



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2026 – 12:10 AM JST

PDB ID : 27LJ / pdb_000027lj
Title : the structure of cis-isoeugenol synthase AtaIGS1 mutant
Authors : Long, G.F.; Wang, G.Q.
Deposited on : 2026-06-04
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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

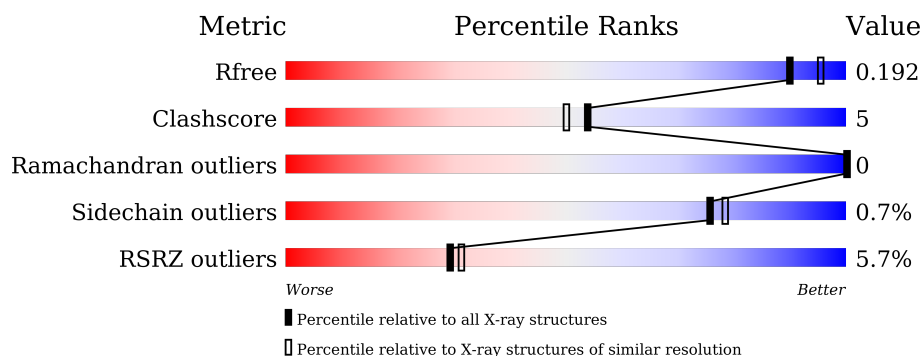
1 Overall quality at a glance

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	312	6% 88% 10% .
1	B	312	5% 93% 5% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	405	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5502 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.

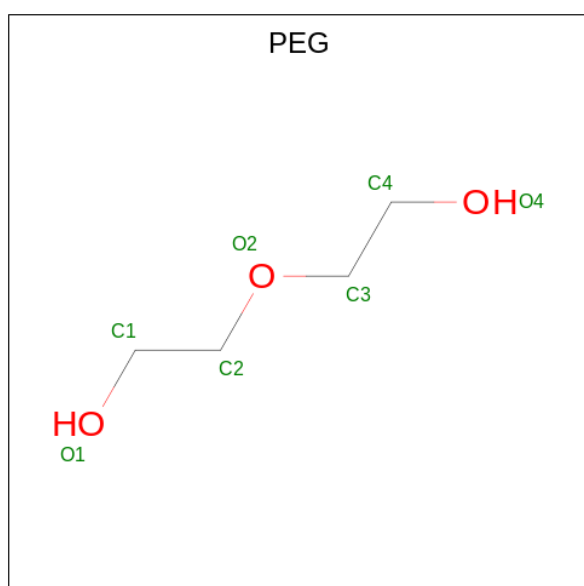
- Molecule 1 is a protein called Isoeugenol synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2404	1531	415	451	7			
1	B	306	Total	C	N	O	S	0	0	0
			2404	1531	415	451	7			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cl	0	0
			4	4		
2	B	5	Total	Cl	0	0
			5	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).

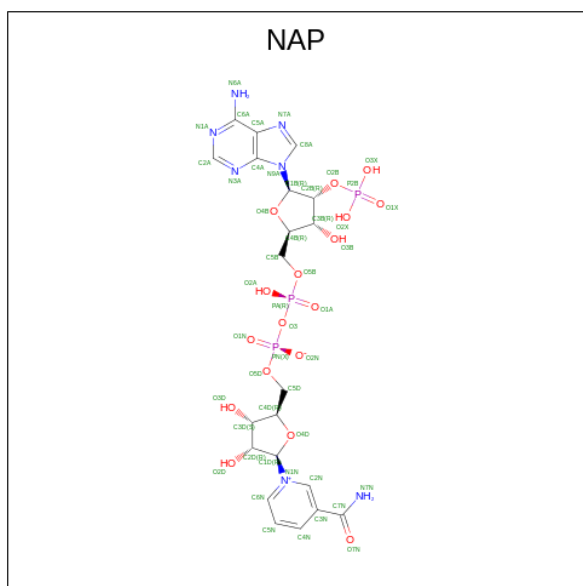


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

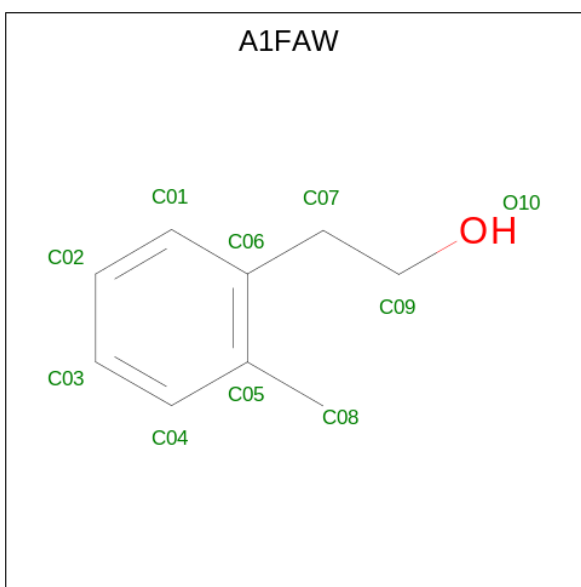
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



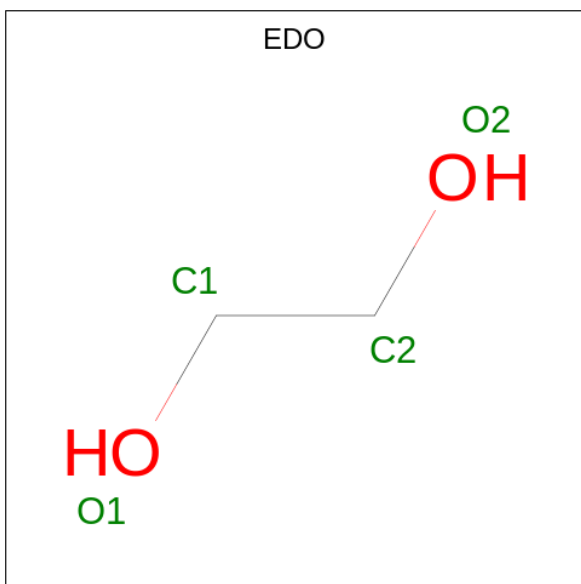
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is 2-(2-methylphenyl)ethanol (CCD ID: A1FAW) (formula: C₉H₁₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	9	1		
6	B	1	Total	C	O	0	0
			10	9	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

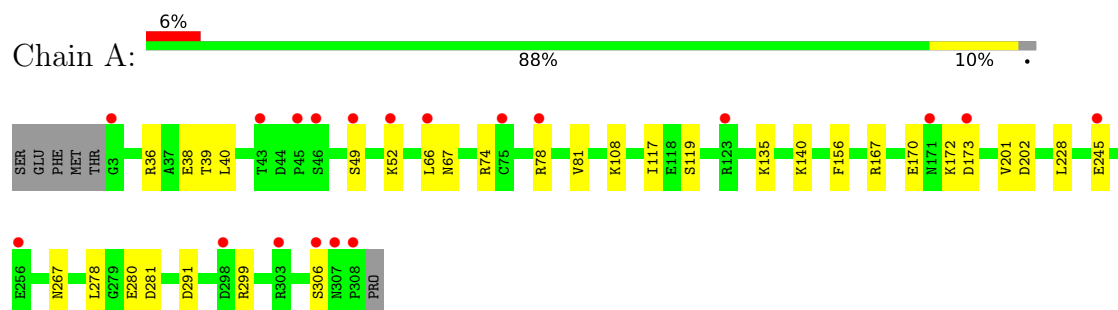
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	281	Total 281	O 281	0	0
8	B	275	Total 275	O 275	0	0

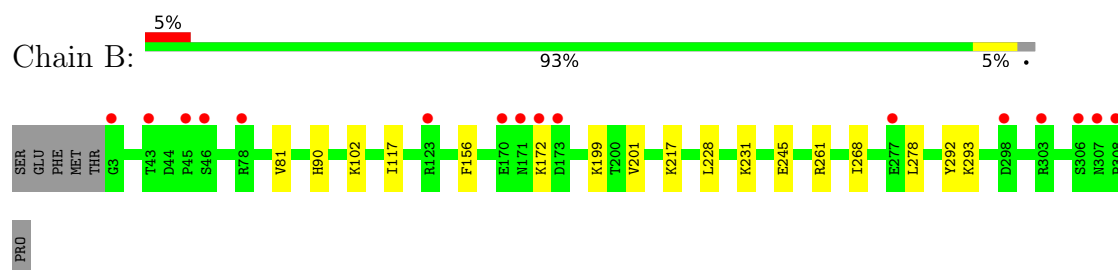
3 Residue-property plots

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: Isoeugenol synthase 1



• Molecule 1: Isoeugenol synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.26Å 177.57Å 71.53Å 90.00° 94.06° 90.00°	Depositor
Resolution (Å)	41.16 – 1.90 41.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.16-1.90) 99.5 (41.16-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, R_{free}	0.168 , 0.192 0.168 , 0.192	Depositor DCC
R_{free} test set	1993 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5502	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: NAP, NA, CL, PEG, EDO, A1FAW

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	0.82	0/2447	0.79	1/3312 (0.0%)
1	B	0.80	0/2447	0.75	0/3312
All	All	0.81	0/4894	0.77	1/6624 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	GLU	CA-CB-CG	-9.82	94.46	114.10

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	2404	0	2460	28	0
1	B	2404	0	2460	14	0
2	A	4	0	0	1	0
2	B	5	0	0	4	0
3	A	7	0	10	0	0
4	A	2	0	0	0	0
5	A	48	0	24	2	0
5	B	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	0	2	0
6	B	10	0	0	2	0
7	B	4	0	6	0	0
8	A	281	0	0	13	2
8	B	275	0	0	11	3
All	All	5502	0	4985	49	3

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 5.

All (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)
5:A:408:NAP:O4B	5:A:408:NAP:C1B	1.64	1.23
2:B:405:CL:CL	8:B:686:HOH:O	2.23	0.91
2:B:403:CL:CL	8:B:725:HOH:O	2.25	0.90
2:B:405:CL:CL	8:B:505:HOH:O	2.25	0.89
1:B:231:LYS:NZ	8:B:502:HOH:O	2.05	0.88
1:A:66:LEU:O	8:A:501:HOH:O	1.92	0.86
1:A:49:SER:O	1:A:52:LYS:HE3	1.80	0.80
1:A:38:GLU:OE1	1:A:38:GLU:N	2.15	0.79
2:B:404:CL:CL	8:B:742:HOH:O	2.39	0.77
1:A:78:ARG:NH2	8:A:505:HOH:O	2.23	0.71
1:A:306:SER:HB2	8:A:614:HOH:O	1.94	0.67
1:A:281:ASP:OD1	8:A:502:HOH:O	2.13	0.67
1:B:102:LYS:NZ	8:B:503:HOH:O	2.12	0.64
1:A:117:ILE:H	6:A:409:A1FAW:C04	2.13	0.62
1:B:117:ILE:H	6:B:408:A1FAW:C04	2.13	0.61
1:B:261:ARG:NH1	8:B:505:HOH:O	2.34	0.61
1:A:117:ILE:H	6:A:409:A1FAW:C03	2.15	0.59
1:B:199:LYS:HE3	1:B:292:TYR:HB2	1.84	0.59
1:B:117:ILE:H	6:B:408:A1FAW:C03	2.18	0.56
1:A:173:ASP:OD1	8:A:503:HOH:O	2.18	0.56
1:B:217:LYS:NZ	8:B:501:HOH:O	2.01	0.55
1:A:140:LYS:HE2	8:A:620:HOH:O	2.07	0.53
1:A:49:SER:C	1:A:52:LYS:HE3	2.33	0.52
1:A:49:SER:CA	1:A:52:LYS:HE3	2.39	0.52
1:B:90:HIS:HD2	8:B:639:HOH:O	1.93	0.52
1:A:202:ASP:OD2	8:A:504:HOH:O	2.18	0.51
1:A:67:ASN:HA	8:A:501:HOH:O	2.09	0.51
1:A:81:VAL:HG21	1:A:201:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:OG1	5:A:408:NAP:O2X	2.23	0.48
2:A:404:CL:CL	8:A:714:HOH:O	2.57	0.48
1:A:167:ARG:CZ	1:A:172:LYS:HE2	2.44	0.48
1:A:291:ASP:HB2	8:A:675:HOH:O	2.14	0.48
1:B:172:LYS:HE3	8:B:696:HOH:O	2.13	0.47
1:A:119:SER:OG	1:A:135:LYS:HE3	2.15	0.47
1:A:156:PHE:HZ	1:A:267:ASN:HD22	1.62	0.47
1:B:293:LYS:HA	8:B:707:HOH:O	2.15	0.46
1:A:36:ARG:O	1:A:40:LEU:HD22	2.16	0.46
1:A:299:ARG:HD2	1:A:299:ARG:HA	1.69	0.46
1:A:49:SER:HA	1:A:52:LYS:HE3	1.99	0.45
1:A:74:ARG:NH1	8:A:509:HOH:O	2.40	0.45
5:B:407:NAP:H6N	5:B:407:NAP:H2D	1.83	0.45
1:B:172:LYS:HA	1:B:172:LYS:HD2	1.61	0.44
1:B:81:VAL:HG21	1:B:201:VAL:HG13	2.00	0.44
1:B:156:PHE:CD1	1:B:268:ILE:HD13	2.52	0.43
1:A:81:VAL:HG21	1:A:201:VAL:CG1	2.48	0.43
1:A:108:LYS:NZ	8:A:514:HOH:O	2.44	0.42
1:A:167:ARG:NE	1:A:170:GLU:OE2	2.42	0.41
1:A:280:GLU:HG2	8:A:648:HOH:O	2.20	0.41
1:B:245:GLU:H	1:B:245:GLU:CD	2.29	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:769:HOH:O	8:B:733:HOH:O[2_545]	2.13	0.07
8:B:556:HOH:O	8:B:727:HOH:O[1_455]	2.13	0.07
8:A:729:HOH:O	8:B:704:HOH:O[2_545]	2.18	0.02

