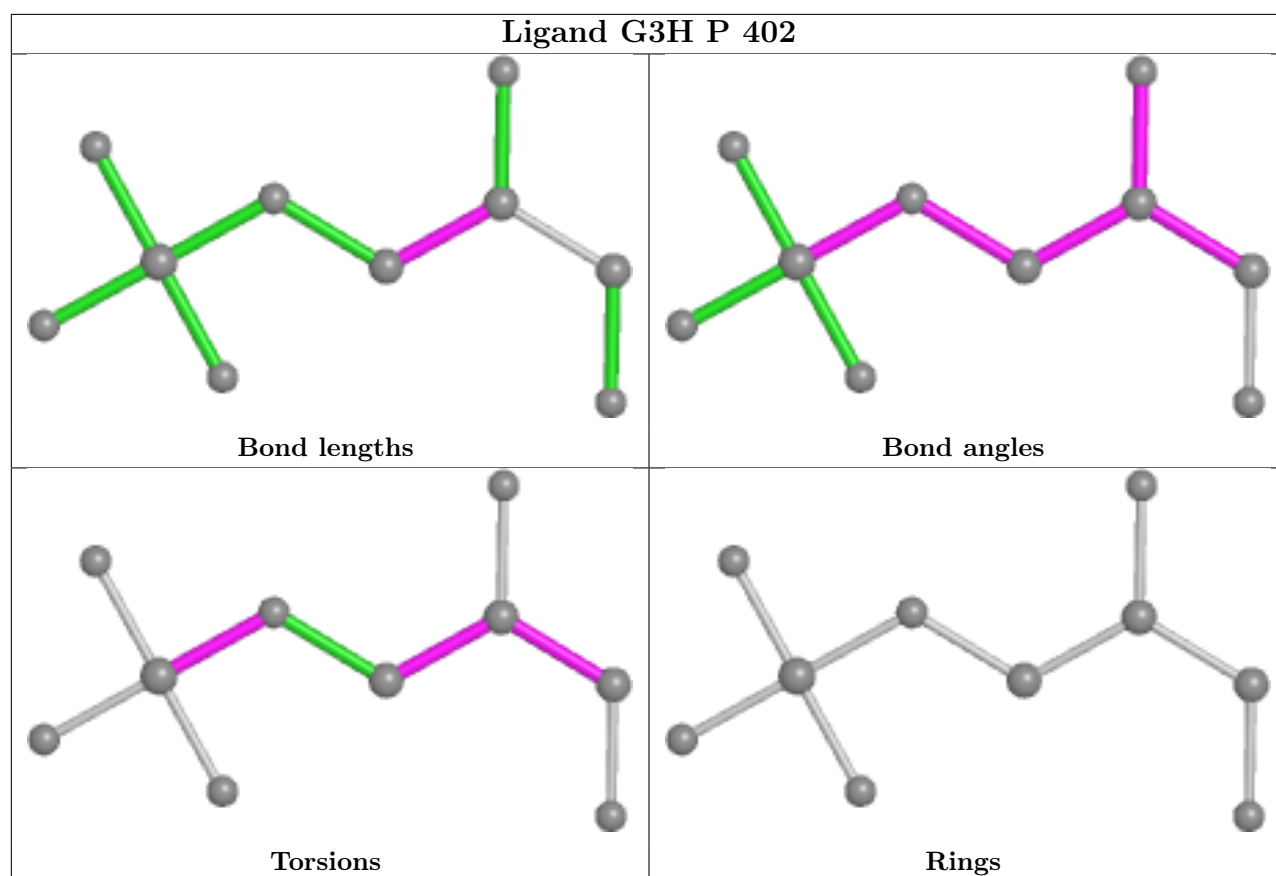












5.7 Other polymers [i](#)

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	O	334/352 (94%)	-0.73	1 (0%) 94 96	16, 23, 37, 58	0
1	P	333/352 (94%)	-0.72	1 (0%) 94 96	17, 25, 43, 66	0
1	Q	333/352 (94%)	-0.61	1 (0%) 94 96	17, 26, 43, 58	0
1	R	333/352 (94%)	-0.27	7 (2%) 63 70	18, 31, 56, 83	0
All	All	1333/1408 (94%)	-0.58	10 (0%) 86 89	16, 26, 48, 83	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	331	ALA	2.9
1	R	86	LYS	2.9
1	R	110	LEU	2.4
1	P	1	MET	2.3
1	Q	1	MET	2.2

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 [i](#)

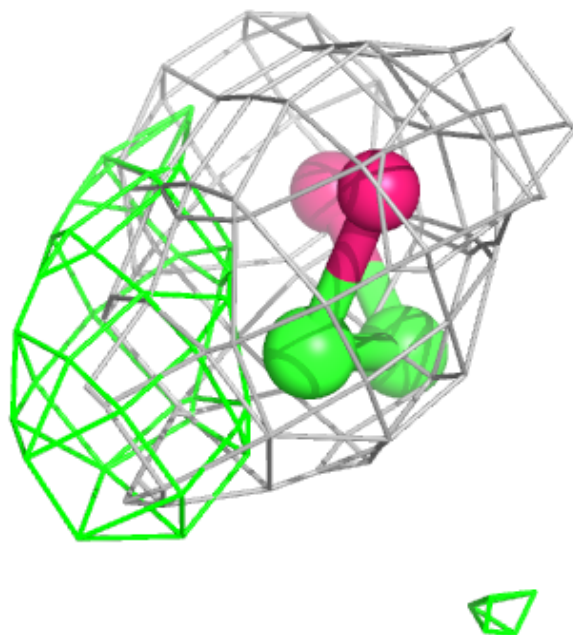
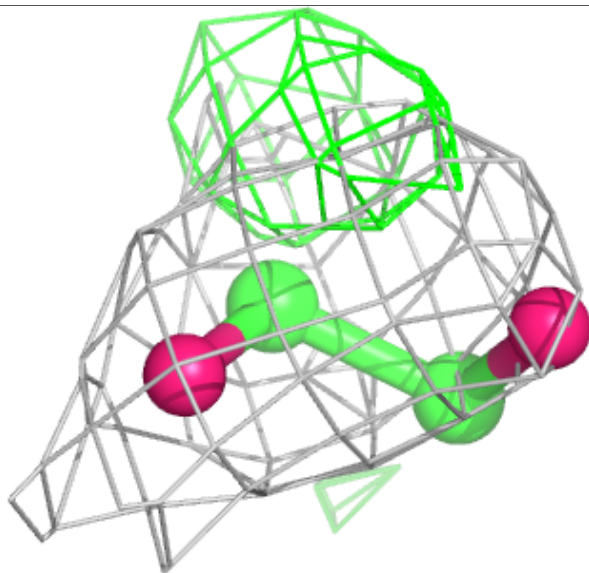
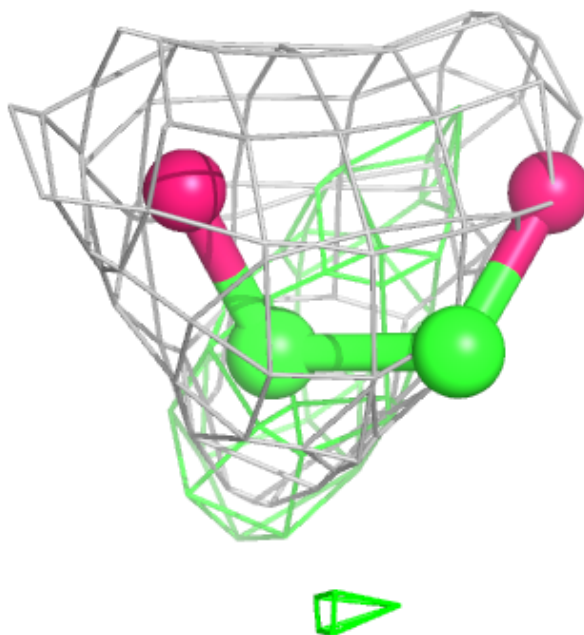
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	R	404	4/4	0.76	0.24	47,53,60,62	0
5	EDO	O	405	4/4	0.80	0.25	38,43,44,49	0
4	PO4	Q	403	5/5	0.82	0.22	69,81,89,99	0
5	EDO	P	404	4/4	0.83	0.17	44,45,46,50	0
5	EDO	R	405	4/4	0.84	0.19	40,42,49,51	0
4	PO4	O	404	5/5	0.86	0.25	66,68,76,95	0
4	PO4	R	403	5/5	0.86	0.26	59,72,81,92	0
4	PO4	P	403	5/5	0.91	0.26	52,56,67,68	0
5	EDO	Q	404[A]	4/4	0.92	0.21	20,22,22,23	4
5	EDO	Q	404[B]	4/4	0.92	0.21	25,25,27,27	4
7	G3H	P	402	10/10	0.94	0.14	34,41,49,57	0
3	DG4	O	402	15/15	0.95	0.15	24,42,59,60	15
6	CL	Q	405	1/1	0.96	0.08	45,45,45,45	0
6	CL	R	406	1/1	0.97	0.05	34,34,34,34	0
4	PO4	O	403	5/5	0.97	0.10	48,48,50,60	0
7	G3H	Q	402[A]	10/10	0.97	0.15	27,33,35,36	10
7	G3H	Q	402[B]	10/10	0.97	0.15	25,29,34,36	10
7	G3H	R	402	10/10	0.97	0.14	29,38,55,64	0
2	NAD	P	401	44/44	0.98	0.07	17,22,25,27	0
2	NAD	Q	401	44/44	0.98	0.09	17,22,27,29	0
2	NAD	R	401	44/44	0.98	0.08	22,24,28,29	0
6	CL	P	405	1/1	0.98	0.05	29,29,29,29	0
2	NAD	O	401	44/44	0.98	0.08	16,19,22,22	0
6	CL	O	408	1/1	0.99	0.07	34,34,34,34	0
6	CL	O	406	1/1	0.99	0.04	28,28,28,28	0
6	CL	O	407	1/1	0.99	0.06	27,27,27,27	0
6	CL	Q	406	1/1	0.99	0.04	27,27,27,27	0
6	CL	Q	407	1/1	0.99	0.04	30,30,30,30	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.

