



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:16 PM UTC

PDB ID : 8AB3 / pdb_00008ab3
Title : Crystal Structure of the Lactate Dehydrogenase of Cyanobacterium Aponinum
in complex with oxamate, NADH and FBP.
Authors : Robin, A.Y.; Girard, E.; Madern, D.
Deposited on : 2022-07-04
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

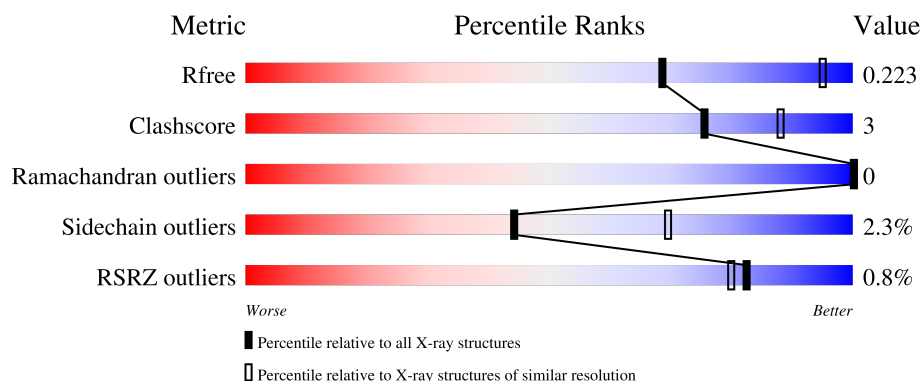
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	337	
1	B	337	
1	C	337	
1	D	337	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10654 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2498	1589	410	486	13			
1	B	328	Total	C	N	O	S	0	1	0
			2459	1567	401	478	13			
1	C	330	Total	C	N	O	S	0	1	0
			2491	1587	411	480	13			
1	D	328	Total	C	N	O	S	0	1	0
			2475	1578	406	478	13			

There are 24 discrepancies between the modelled and reference sequences:

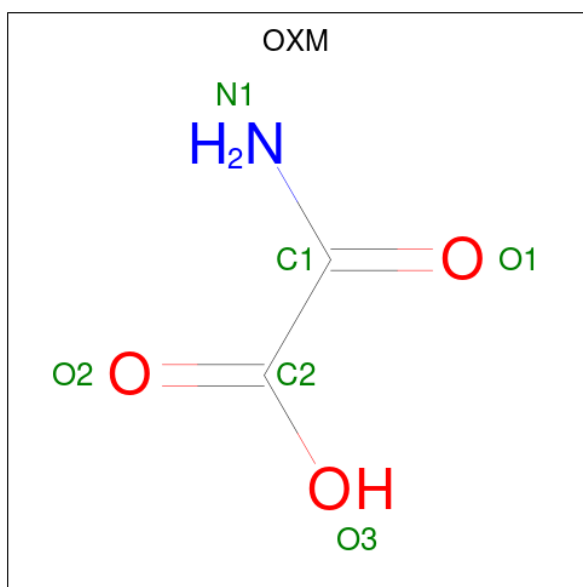
Chain	Residue	Modelled	Actual	Comment	Reference
A	334	HIS	-	expression tag	UNP K9Z684
A	335	HIS	-	expression tag	UNP K9Z684
A	336	HIS	-	expression tag	UNP K9Z684
A	337	HIS	-	expression tag	UNP K9Z684
A	338	HIS	-	expression tag	UNP K9Z684
A	339	HIS	-	expression tag	UNP K9Z684
B	334	HIS	-	expression tag	UNP K9Z684
B	335	HIS	-	expression tag	UNP K9Z684
B	336	HIS	-	expression tag	UNP K9Z684
B	337	HIS	-	expression tag	UNP K9Z684
B	338	HIS	-	expression tag	UNP K9Z684
B	339	HIS	-	expression tag	UNP K9Z684
C	334	HIS	-	expression tag	UNP K9Z684
C	335	HIS	-	expression tag	UNP K9Z684
C	336	HIS	-	expression tag	UNP K9Z684
C	337	HIS	-	expression tag	UNP K9Z684
C	338	HIS	-	expression tag	UNP K9Z684
C	339	HIS	-	expression tag	UNP K9Z684
D	334	HIS	-	expression tag	UNP K9Z684
D	335	HIS	-	expression tag	UNP K9Z684
D	336	HIS	-	expression tag	UNP K9Z684