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	304/312 (97%)	300 (99%)	4 (1%)	0	100	100
1	B	304/312 (97%)	300 (99%)	4 (1%)	0	100	100
All	All	608/624 (97%)	600 (99%)	8 (1%)	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	267/273 (98%)	265 (99%)	2 (1%)	76	78
1	B	267/273 (98%)	265 (99%)	2 (1%)	76	78
All	All	534/546 (98%)	530 (99%)	4 (1%)	76	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	LEU
1	A	278	LEU
1	B	228	LEU
1	B	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	307	ASN
1	B	307	ASN

5.3.3 RNA ⓘ

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 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	PEG	A	405	-	6,6,6	0.43	0	5,5,5	0.52	0
5	NAP	A	408	-	49,52,52	3.94	19 (38%)	69,80,80	1.97	15 (21%)
6	A1FAW	B	408	-	10,10,10	0.90	1 (10%)	11,12,12	2.00	3 (27%)
5	NAP	B	407	-	49,52,52	3.81	16 (32%)	69,80,80	1.73	14 (20%)
7	EDO	B	406	-	3,3,3	0.59	0	2,2,2	0.20	0
6	A1FAW	A	409	-	10,10,10	1.04	1 (10%)	11,12,12	1.71	2 (18%)

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
3	PEG	A	405	-	-	3/4/4/4	-
5	NAP	A	408	-	-	9/35/67/67	0/5/5/5
6	A1FAW	B	408	-	-	0/3/3/3	0/1/1/1
5	NAP	B	407	-	-	8/35/67/67	0/5/5/5
7	EDO	B	406	-	-	0/1/1/1	-
6	A1FAW	A	409	-	-	2/3/3/3	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	407	NAP	O4D-C1D	13.67	1.60	1.41
5	A	408	NAP	O4D-C1D	13.67	1.60	1.41
5	B	407	NAP	C2D-C1D	-12.52	1.34	1.53
5	A	408	NAP	C2D-C1D	-12.23	1.35	1.53
5	A	408	NAP	O4B-C1B	9.28	1.64	1.42
5	A	408	NAP	C2B-C1B	-8.16	1.32	1.53
5	A	408	NAP	C7N-N7N	8.05	1.48	1.33
5	B	407	NAP	O4B-C1B	8.01	1.61	1.42
5	B	407	NAP	C7N-N7N	8.00	1.48	1.33
5	B	407	NAP	C2B-C1B	-7.71	1.33	1.53
5	A	408	NAP	C6A-N6A	5.48	1.47	1.34
5	A	408	NAP	P2B-O2B	5.30	1.69	1.59
5	A	408	NAP	O4B-C4B	-5.01	1.33	1.45
5	B	407	NAP	C6A-N6A	4.98	1.46	1.34
5	A	408	NAP	O4D-C4D	-4.55	1.34	1.45
5	B	407	NAP	O4B-C4B	-4.45	1.35	1.45
5	B	407	NAP	O4D-C4D	-4.42	1.35	1.45
5	B	407	NAP	P2B-O2B	3.97	1.66	1.59
5	B	407	NAP	C3N-C7N	3.89	1.56	1.50
5	A	408	NAP	O2D-C2D	3.52	1.51	1.43
5	A	408	NAP	O3B-C3B	-3.04	1.35	1.43
5	A	408	NAP	C3B-C2B	2.99	1.59	1.52
5	B	407	NAP	C3B-C2B	2.95	1.59	1.52
5	A	408	NAP	C3N-C7N	2.85	1.54	1.50
5	B	407	NAP	O2D-C2D	2.67	1.49	1.43
5	B	407	NAP	PA-O5B	2.49	1.69	1.59
5	A	408	NAP	O2B-C2B	2.42	1.52	1.44
5	A	408	NAP	PA-O5B	2.38	1.68	1.59
5	A	408	NAP	C2A-N3A	2.33	1.38	1.33
6	A	409	A1FAW	C06-C05	-2.32	1.36	1.40
5	B	407	NAP	C2N-N1N	2.18	1.37	1.35
6	B	408	A1FAW	C06-C05	-2.16	1.37	1.40
5	A	408	NAP	C2N-C3N	2.11	1.42	1.39
5	A	408	NAP	C8A-N7A	2.08	1.35	1.31
5	B	407	NAP	C8A-N7A	2.05	1.35	1.31
5	B	407	NAP	C6N-C5N	2.04	1.43	1.38
5	A	408	NAP	C6N-C5N	2.01	1.43	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	NAP	C5A-C4A-N3A	-6.61	118.13	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	407	NAP	N3A-C2A-N1A	-5.61	119.82	128.60
5	A	408	NAP	N3A-C2A-N1A	-5.41	120.13	128.60
5	B	407	NAP	C5A-C4A-N3A	-5.35	119.77	126.75
6	B	408	A1FAW	C07-C06-C05	-5.28	116.32	121.83
5	A	408	NAP	N9A-C8A-N7A	-4.31	108.02	113.91
6	A	409	A1FAW	C07-C06-C05	-4.19	117.45	121.83
5	A	408	NAP	C2A-N3A-C4A	4.10	121.43	111.75
5	A	408	NAP	C6N-N1N-C2N	-4.09	118.24	121.97
5	A	408	NAP	C5A-N7A-C8A	4.05	109.27	103.51
5	A	408	NAP	N3A-C4A-N9A	3.94	133.57	127.08
5	B	407	NAP	N9A-C8A-N7A	-3.87	108.61	113.91
5	B	407	NAP	N3A-C4A-N9A	3.75	133.27	127.08
5	B	407	NAP	C2A-N3A-C4A	3.28	119.49	111.75
5	B	407	NAP	O4D-C1D-C2D	-3.23	102.20	106.93
5	A	408	NAP	C3D-C2D-C1D	3.23	105.84	100.98
5	A	408	NAP	O4B-C1B-C2B	-3.17	101.01	106.57
5	A	408	NAP	C6A-C5A-C4A	2.88	121.06	117.18
5	A	408	NAP	C4A-C5A-N7A	-2.83	107.17	110.62
6	B	408	A1FAW	C08-C05-C06	-2.62	118.84	121.99
5	B	407	NAP	C5A-N7A-C8A	2.61	107.22	103.51
5	A	408	NAP	N6A-C6A-N1A	-2.58	112.70	118.35
5	B	407	NAP	C6A-C5A-C4A	2.57	120.64	117.18
5	B	407	NAP	C6N-N1N-C2N	-2.51	119.69	121.97
5	B	407	NAP	PN-O3-PA	-2.44	124.46	132.83
5	B	407	NAP	O4B-C1B-C2B	-2.44	102.30	106.57
5	A	408	NAP	O7N-C7N-N7N	-2.37	119.21	122.58
6	A	409	A1FAW	C08-C05-C06	-2.28	119.25	121.99
5	B	407	NAP	C4A-N9A-C1B	-2.20	121.35	126.59
5	B	407	NAP	C4A-N9A-C8A	2.18	108.09	105.73
5	A	408	NAP	C5A-C4A-N9A	2.16	108.30	105.78
5	A	408	NAP	O4D-C1D-C2D	-2.11	103.85	106.93
5	B	407	NAP	C3D-C2D-C1D	2.01	104.00	100.98
6	B	408	A1FAW	C07-C06-C01	2.01	123.76	119.37

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	408	NAP	C5B-O5B-PA-O3
5	A	408	NAP	O4D-C1D-N1N-C2N
5	A	408	NAP	O4D-C1D-N1N-C6N
5	A	408	NAP	C2D-C1D-N1N-C2N