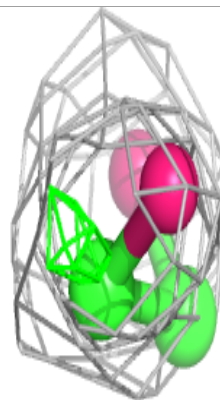
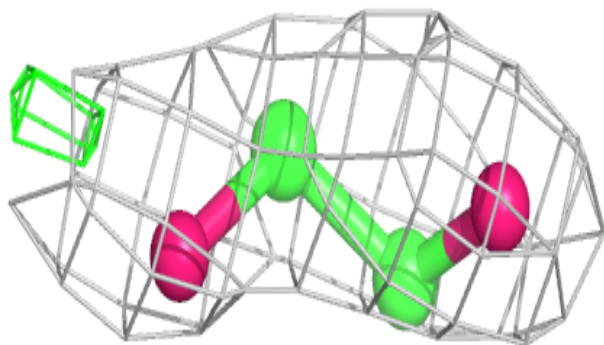
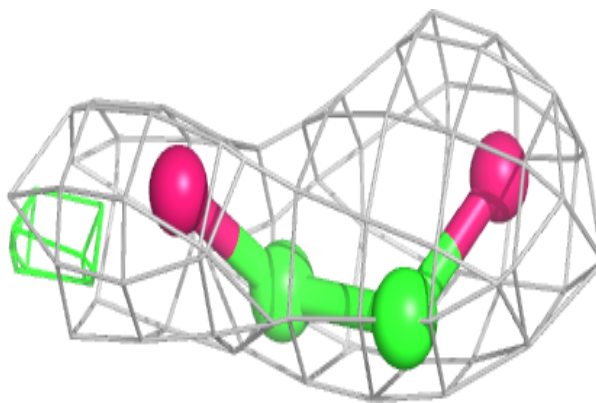
Electron density around EDO R 404:

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



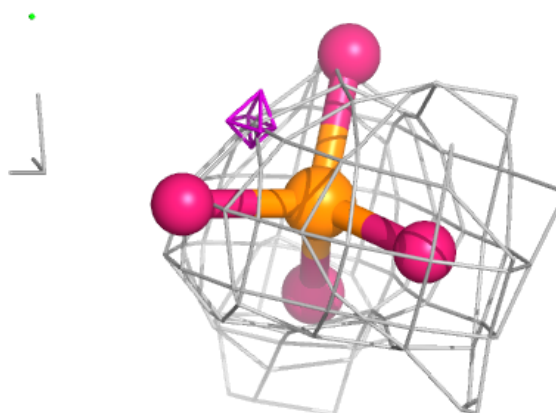
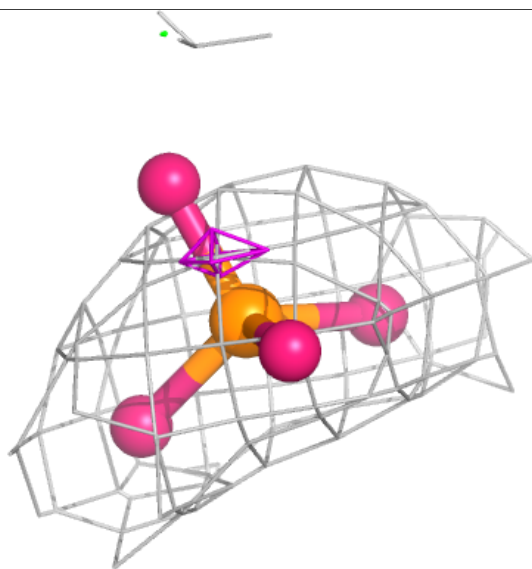
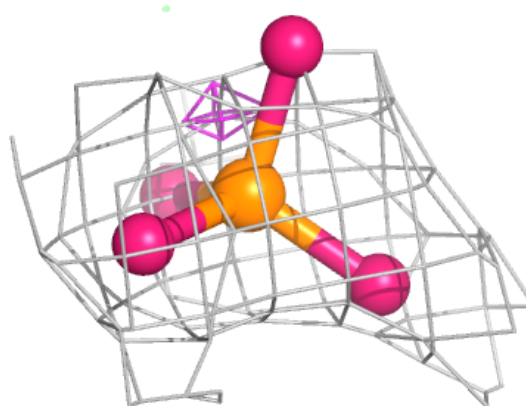
Electron density around EDO O 405:

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



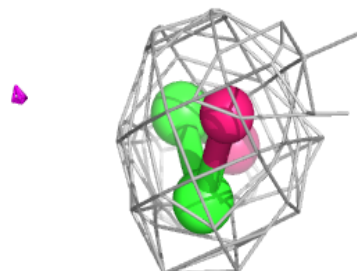
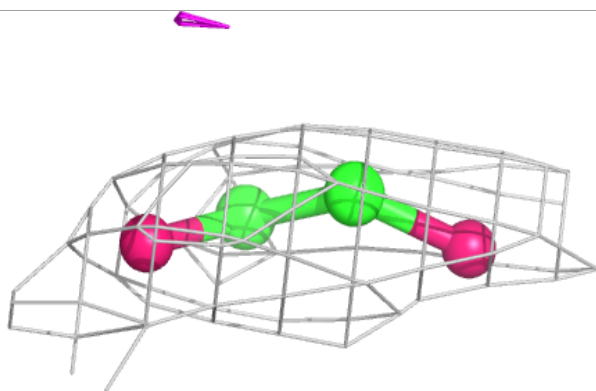
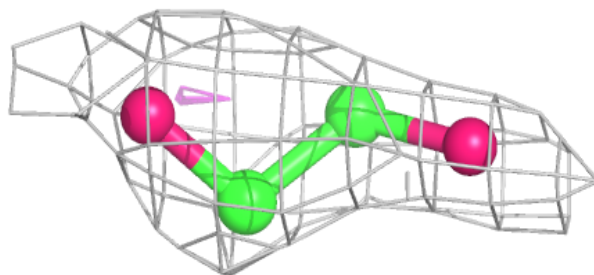
Electron density around PO4 Q 403:

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

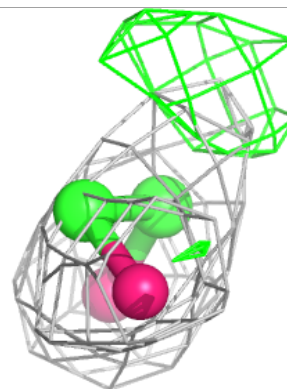
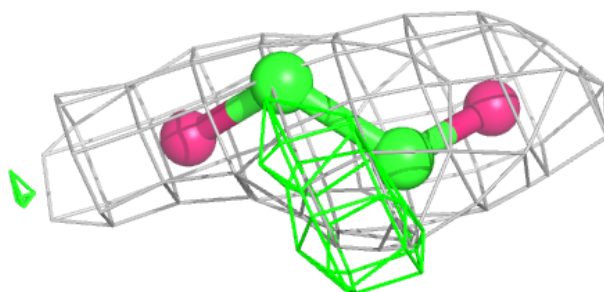
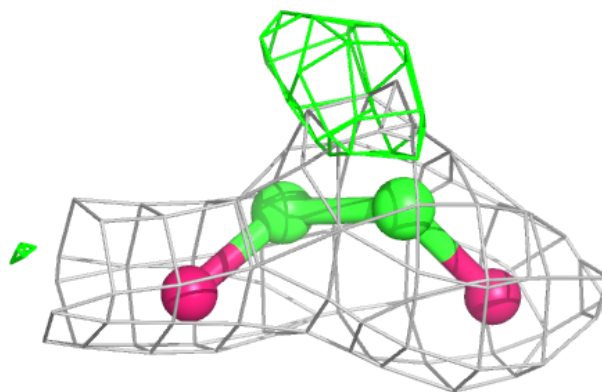


Electron density around EDO P 404:

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

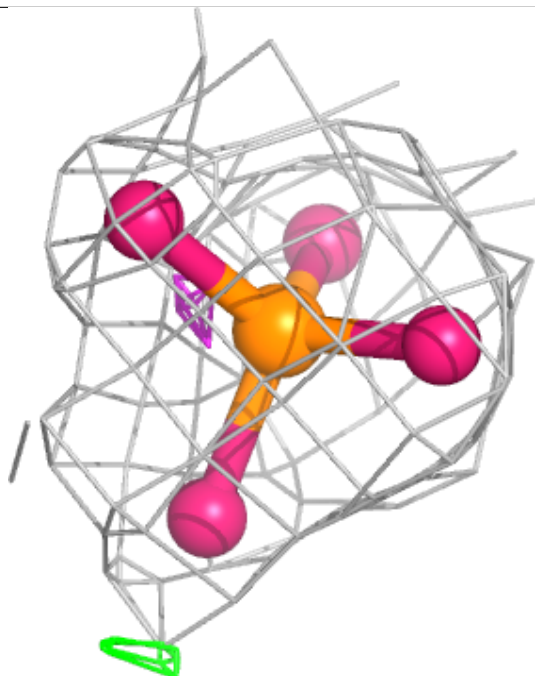
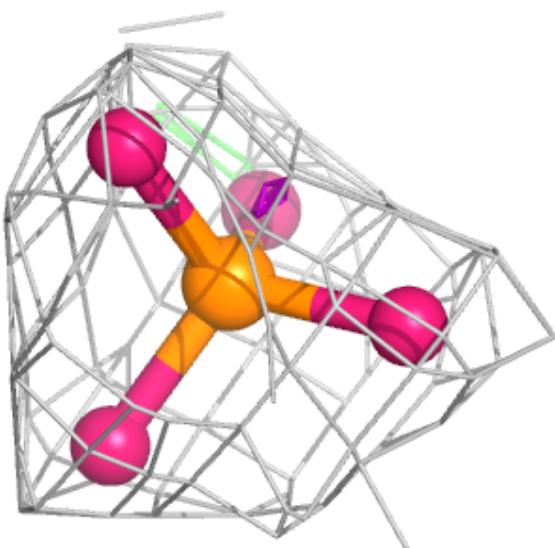
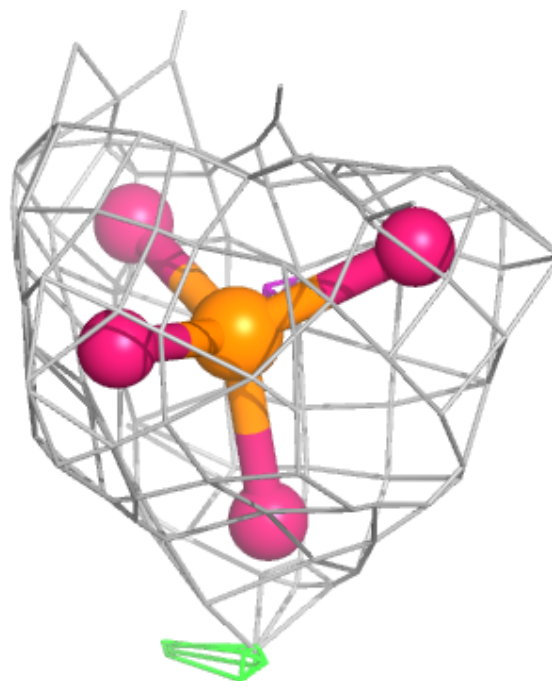
**Electron density around EDO R 405:**

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



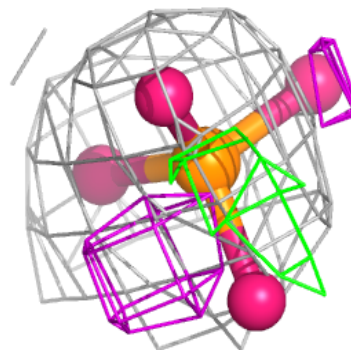
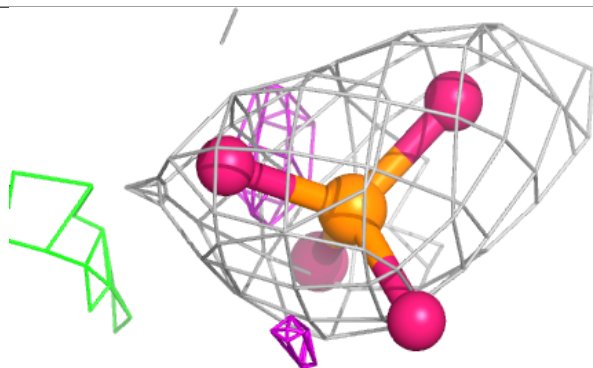
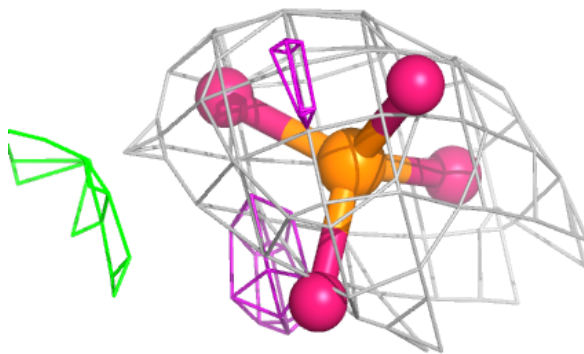
Electron density around PO4 O 404:

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



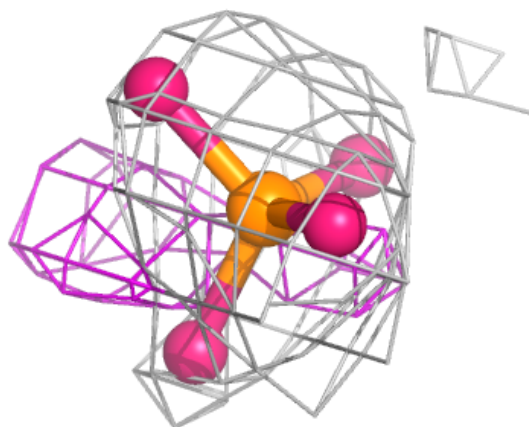
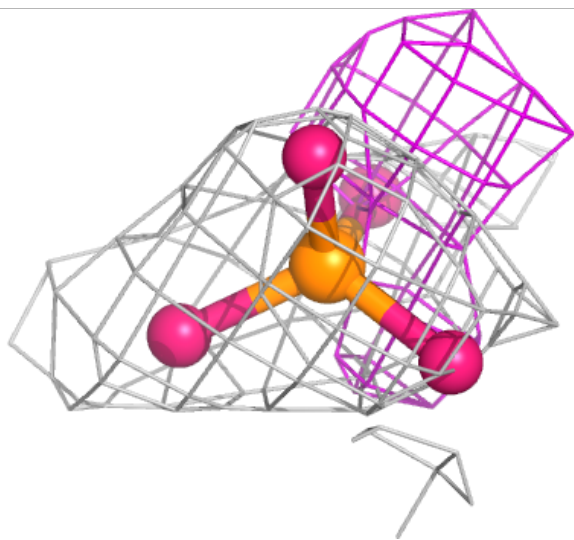
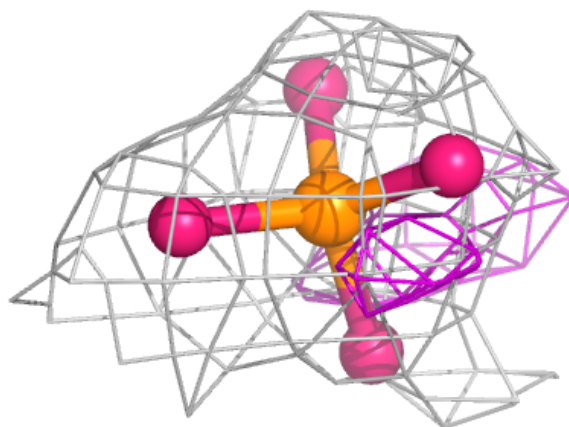
Electron density around PO4 R 403:

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



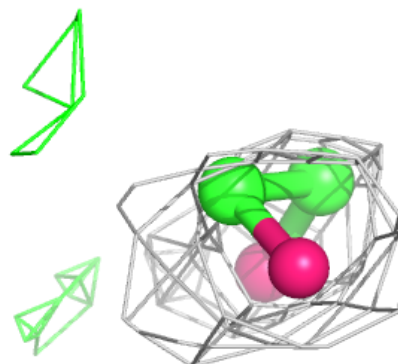
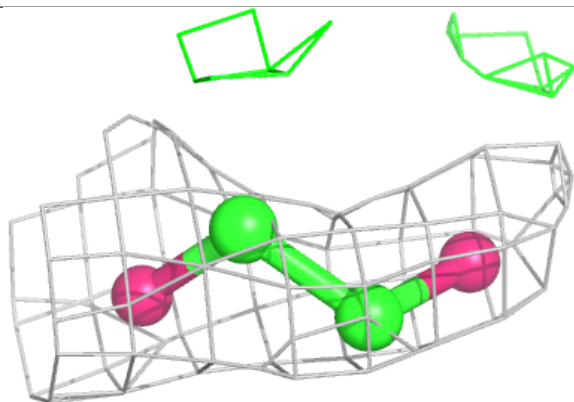
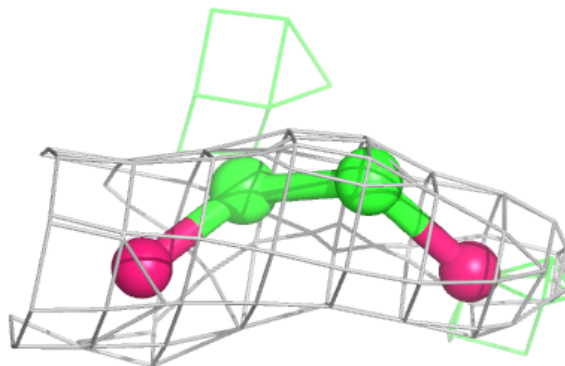
Electron density around PO4 P 403:

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

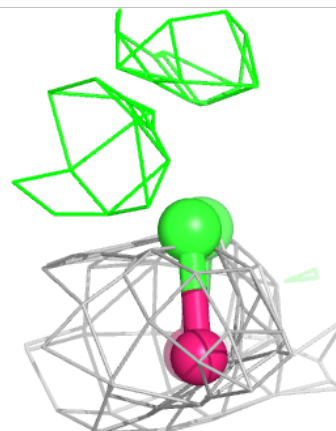
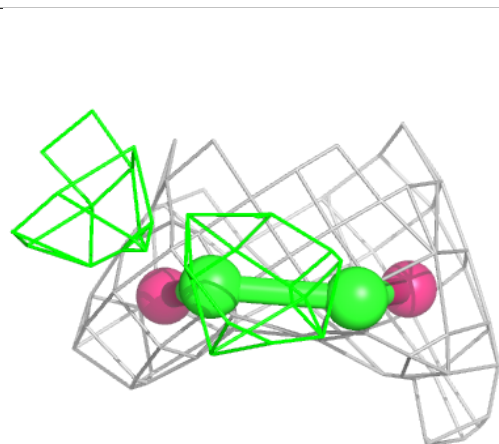
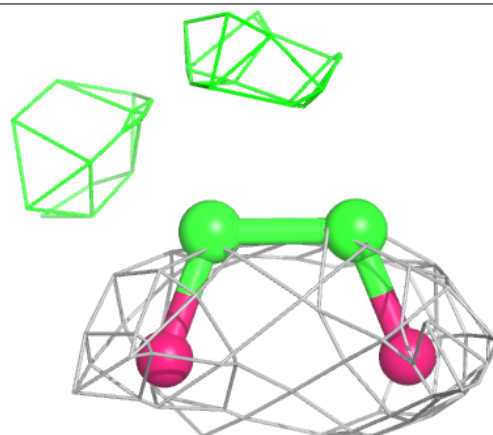


Electron density around EDO Q 404 (A):

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

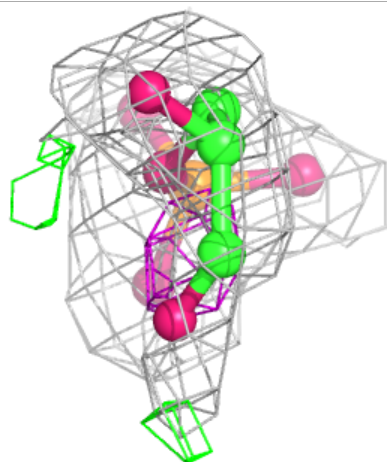
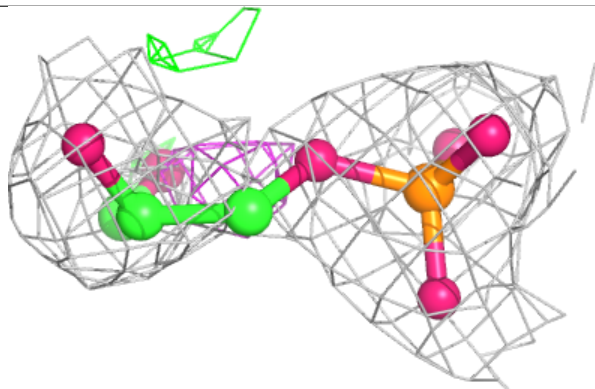
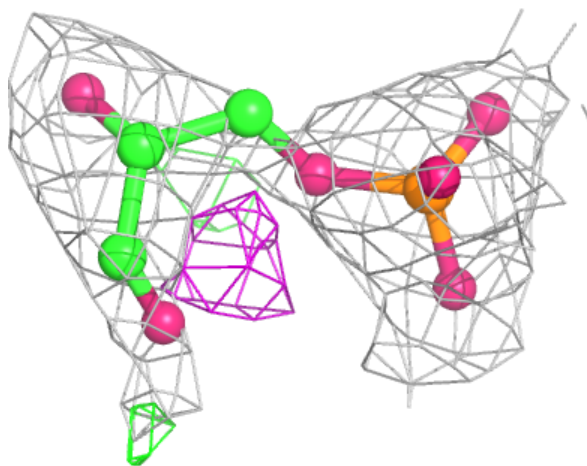
**Electron density around EDO Q 404 (B):**

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



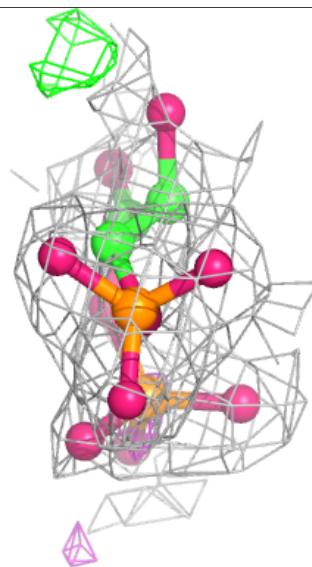
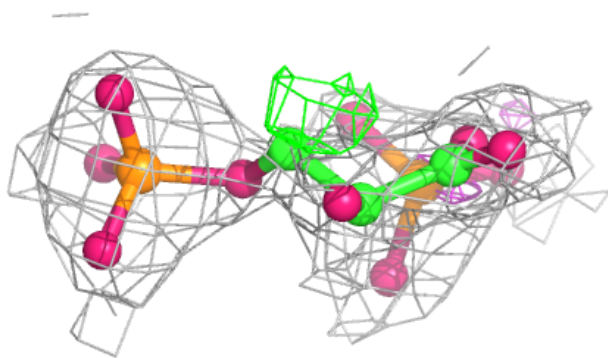
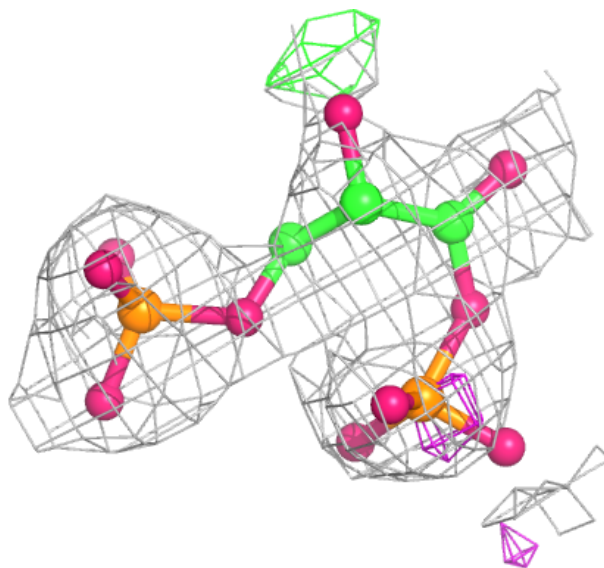
Electron density around G3H P 402:

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



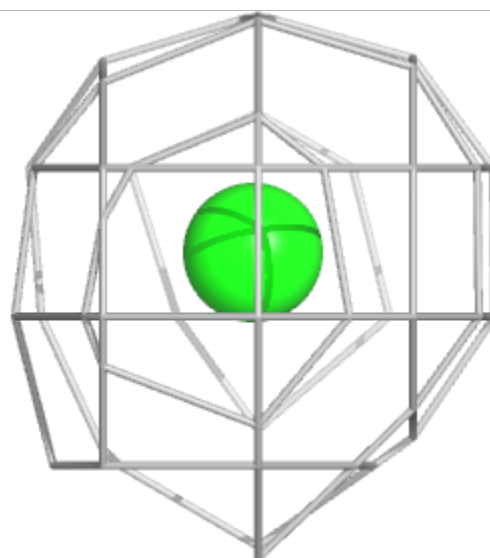
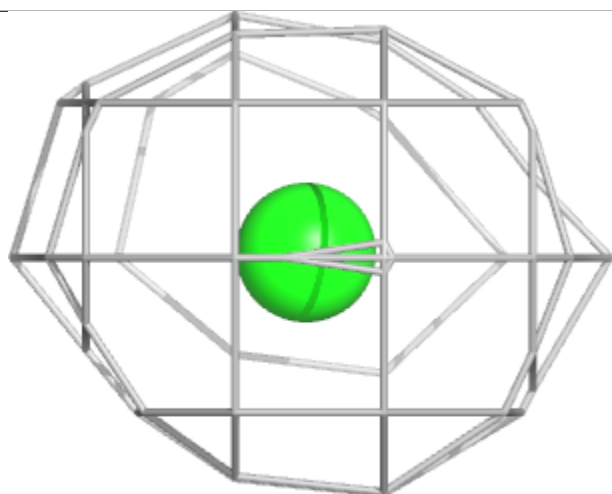
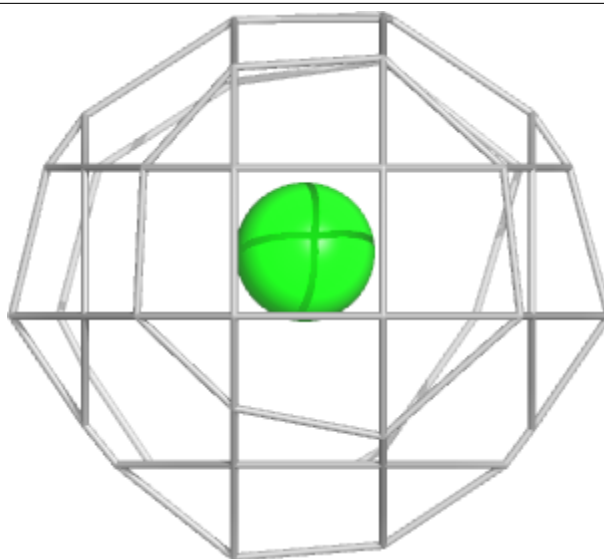
Electron density around DG4 O 402:

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



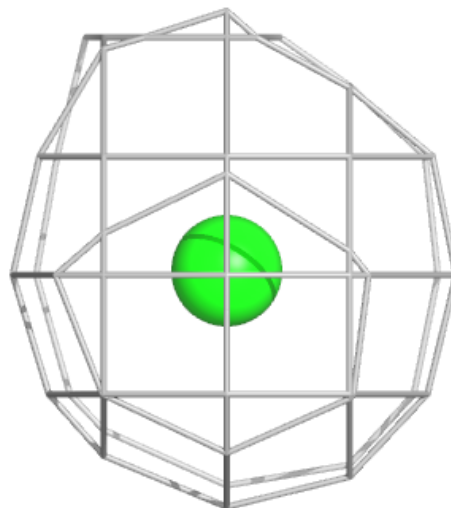
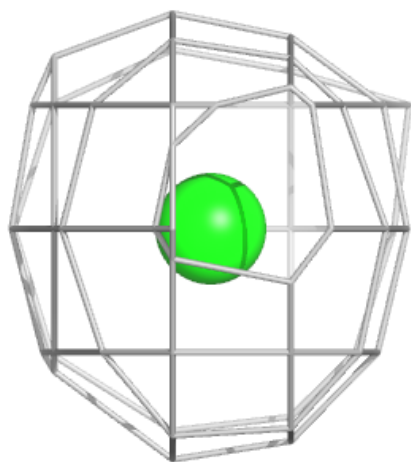
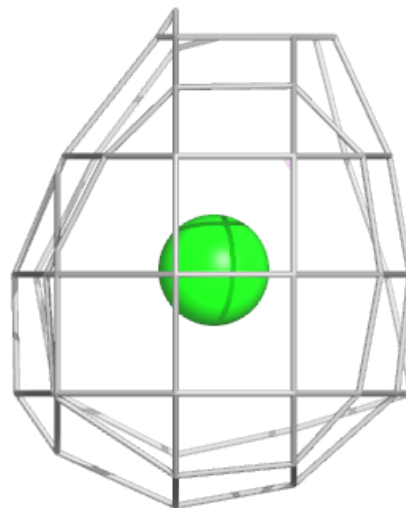
Electron density around CL Q 405:

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



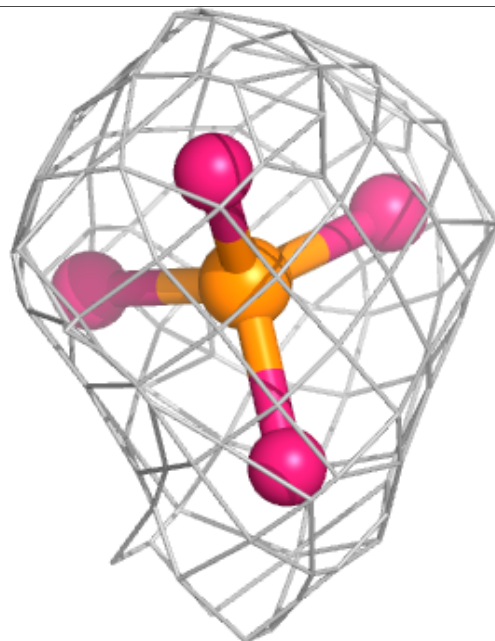
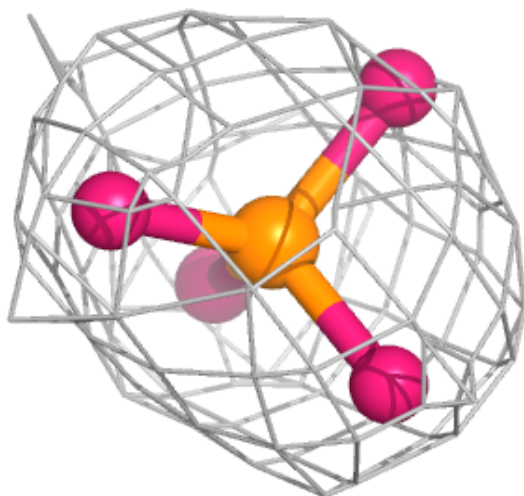
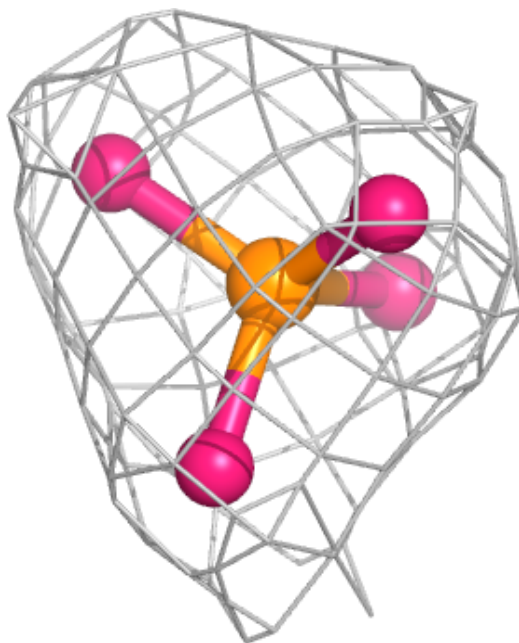
Electron density around CL R 406:

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



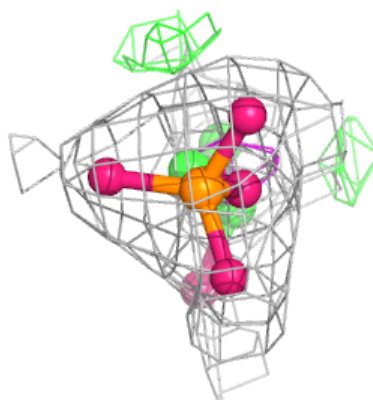
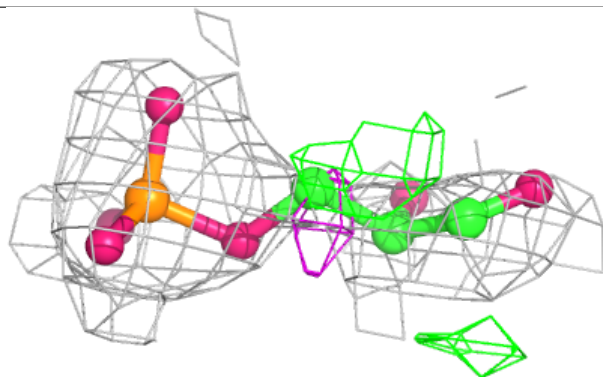
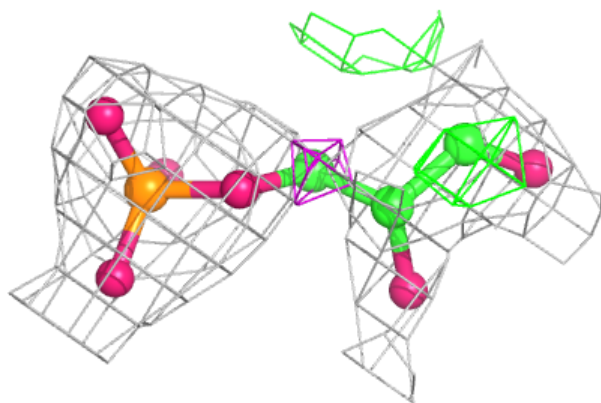
Electron density around PO4 O 403:

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

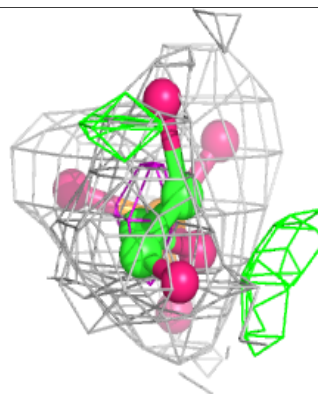
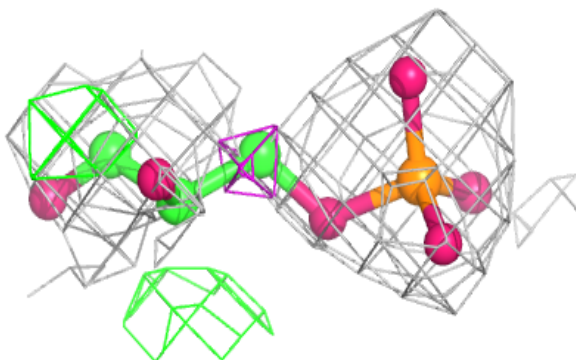
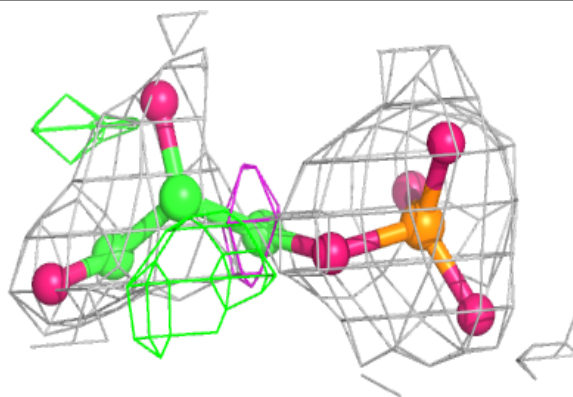


Electron density around G3H Q 402 (A):