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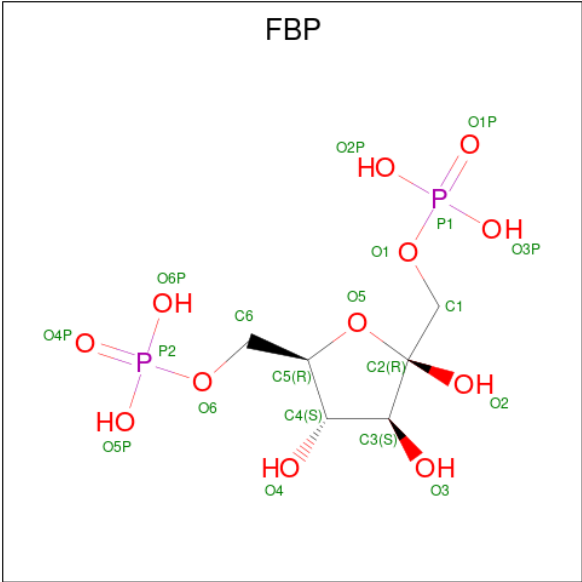
Chain	Residue	Modelled	Actual	Comment	Reference
D	337	HIS	-	expression tag	UNP K9Z684
D	338	HIS	-	expression tag	UNP K9Z684
D	339	HIS	-	expression tag	UNP K9Z684

- Molecule 2 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$) (labeled as "Ligand of Interest" by depositor).



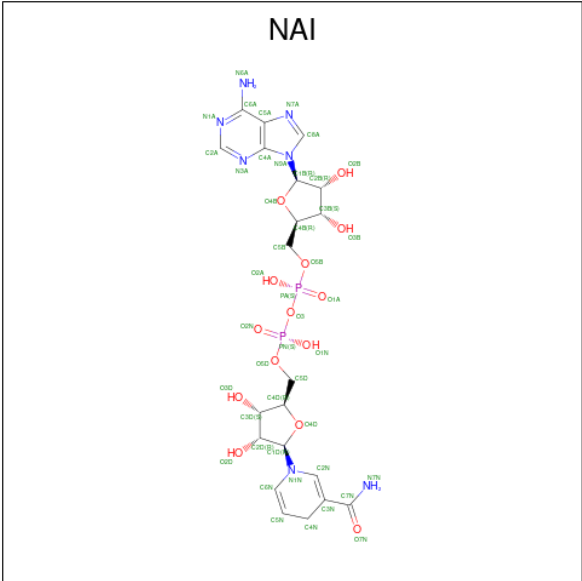
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	2	1	3		
2	B	1	Total	C	N	O	0	0
			6	2	1	3		
2	C	1	Total	C	N	O	0	0
			6	2	1	3		
2	D	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	C	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	108	Total	O	0	0
			108	108		
5	C	147	Total	O	0	0
			147	147		
5	D	108	Total	O	0	0
			108	108		

HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.37Å 111.50Å 101.79Å 90.00° 99.78° 90.00°	Depositor
Resolution (Å)	100.31 – 2.62 100.31 – 2.62	Depositor ED
% Data completeness (in resolution range)	99.3 (100.31-2.62) 99.3 (100.31-2.62)	Depositor ED
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.4 (8-JUN-2022), BUSTER 2.10.4 (8-JUN-2022)	Depositor
R, R_{free}	0.186 , 0.232 0.178 , 0.223	Depositor DC
R_{free} test set	2317 reflections (4.98%)	wwPDB
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.2	ED
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	0.95	ED
Total number of atoms	10654	wwPDB
Average B, all atoms (Å ²)	39.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: FBP, NAI, OXM