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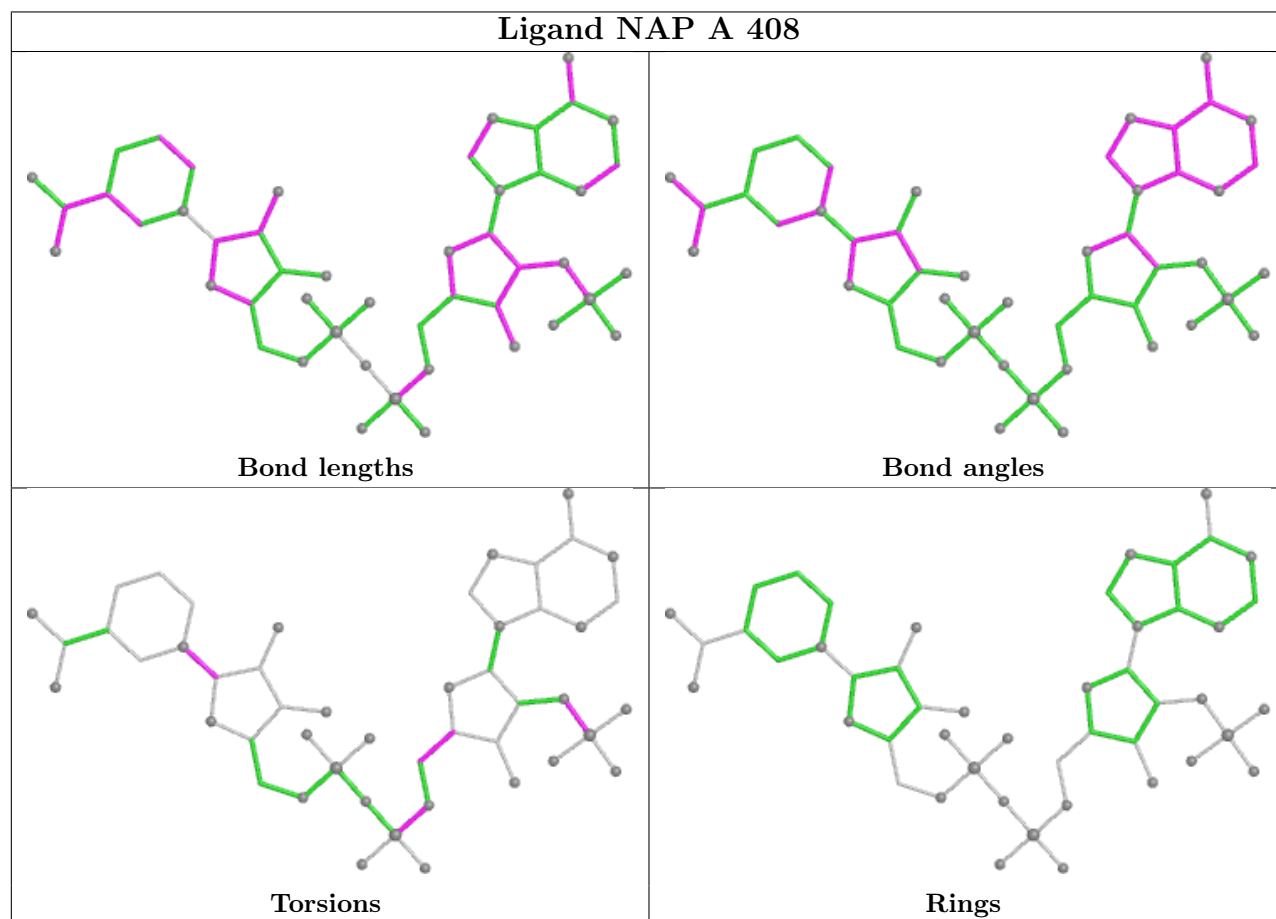
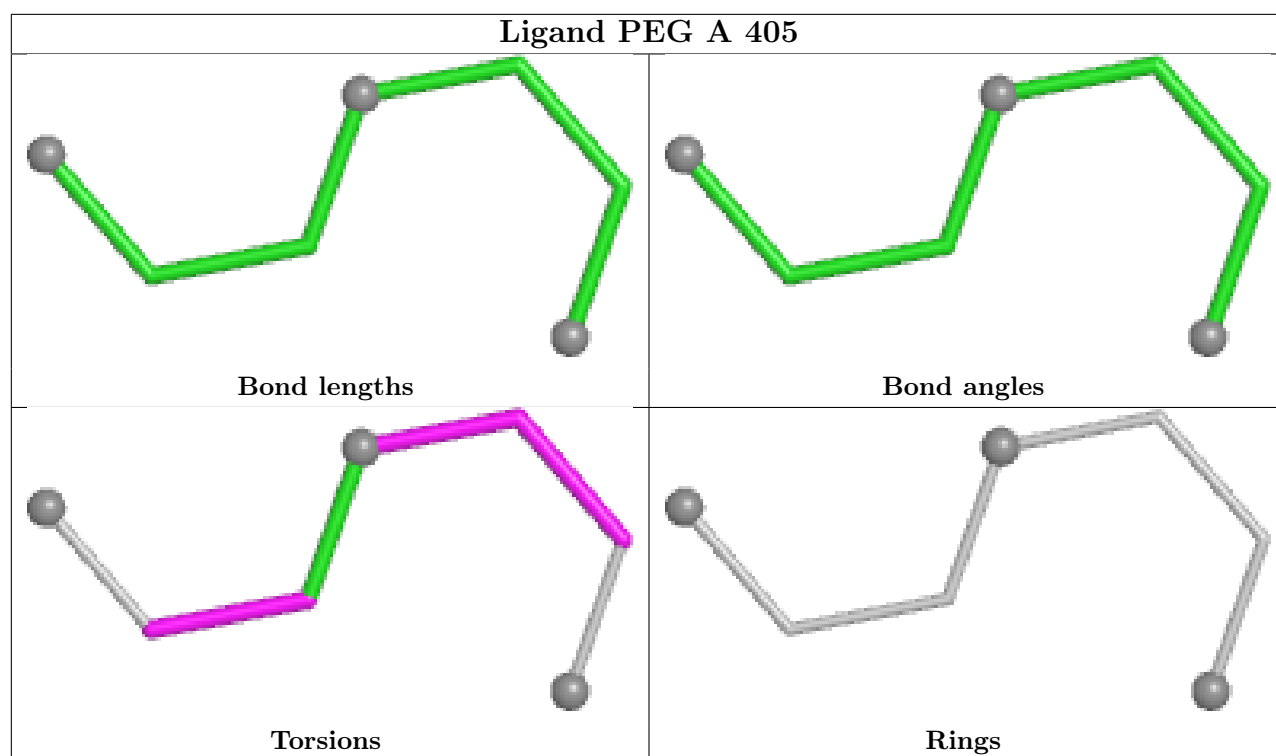
Mol	Chain	Res	Type	Atoms
5	A	408	NAP	C2D-C1D-N1N-C6N
5	B	407	NAP	O4D-C1D-N1N-C2N
5	B	407	NAP	O4D-C1D-N1N-C6N
5	B	407	NAP	C2D-C1D-N1N-C2N
5	B	407	NAP	C2D-C1D-N1N-C6N
6	A	409	A1FAW	C01-C06-C07-C09
6	A	409	A1FAW	C05-C06-C07-C09
5	A	408	NAP	O4B-C4B-C5B-O5B
3	A	405	PEG	O1-C1-C2-O2
3	A	405	PEG	O2-C3-C4-O4
5	B	407	NAP	C2B-O2B-P2B-O1X
5	A	408	NAP	C2B-O2B-P2B-O1X
5	A	408	NAP	C2B-O2B-P2B-O2X
5	B	407	NAP	C2B-O2B-P2B-O3X
5	B	407	NAP	C5D-O5D-PN-O3
3	A	405	PEG	C4-C3-O2-C2
5	B	407	NAP	O4B-C4B-C5B-O5B
5	A	408	NAP	C5B-O5B-PA-O1A

There are no ring outliers.

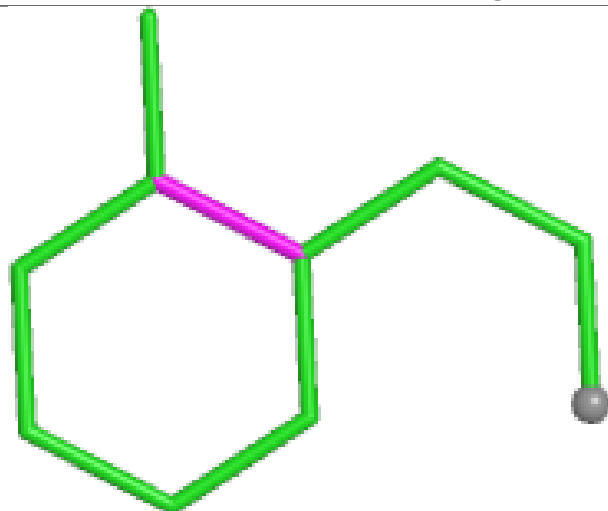
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	NAP	2	0
6	B	408	A1FAW	2	0
5	B	407	NAP	1	0
6	A	409	A1FAW	2	0

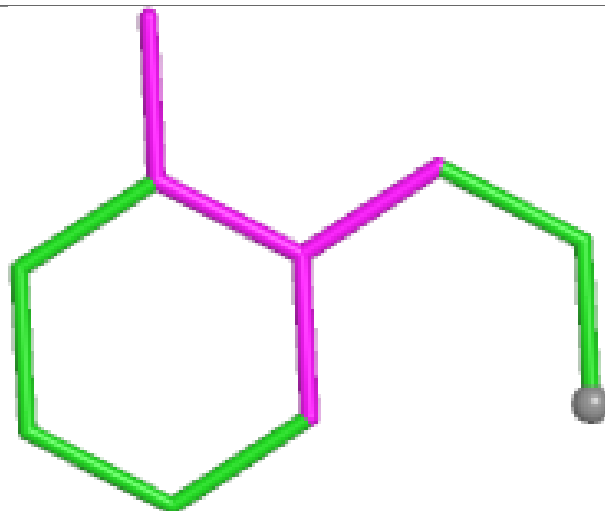
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



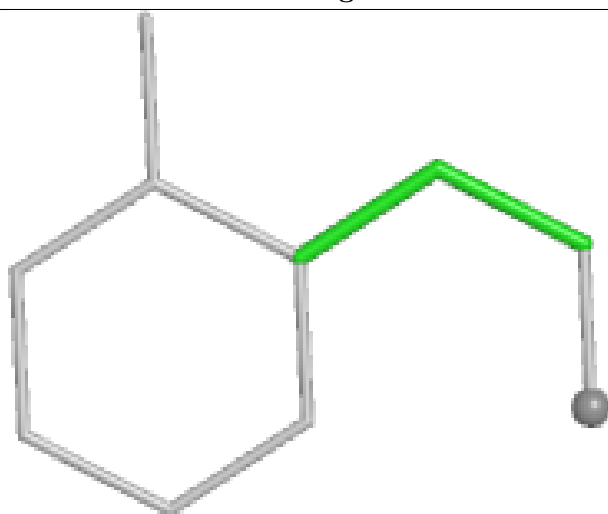
Ligand A1FAW B 408



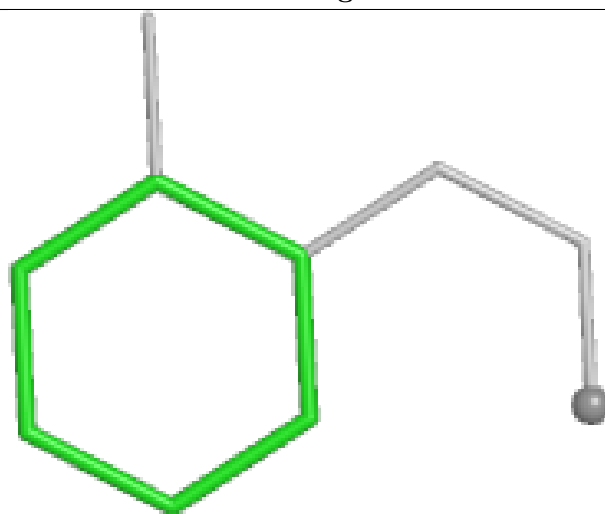
Bond lengths



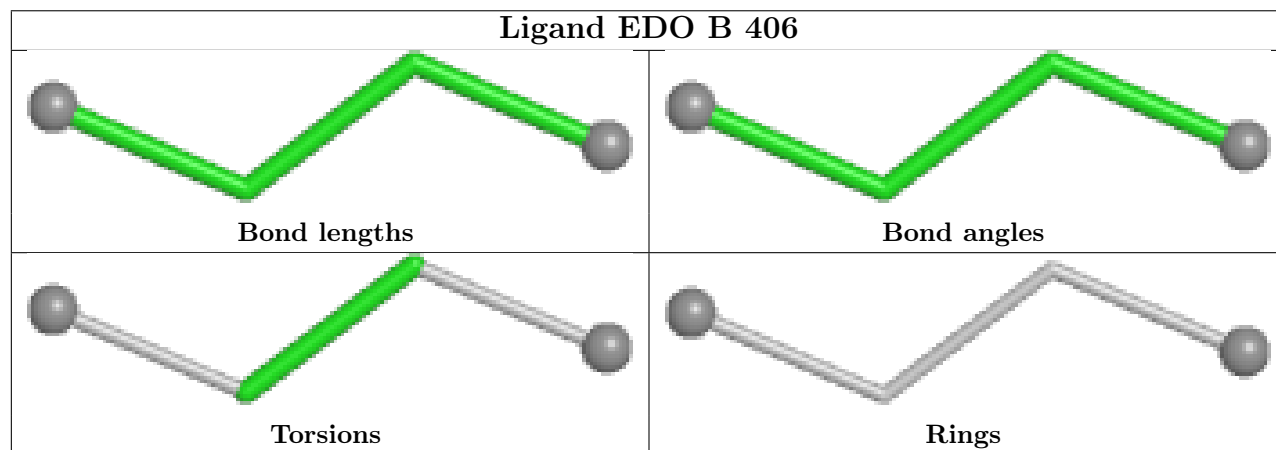
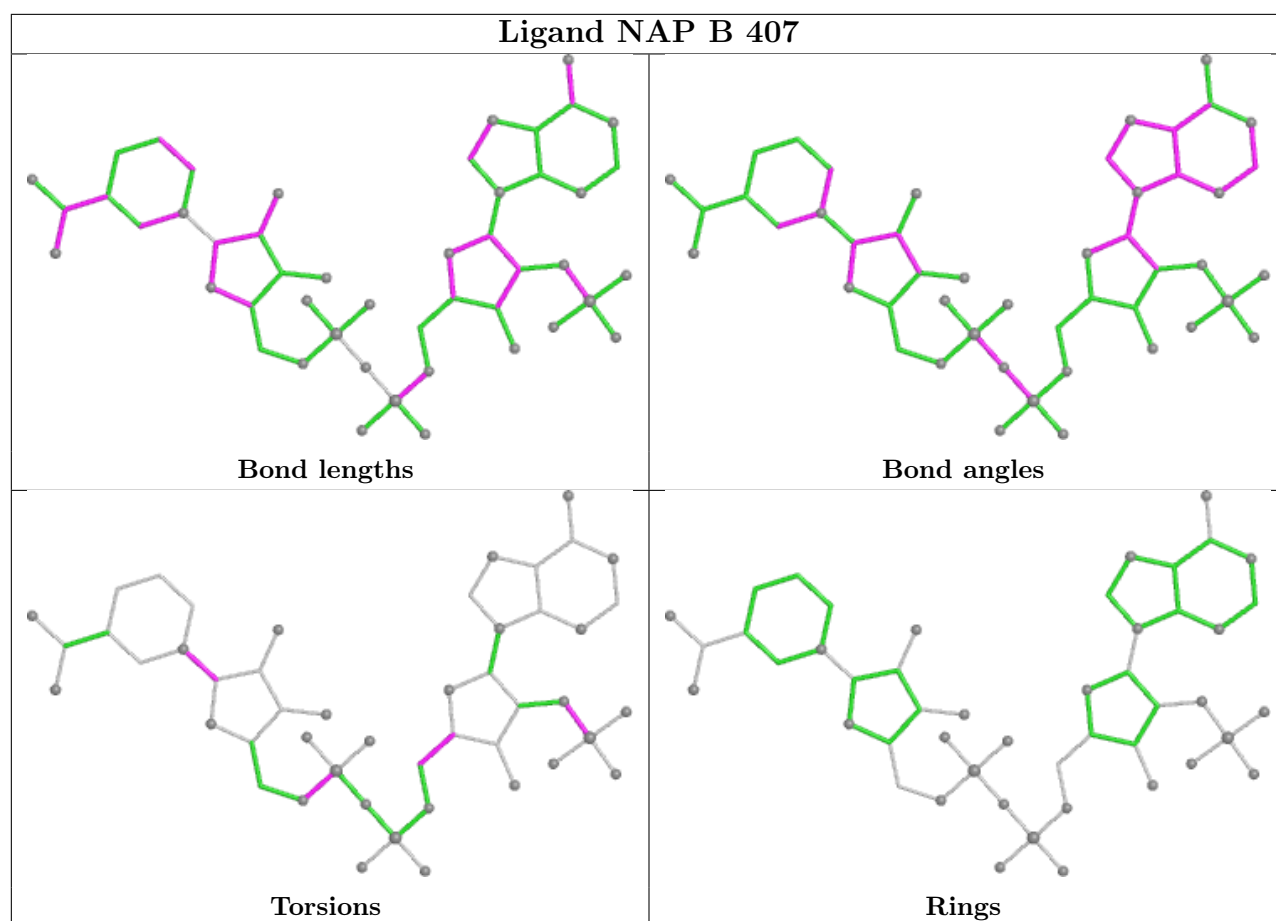
Bond angles