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

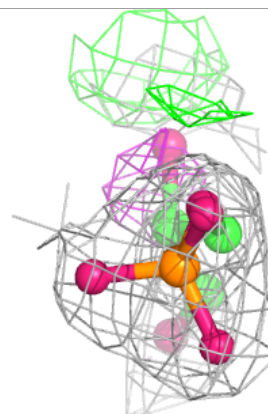
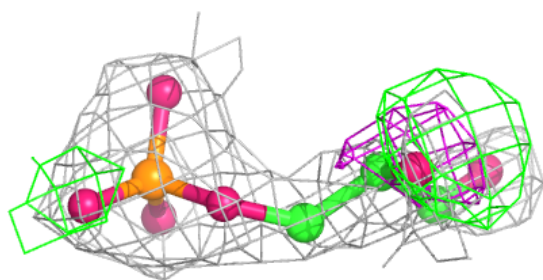
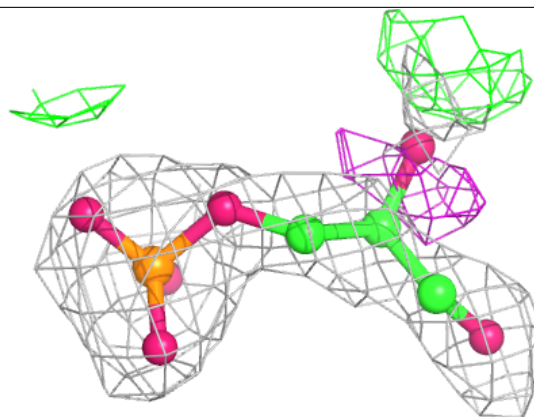
**Electron density around G3H Q 402 (B):**

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

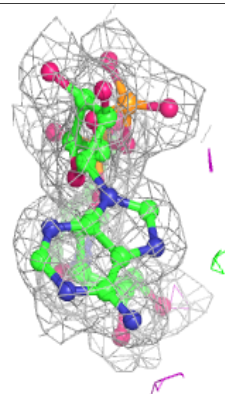
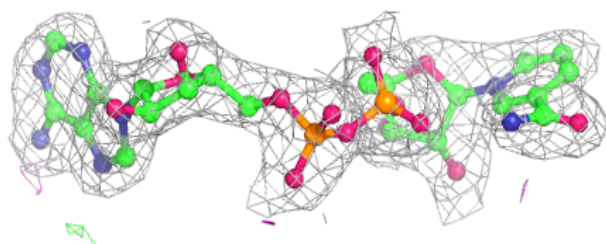
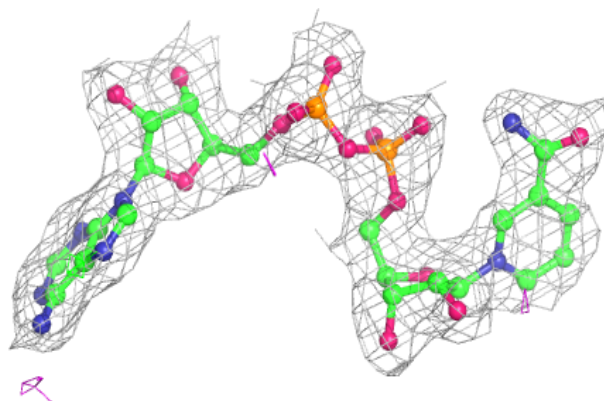


Electron density around G3H R 402:

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

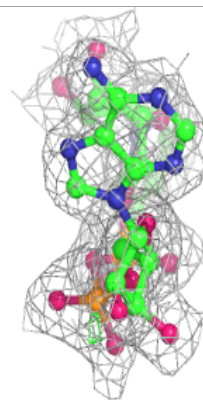
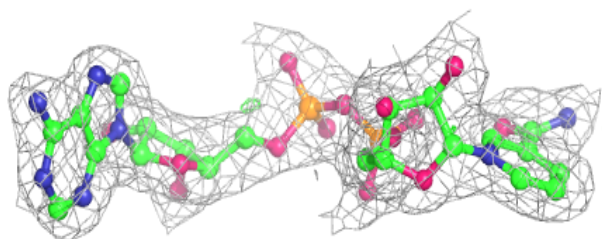
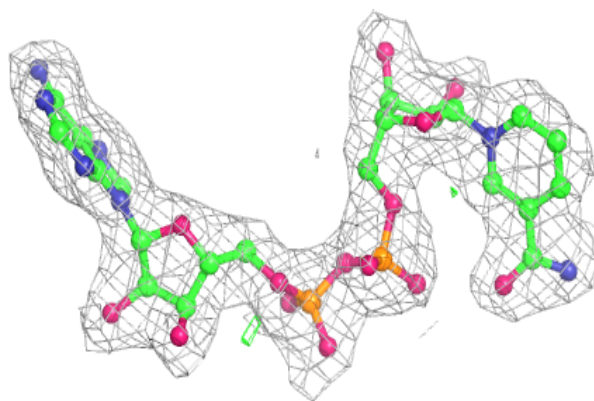
**Electron density around NAD P 401:**

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

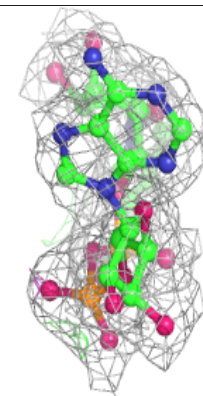
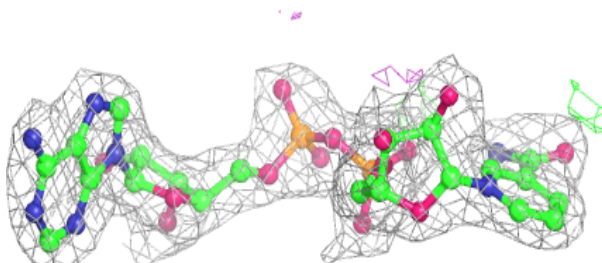
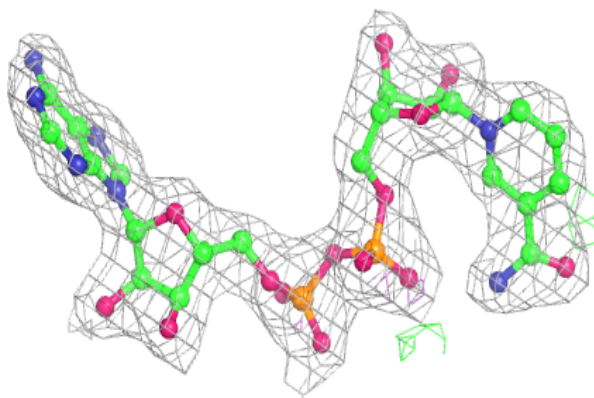


Electron density around NAD Q 401:

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

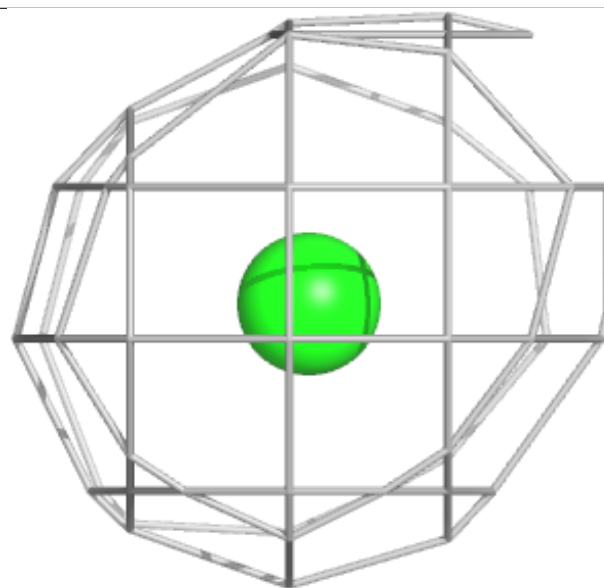
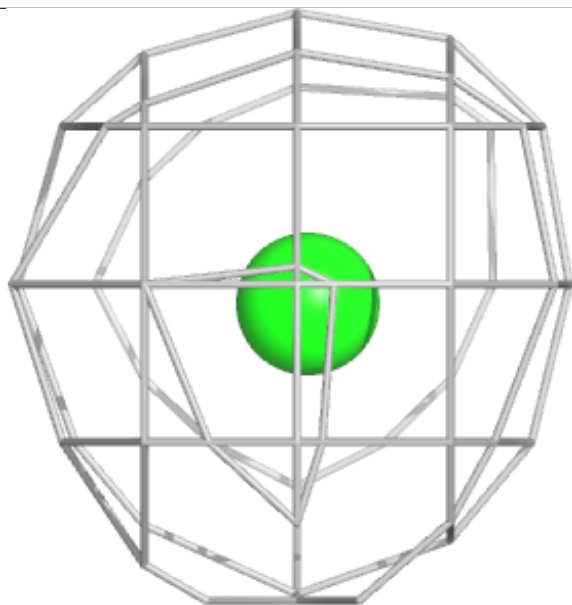
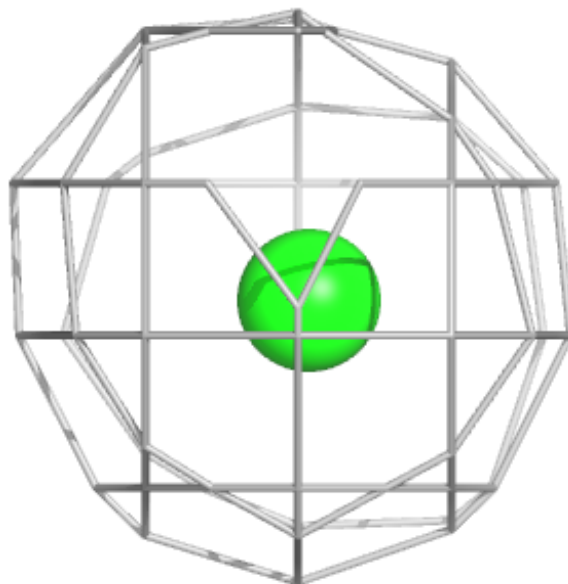
**Electron density around NAD R 401:**