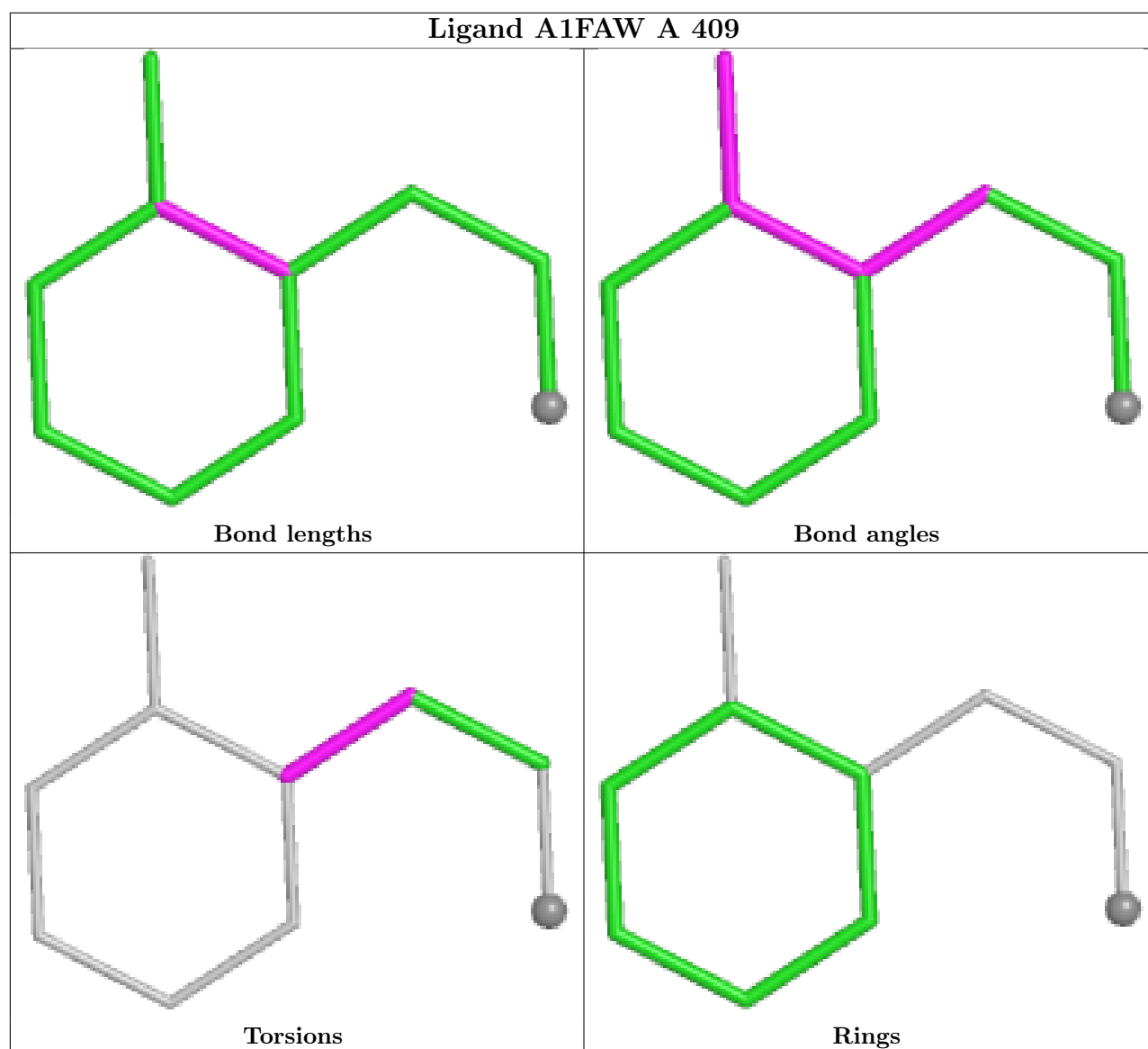


Torsions



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

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	306/312 (98%)	-0.18	19 (6%) 26 28	16, 27, 68, 98	0
1	B	306/312 (98%)	-0.20	16 (5%) 33 35	17, 27, 64, 100	0
All	All	612/624 (98%)	-0.19	35 (5%) 29 31	16, 27, 66, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ASP	4.2
1	A	308	PRO	4.2
1	A	43	THR	3.7
1	B	173	ASP	3.6
1	B	172	LYS	3.5
1	B	298	ASP	3.5
1	B	308	PRO	3.3
1	A	52	LYS	3.3
1	B	43	THR	3.0
1	A	171	ASN	2.9
1	B	307	ASN	2.9
1	A	78	ARG	2.8
1	A	46	SER	2.8
1	B	78	ARG	2.7
1	A	307	ASN	2.7
1	A	245	GLU	2.7
1	A	3	GLY	2.7
1	B	123	ARG	2.6
1	B	171	ASN	2.6
1	B	306	SER	2.5
1	A	123	ARG	2.4
1	B	3	GLY	2.4
1	A	49	SER	2.4
1	A	256	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	75	CYS	2.3
1	A	66	LEU	2.3
1	B	45	PRO	2.2
1	B	46	SER	2.2
1	A	173	ASP	2.2
1	A	45	PRO	2.2
1	B	303	ARG	2.1
1	A	303	ARG	2.1
1	A	306	SER	2.1
1	B	170	GLU	2.0
1	B	277	GLU	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.

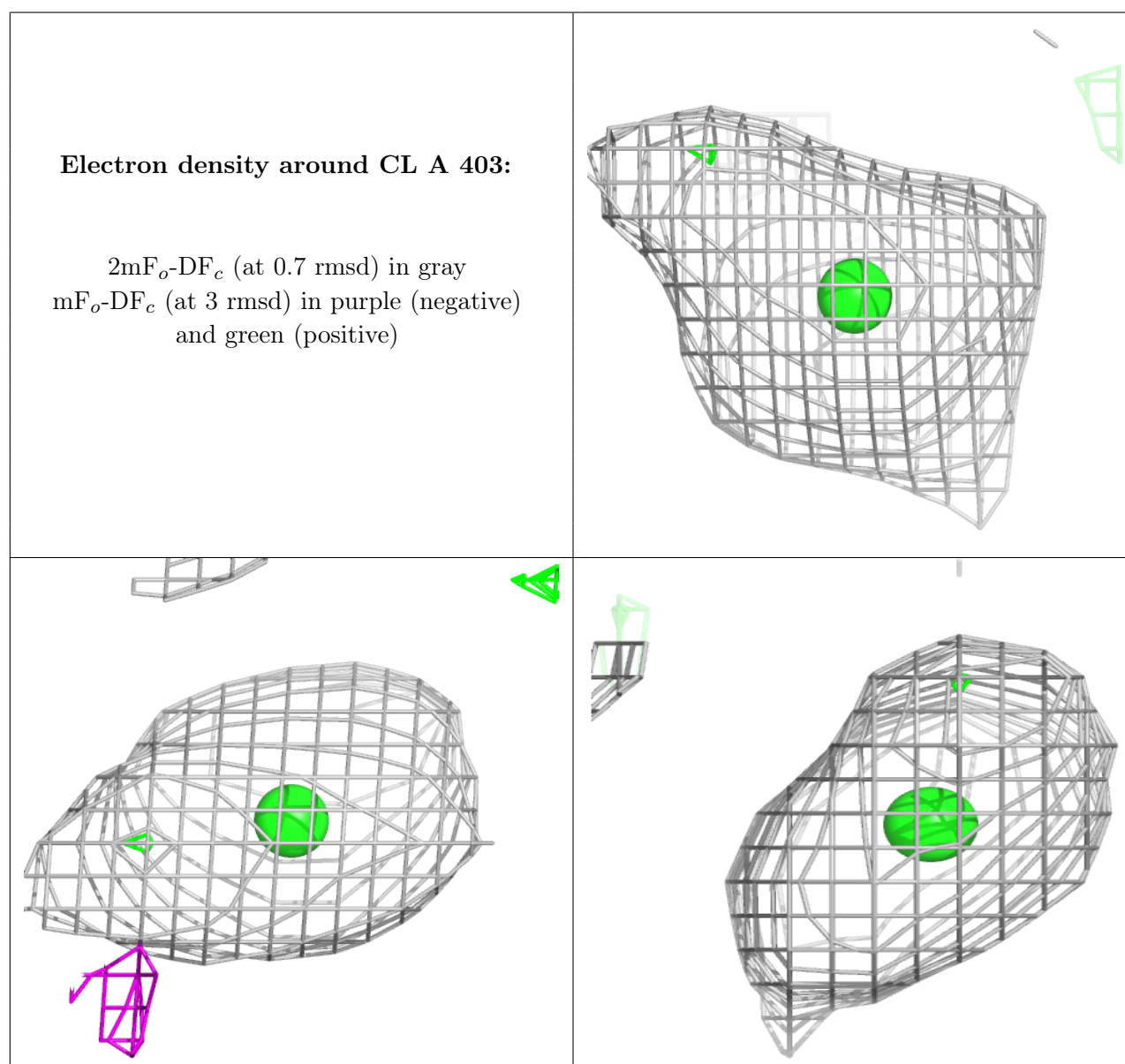
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	403	1/1	0.84	0.13	82,82,82,82	0
2	CL	B	402	1/1	0.84	0.21	78,78,78,78	0
2	CL	B	404	1/1	0.85	0.17	95,95,95,95	0
4	NA	A	406	1/1	0.86	0.19	70,70,70,70	0
2	CL	A	404	1/1	0.88	0.16	78,78,78,78	0
2	CL	A	402	1/1	0.88	0.17	72,72,72,72	0
7	EDO	B	406	4/4	0.89	0.15	50,53,55,55	0
6	A1FAW	B	408	10/10	0.90	0.17	29,45,73,80	0
3	PEG	A	405	7/7	0.91	0.13	54,56,59,59	0
6	A1FAW	A	409	10/10	0.91	0.16	26,53,72,77	0
2	CL	B	403	1/1	0.93	0.11	67,67,67,67	0
4	NA	A	407	1/1	0.94	0.21	49,49,49,49	0