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



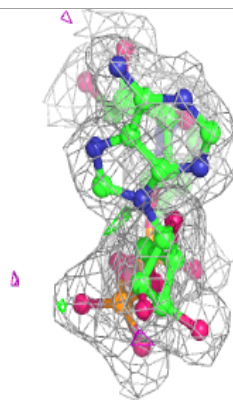
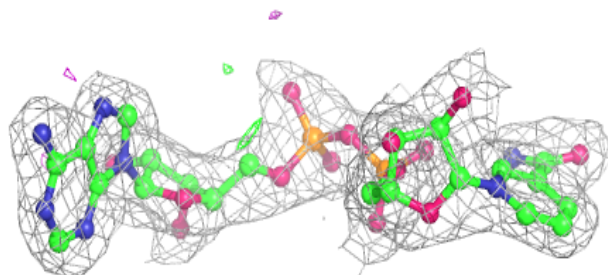
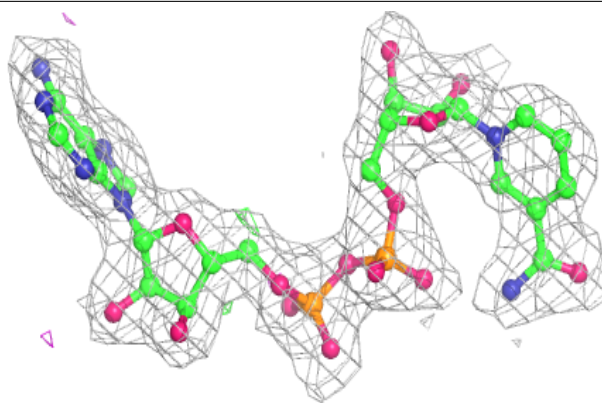
Electron density around CL P 405:

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



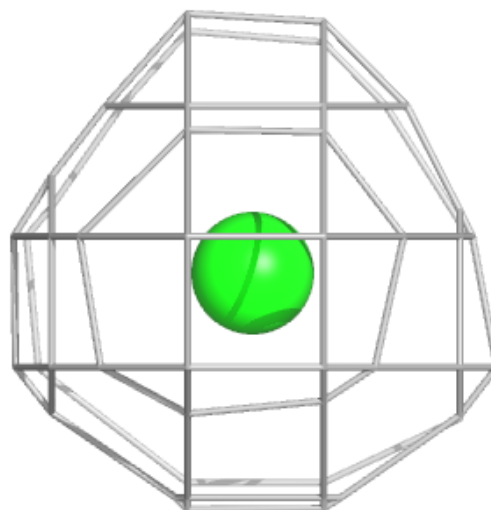
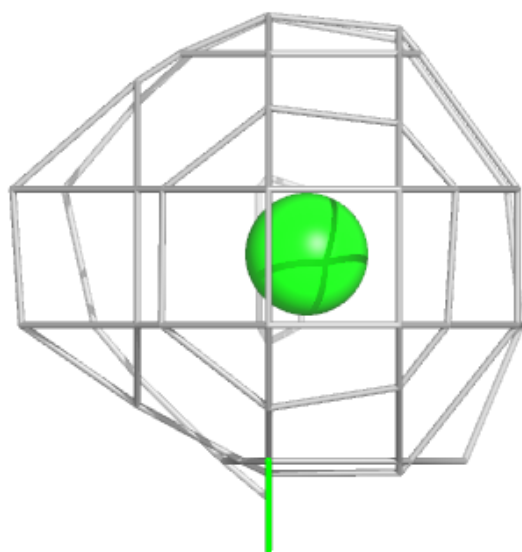
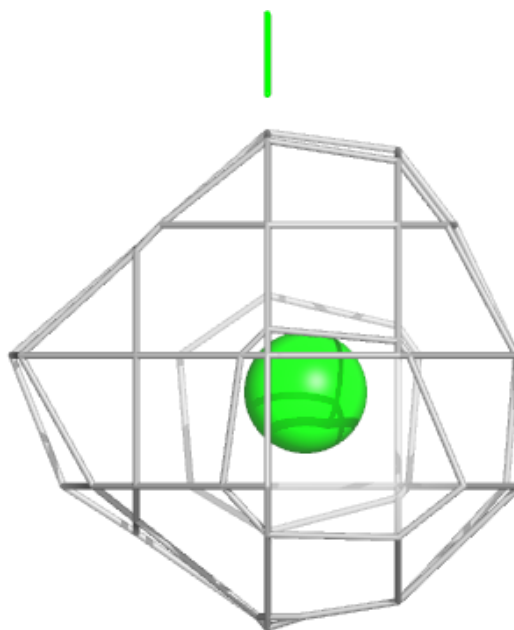
Electron density around NAD O 401:

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



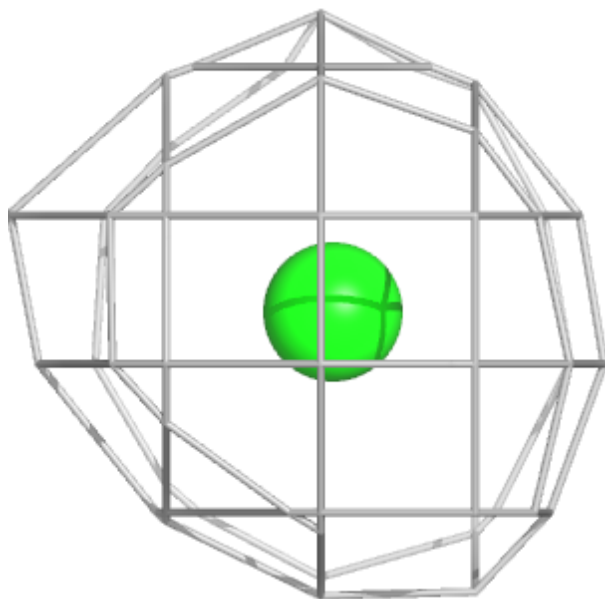
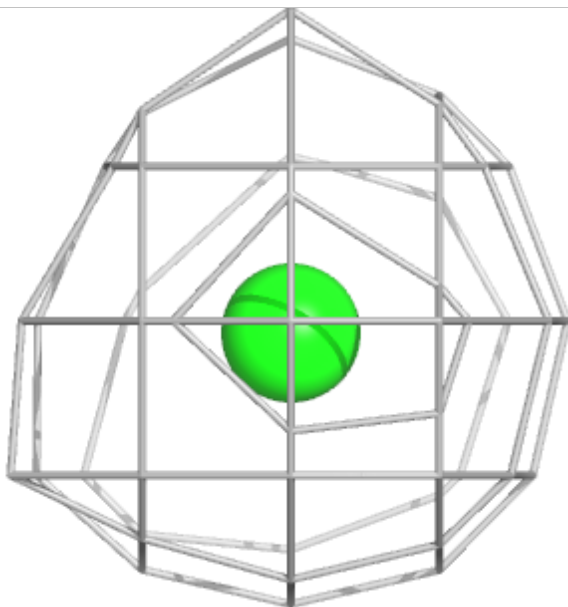
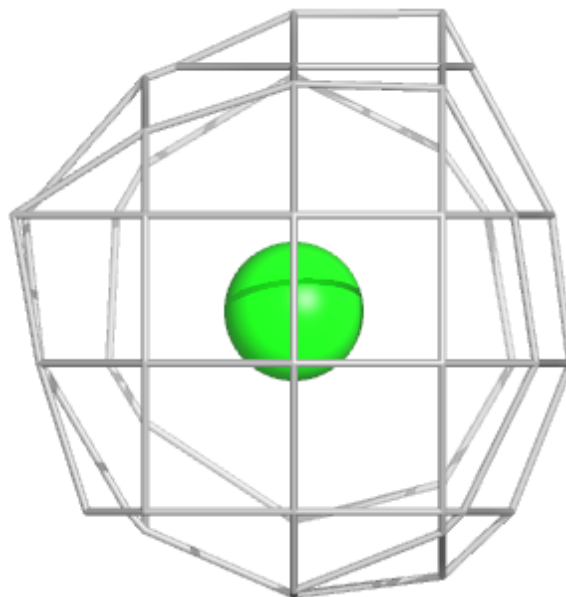
Electron density around CL O 408:

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



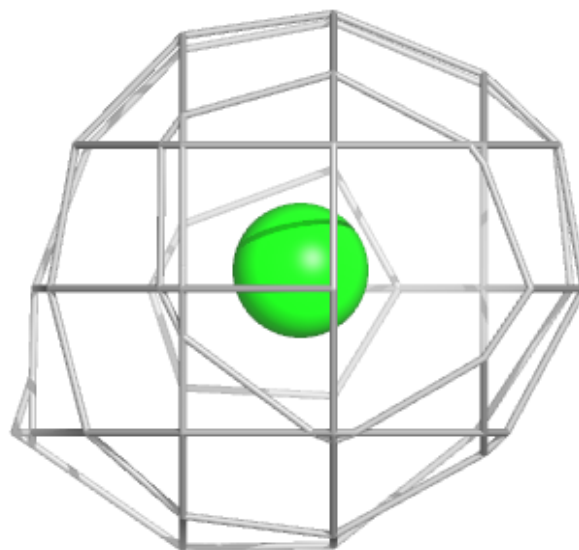
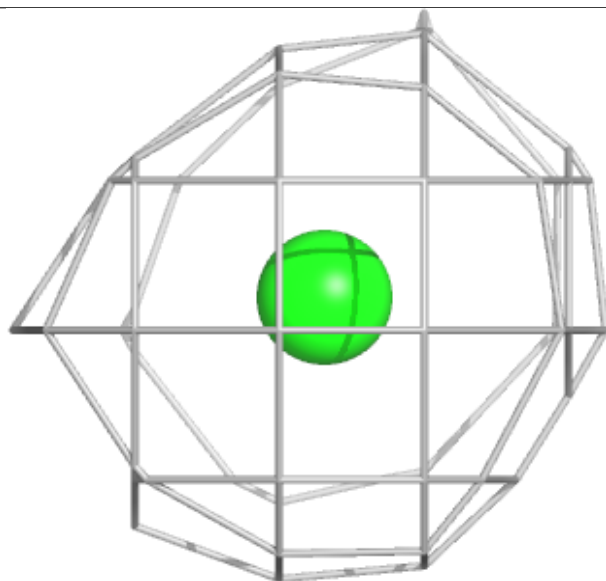
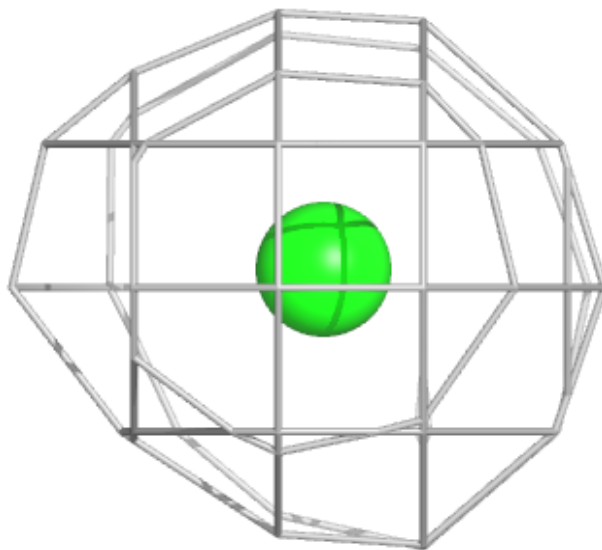
Electron density around CL O 406:

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



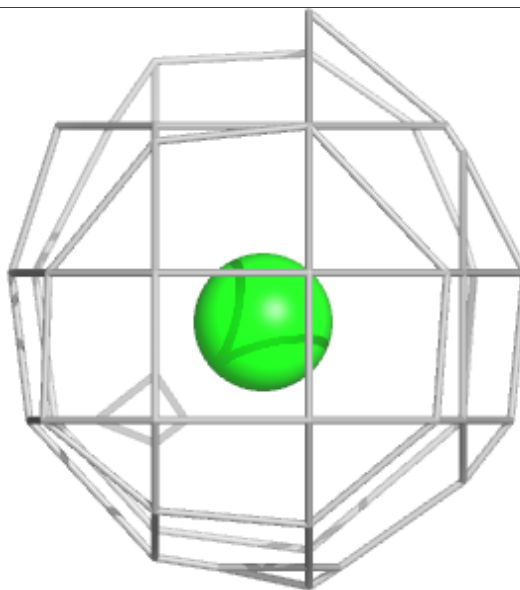
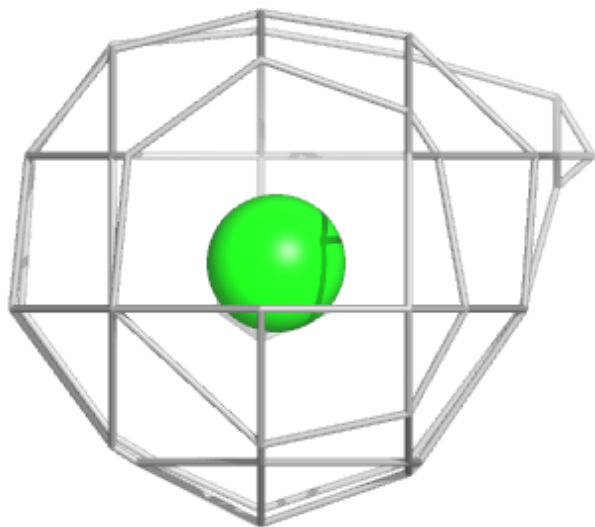
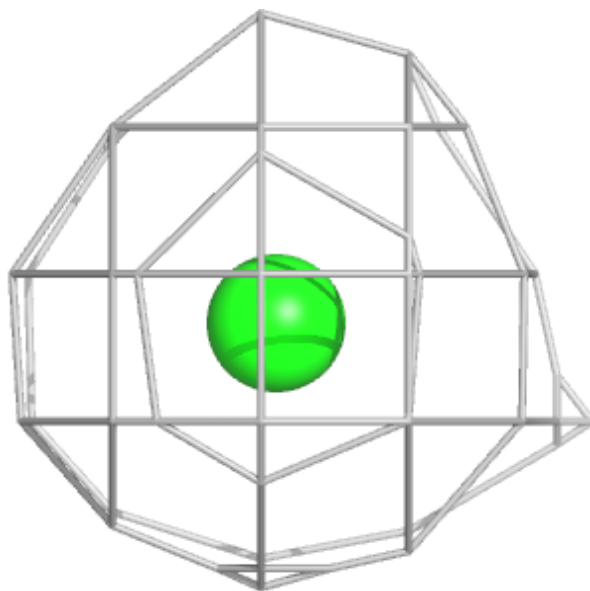
Electron density around CL O 407:

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



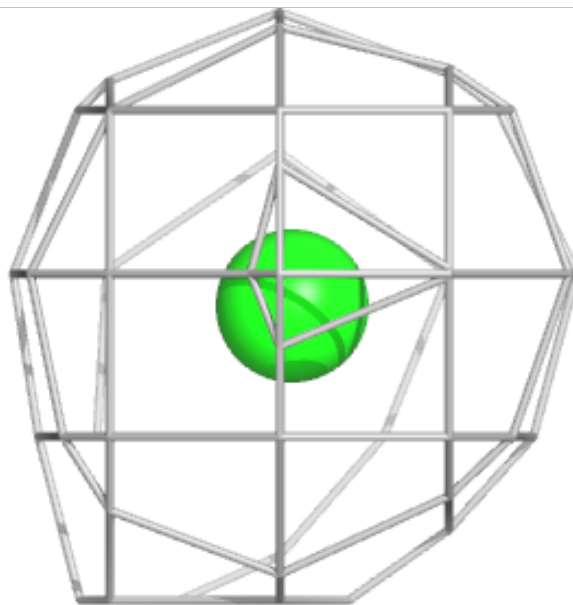
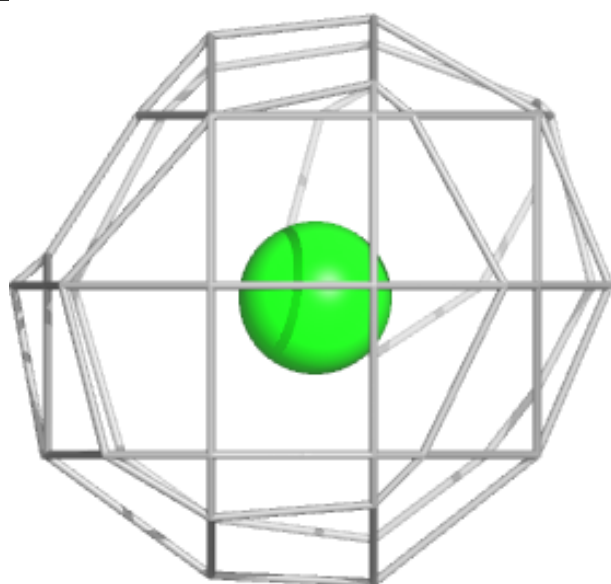
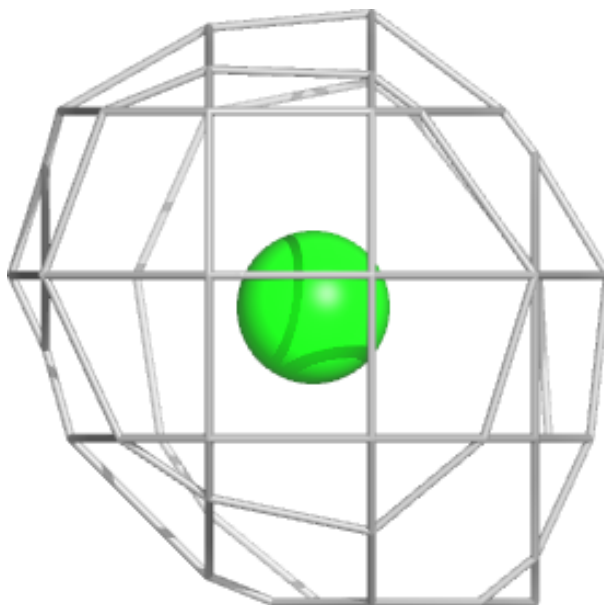
Electron density around CL Q 406:

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



Electron density around CL Q 407:

$2mF_o-DF_c$ (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.