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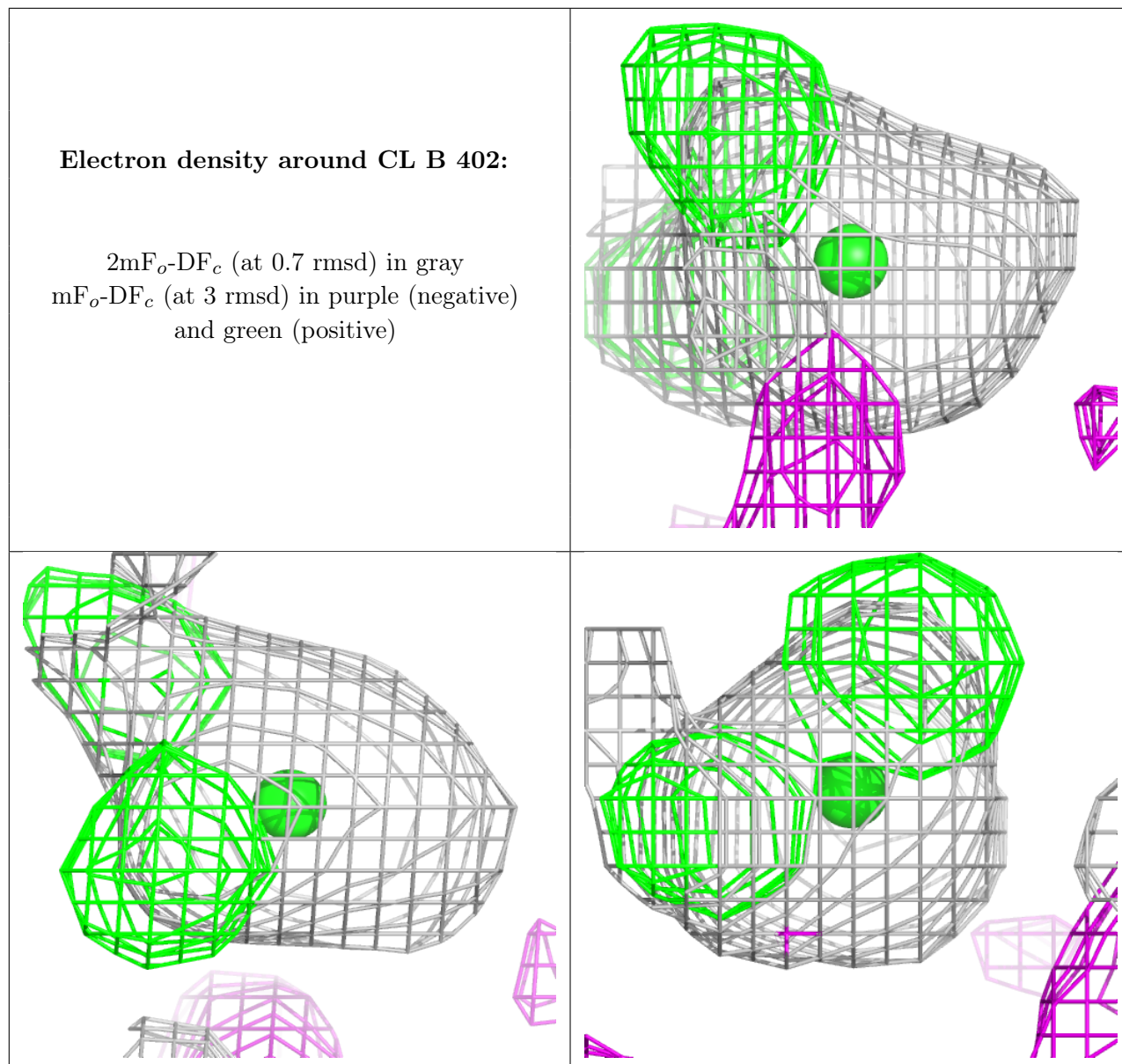
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	401	1/1	0.94	0.15	79,79,79,79	0
5	NAP	A	408	48/48	0.95	0.09	27,42,56,57	0
2	CL	B	405	1/1	0.96	0.14	81,81,81,81	0
2	CL	B	401	1/1	0.96	0.15	80,80,80,80	0
5	NAP	B	407	48/48	0.97	0.07	22,33,39,40	0

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.



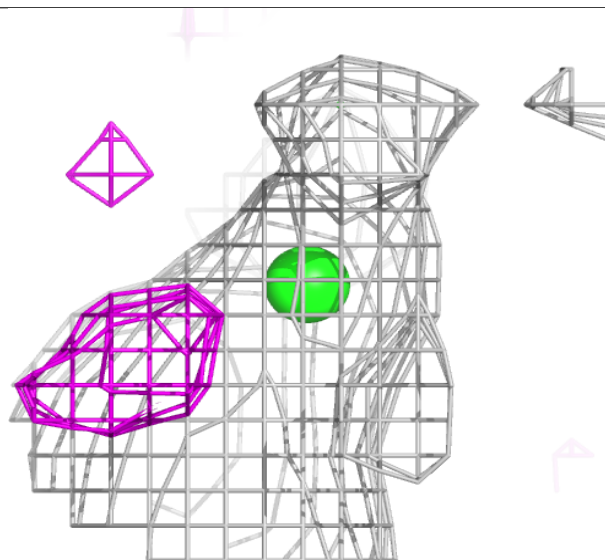
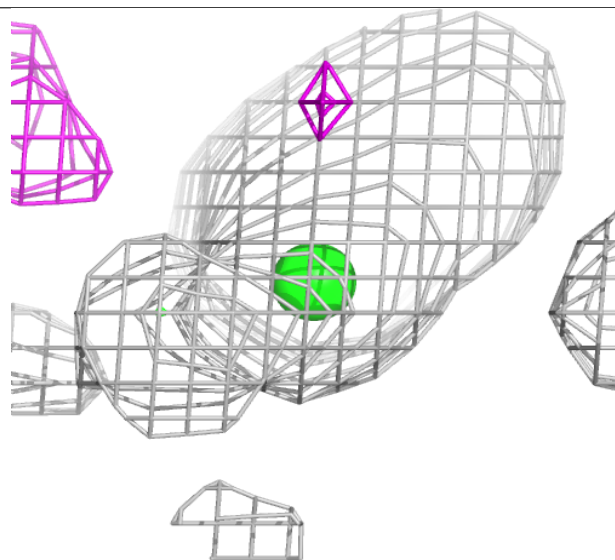
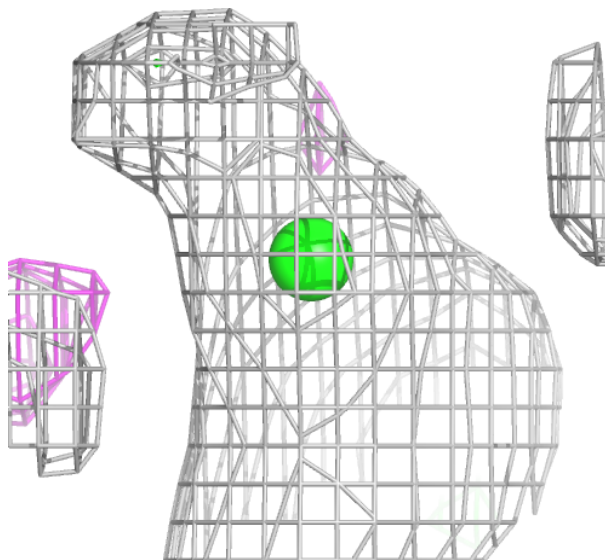
Electron density around CL B 402:

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



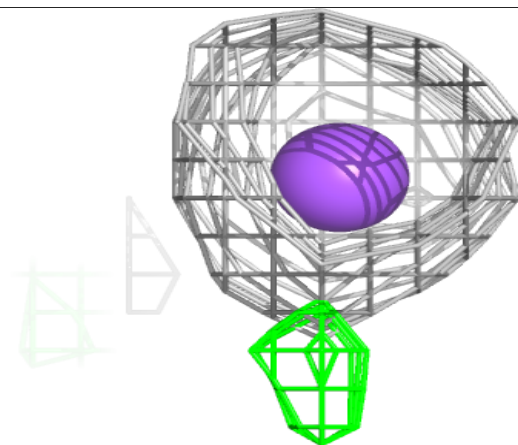
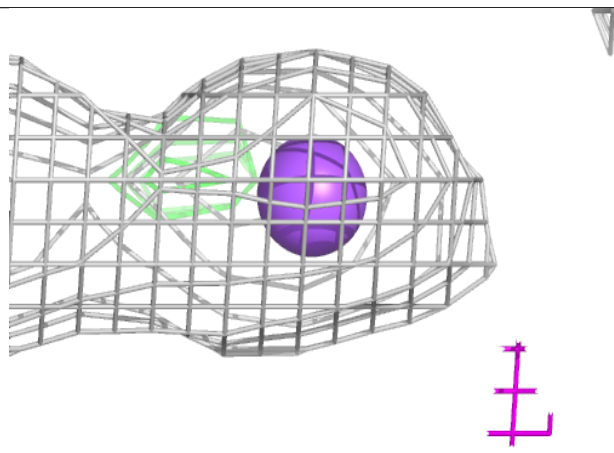
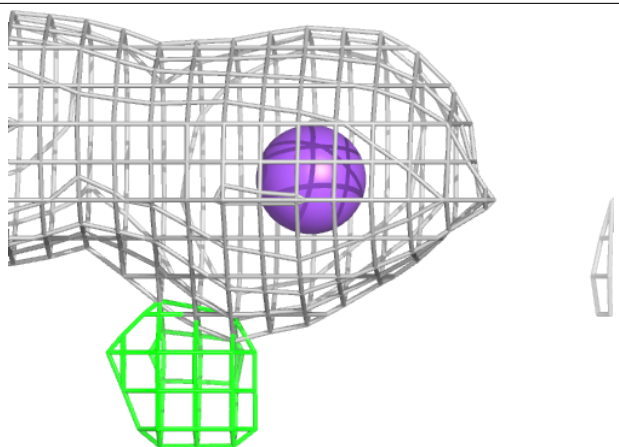
Electron density around CL B 404:

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



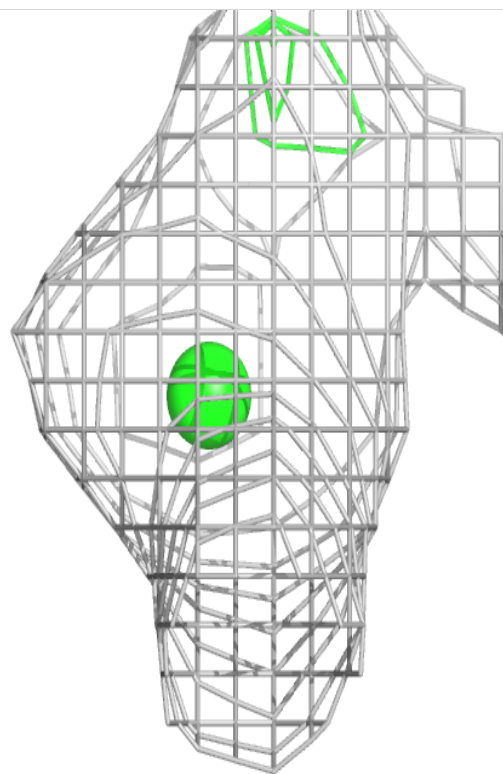
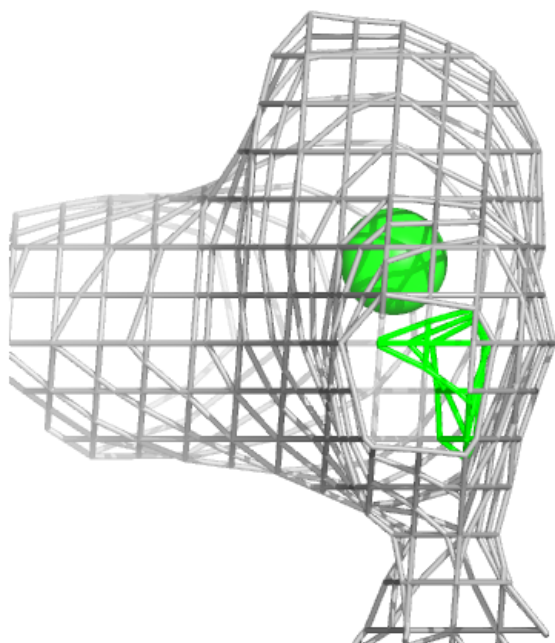
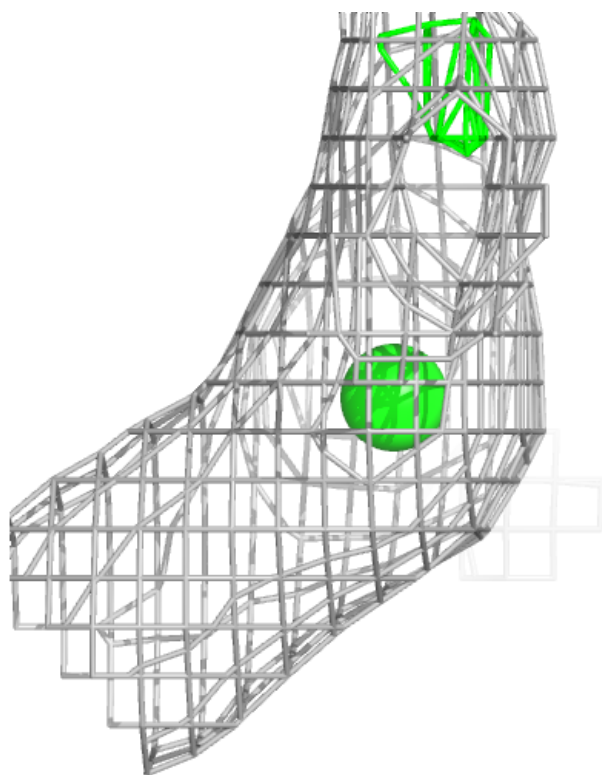
Electron density around NA A 406:

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



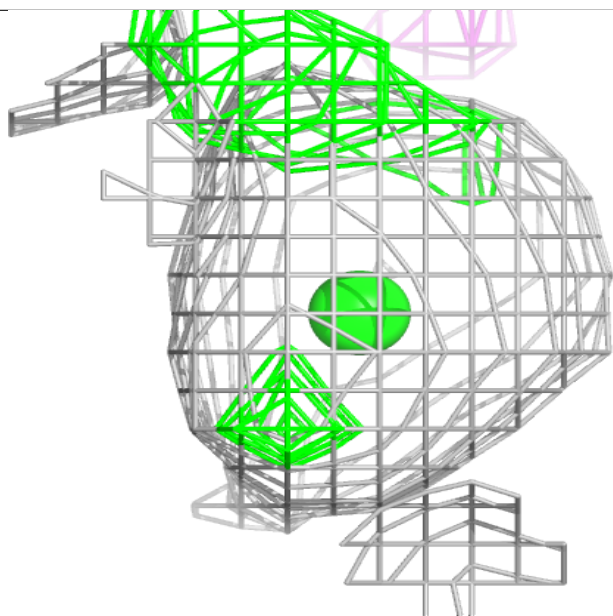
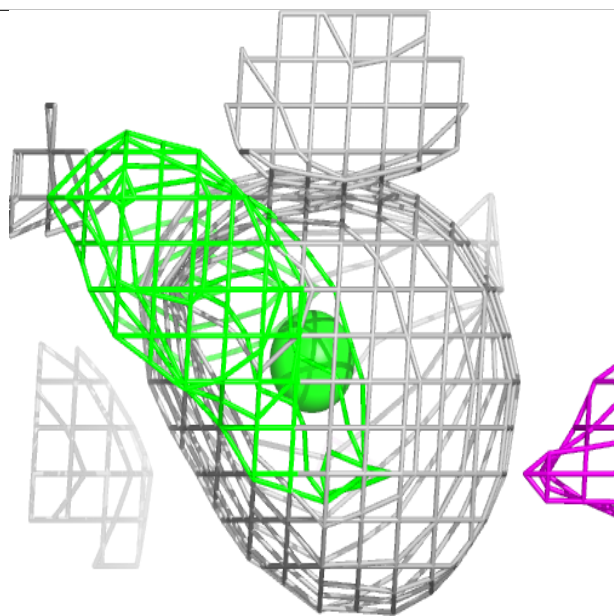
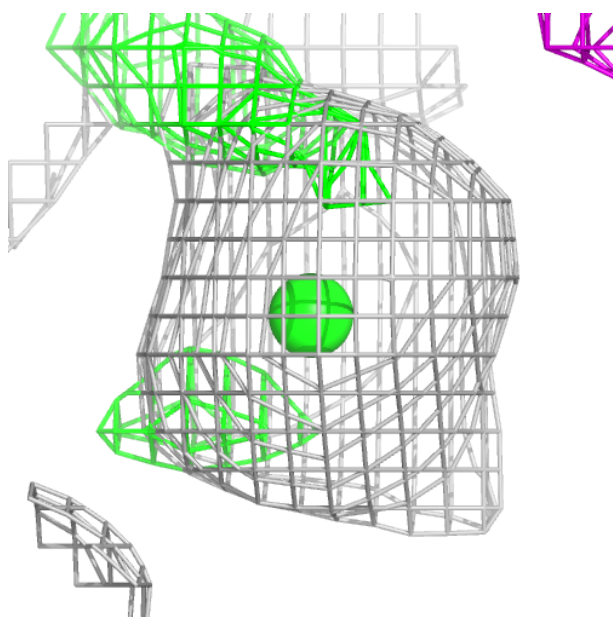
Electron density around CL A 404:

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



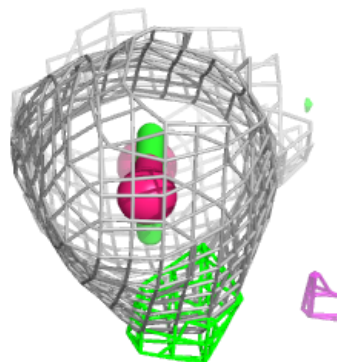
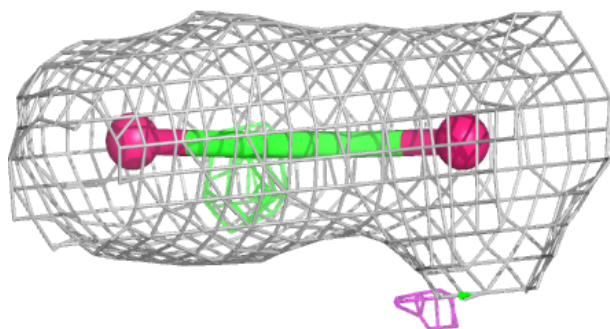
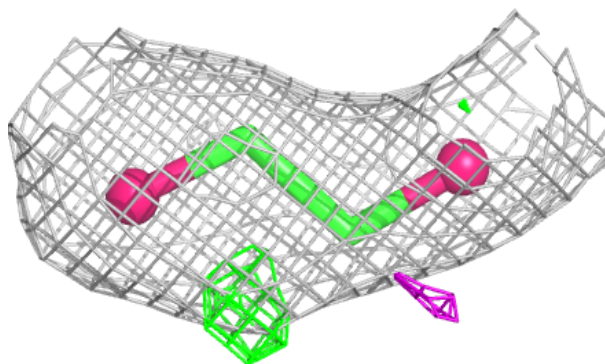
Electron density around CL A 402:

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



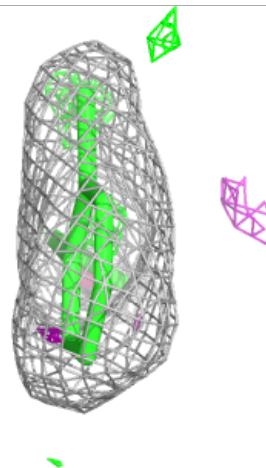
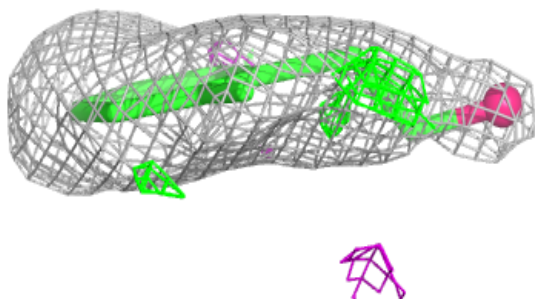
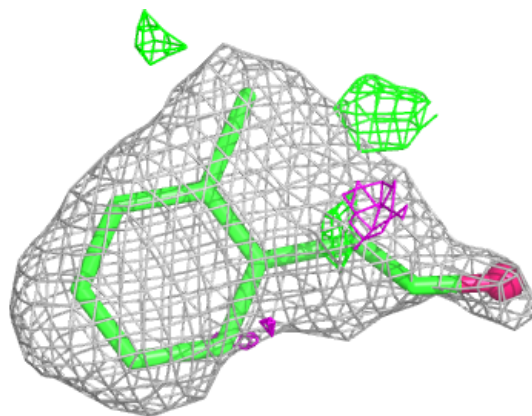
Electron density around EDO B 406:

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



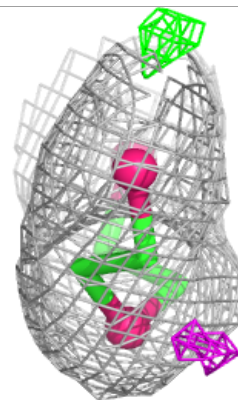
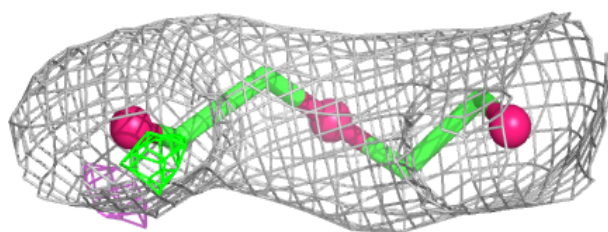
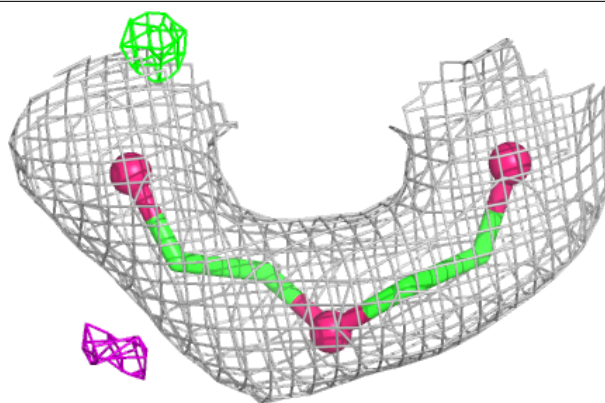
Electron density around A1FAW B 408:

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

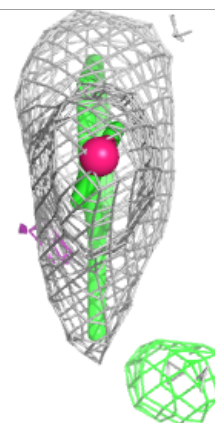
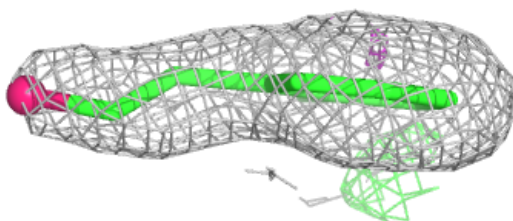
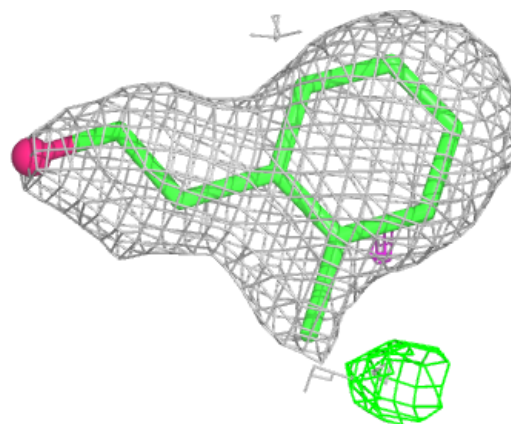


Electron density around PEG A 405:

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

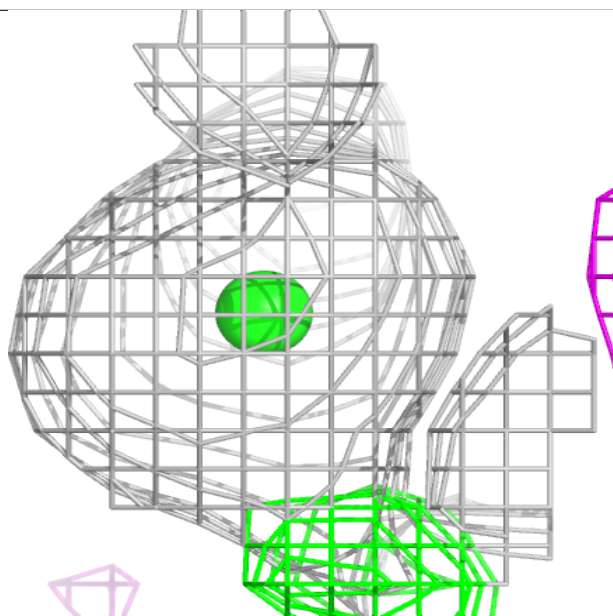
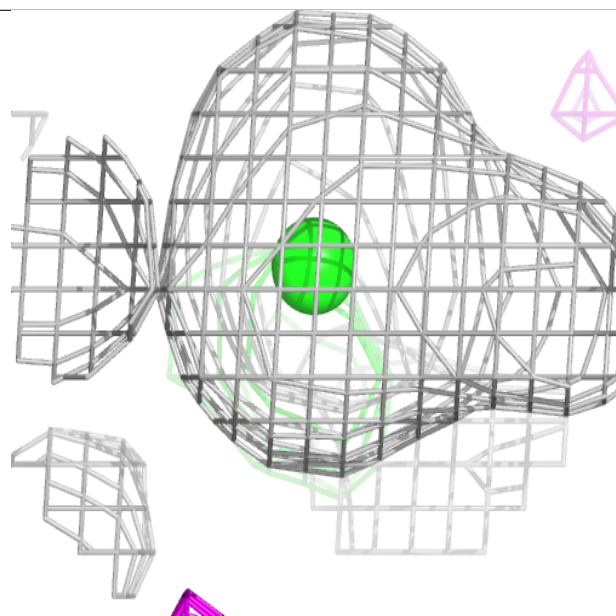
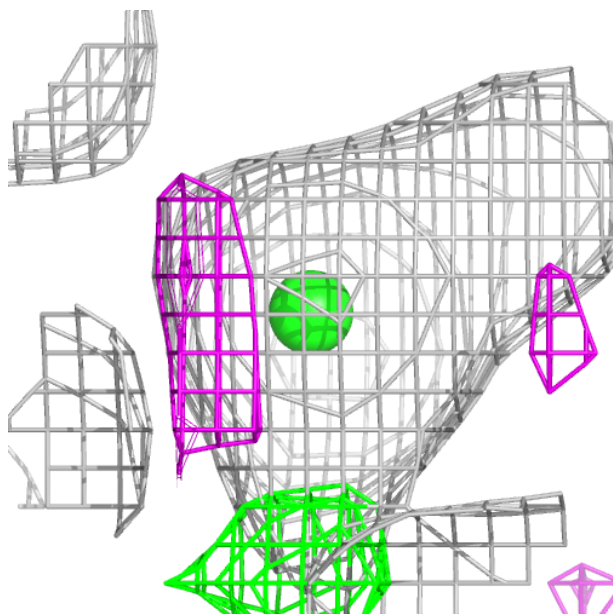
**Electron density around A1FAW A 409:**

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



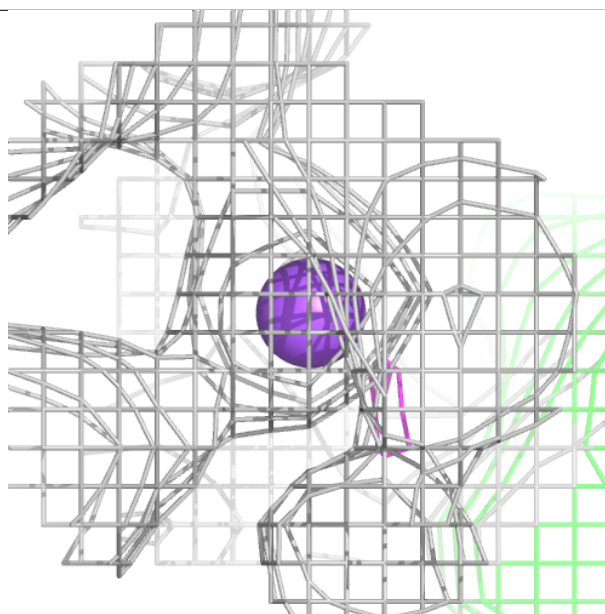
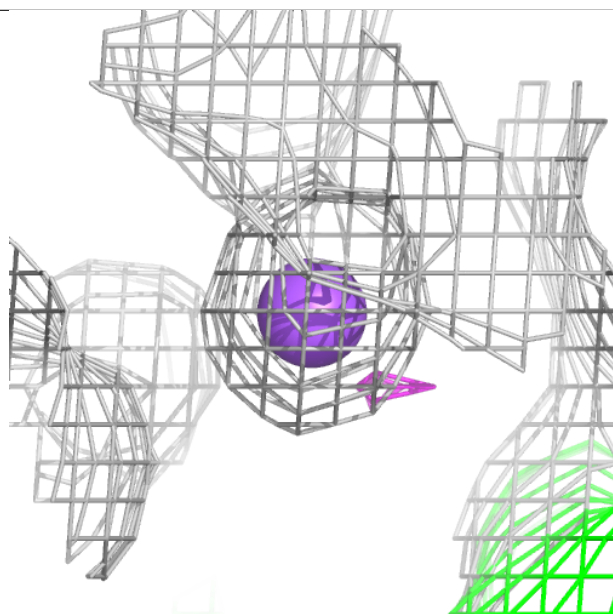
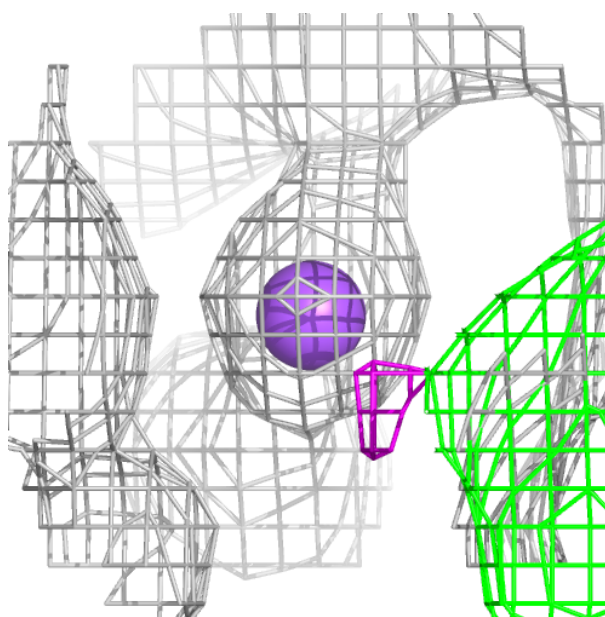
Electron density around CL B 403:

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



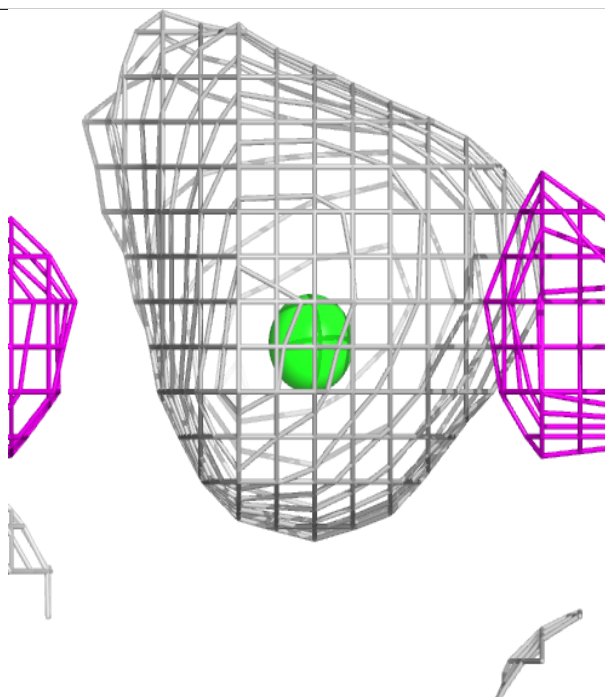
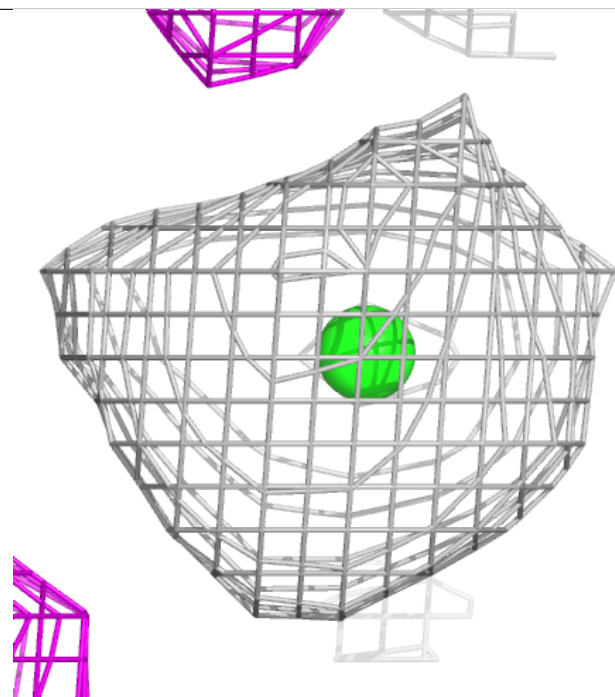
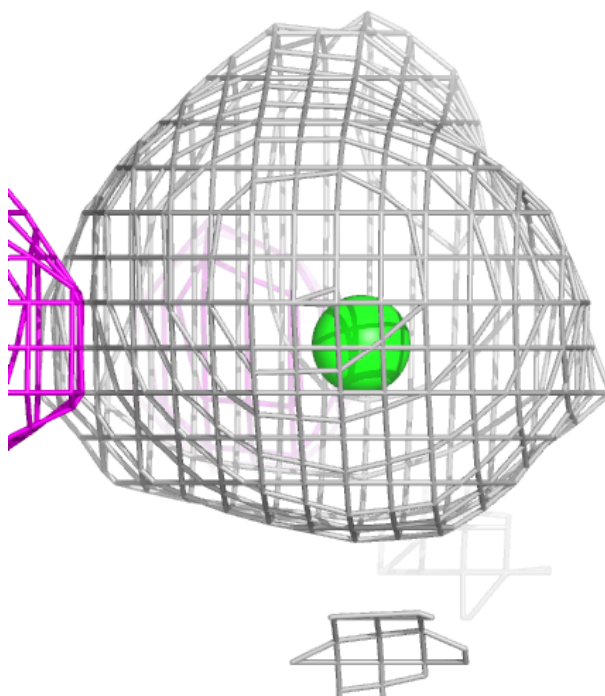
Electron density around NA A 407:

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



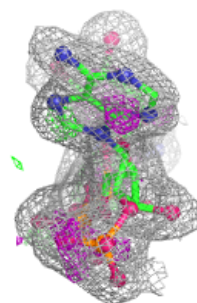
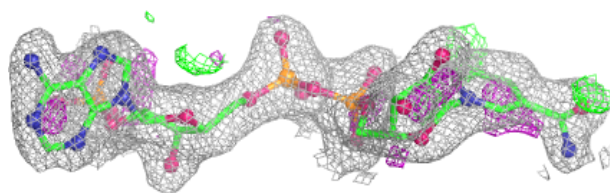
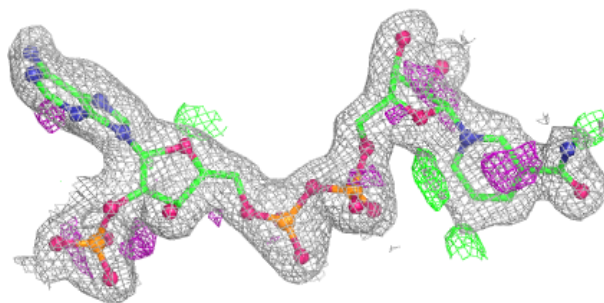
Electron density around CL A 401:

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



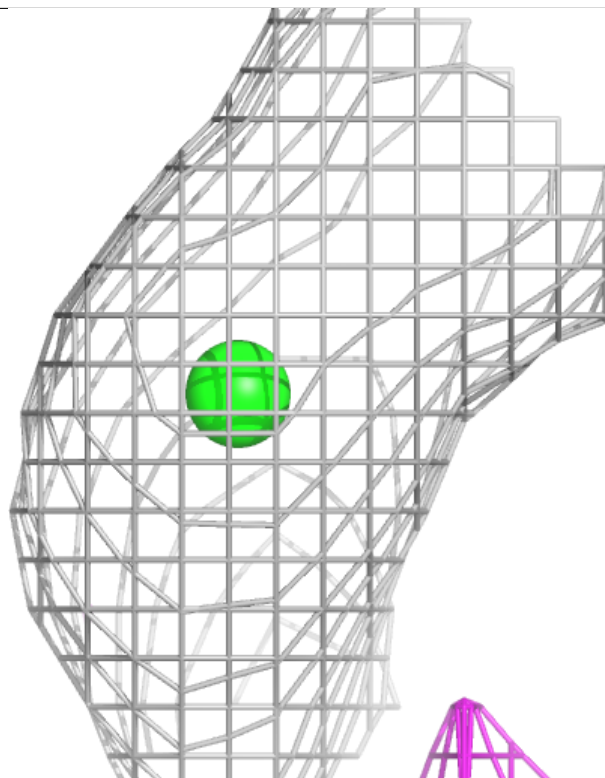
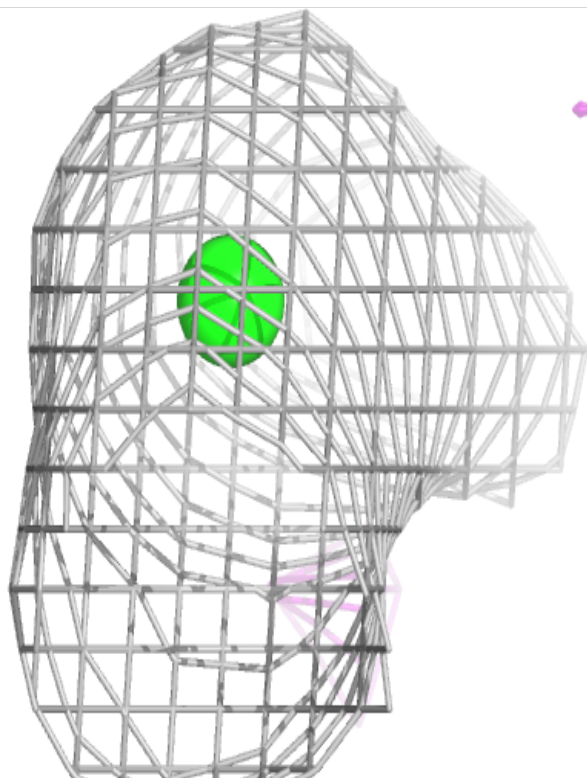
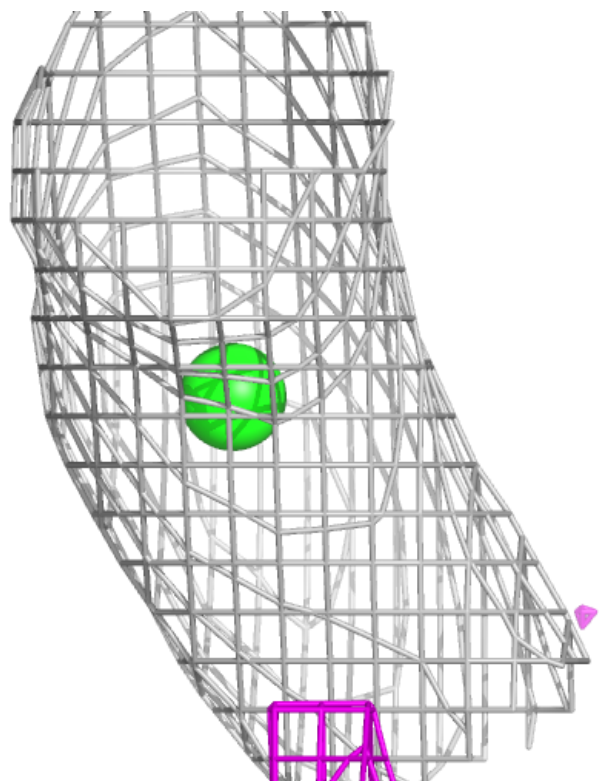
Electron density around NAP A 408:

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



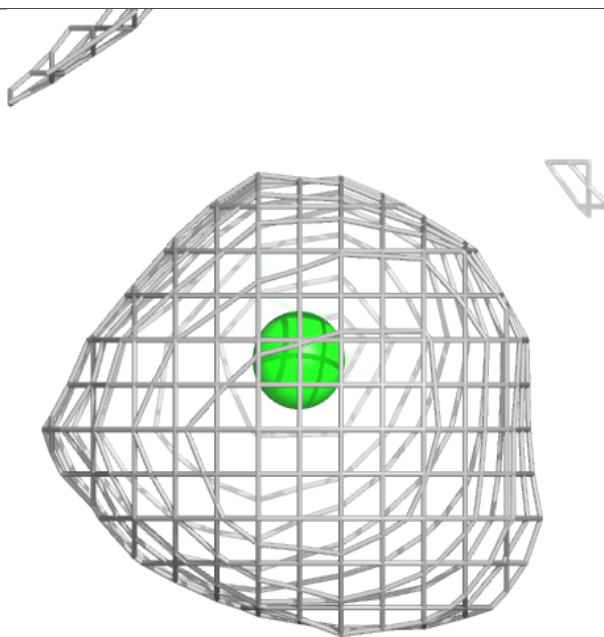
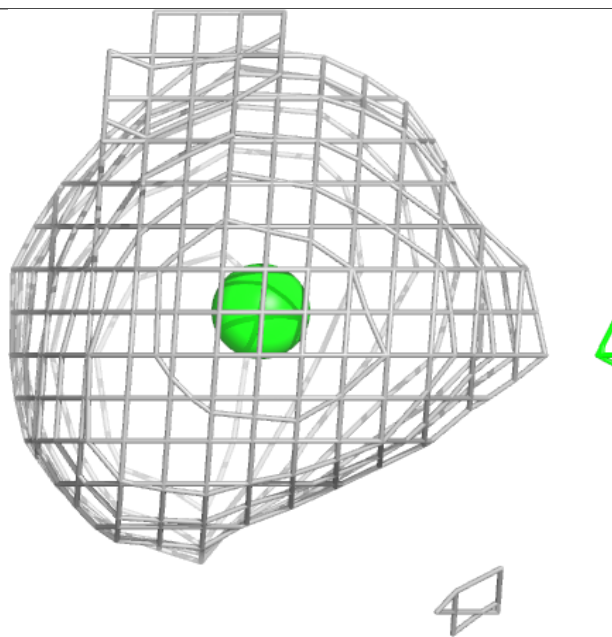
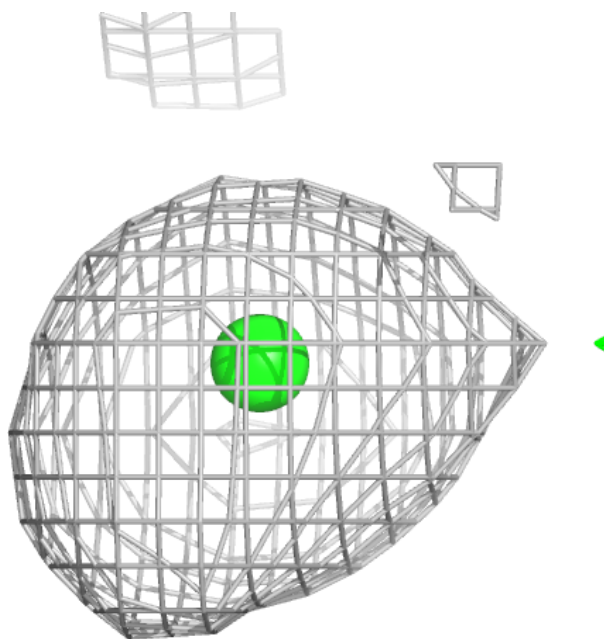
Electron density around CL B 405:

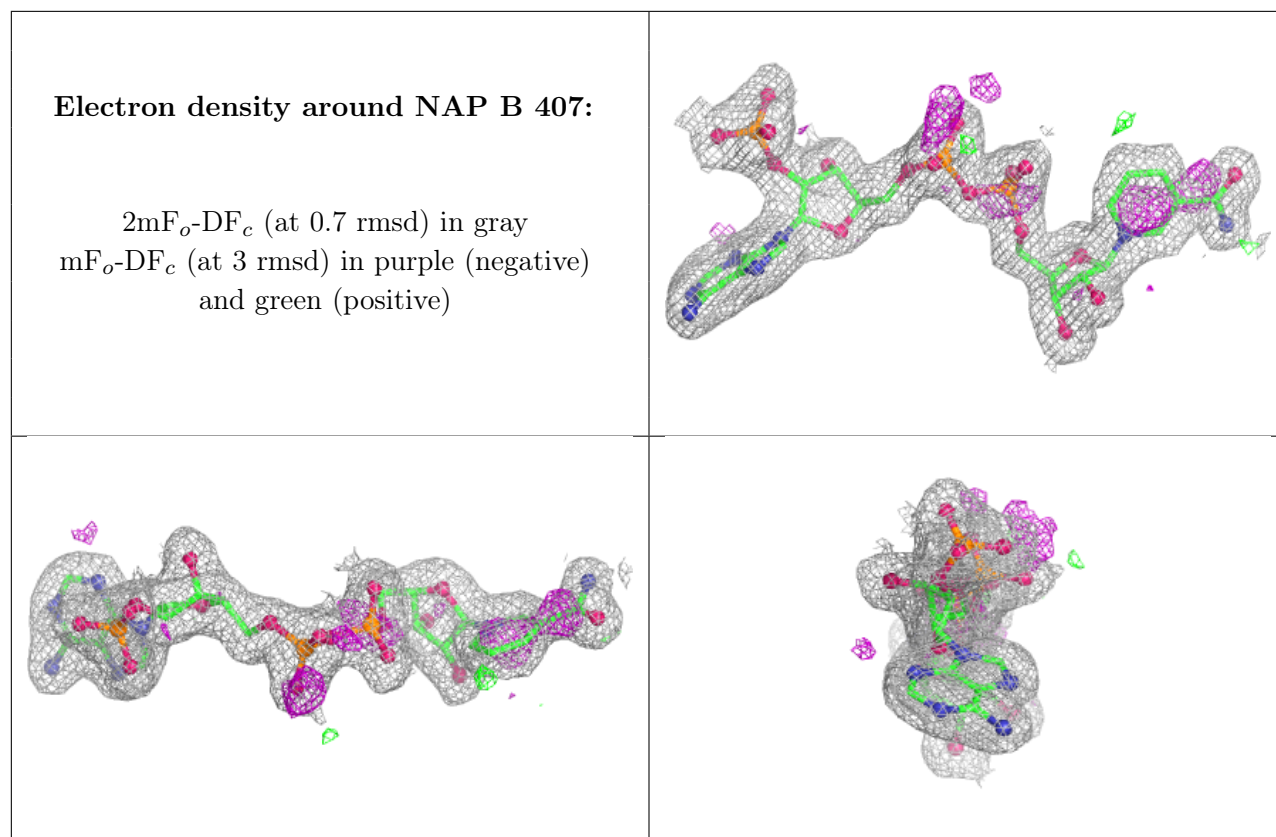
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL B 401:

$2mF_o-DF_c$ (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.