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	0.68	0/2535	1.07	4/3441 (0.1%)
1	B	0.74	1/2496 (0.0%)	1.10	5/3395 (0.1%)
1	C	0.69	0/2528	1.02	0/3433
1	D	0.66	0/2512	1.03	2/3412 (0.1%)
All	All	0.69	1/10071 (0.0%)	1.06	11/13681 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	PRO	CA-C	5.33	1.54	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ILE	N-CA-C	6.51	116.65	110.53
1	A	86	ASN	CA-CB-CG	6.31	118.91	112.60
1	B	200	VAL	N-CA-C	5.81	114.36	107.73
1	B	57	SER	N-CA-C	5.61	117.07	111.07
1	B	112	LEU	N-CA-C	5.56	117.02	111.07
1	D	112	LEU	N-CA-C	5.54	117.00	110.97
1	A	111	LEU	CA-C-N	5.13	127.46	120.54
1	A	111	LEU	C-N-CA	5.13	127.46	120.54
1	D	86	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	171	ARG	CA-C-N	5.02	126.97	120.44
1	B	171	ARG	C-N-CA	5.02	126.97	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2498	0	2539	15	0
1	B	2459	0	2471	21	0
1	C	2491	0	2536	19	0
1	D	2475	0	2517	13	0
2	A	6	0	2	0	0
2	B	6	0	2	0	0
2	C	6	0	2	0	0
2	D	6	0	2	0	0
3	A	20	0	10	0	0
3	C	20	0	10	0	0
4	A	44	0	27	0	0
4	B	44	0	27	1	0
4	C	44	0	27	0	0
4	D	44	0	27	1	0
5	A	128	0	0	1	0
5	B	108	0	0	0	0
5	C	147	0	0	2	0
5	D	108	0	0	0	0
All	All	10654	0	10199	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:SER:HB3	1:B:302:ILE:HD13	1.79	0.63
1:B:168:ASP:OD2	1:B:195:HIS:ND1	2.33	0.61
1:A:28:ILE:HD11	1:A:84:ILE:HD11	1.86	0.57
1:C:270:GLU:HB3	1:D:182:ILE:HA	1.87	0.56
1:B:33:VAL:HG21	4:B:402:NAI:C6N	2.37	0.55
1:C:42:LEU:HD22	1:C:71:MET:HE1	1.90	0.54
1:B:302:ILE:HG22	1:B:303:LYS:HG3	1.90	0.53
1:C:28:ILE:HD11	1:C:84:ILE:HD11	1.89	0.53
1:A:42:LEU:HD22	1:A:71:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LEU:HD22	1:D:71:MET:HE1	1.92	0.52
1:B:218:TRP:O	1:B:221:LEU:HB2	2.11	0.51
1:A:9:LEU:HD12	1:C:282:MET:HE1	1.92	0.51
1:B:42:LEU:HD22	1:B:71:MET:HE1	1.93	0.51
1:A:270:GLU:HB3	1:B:182:ILE:HA	1.93	0.51
1:D:138:VAL:O	4:D:402:NAI:H2N	2.11	0.50
1:D:299:ARG:HB2	1:D:302:ILE:CD1	2.42	0.49
1:D:299:ARG:HB2	1:D:302:ILE:HD11	1.95	0.49
1:A:23:ARG:NH2	1:C:23:ARG:HG3	2.28	0.49
1:A:100:VAL:HG23	1:A:111:LEU:HD22	1.95	0.48
1:B:244:ILE:HG12	1:B:249:TYR:HA	1.94	0.47
1:C:100:VAL:HG23	1:C:111:LEU:HD22	1.95	0.47
1:B:222:PRO:HD2	1:B:225:GLU:HB2	1.97	0.47
1:D:328:PHE:O	1:D:331:ILE:HG13	2.15	0.47
1:C:121:LYS:O	5:C:501:HOH:O	2.21	0.46
1:B:30:LEU:HD21	1:B:52:LEU:HD22	1.98	0.46
1:C:140:ASN:HA	1:C:142:VAL:N	2.31	0.46
1:D:102:GLN:HB3	1:D:111:LEU:HD11	1.96	0.46
1:C:30:LEU:HD21	1:C:52:LEU:HD22	1.98	0.46
1:A:282:MET:HE1	1:A:304:THR:HG21	1.97	0.45
1:D:194:GLU:HG3	1:D:324:LEU:HD21	1.97	0.45
1:D:294:ARG:HG2	1:D:304:THR:HG23	1.99	0.45
1:B:89:ARG:HG2	1:B:129:TYR:HB3	1.99	0.45
1:B:109:LEU:HA	1:B:141:PRO:HG3	1.97	0.45
1:C:187:VAL:HA	1:C:208:VAL:HG12	1.99	0.45
1:A:178:LYS:HE2	5:A:545:HOH:O	2.16	0.45
1:A:294:ARG:HG2	1:A:304:THR:HG23	1.99	0.44
1:C:182:ILE:HA	1:D:270:GLU:HB3	1.97	0.44
1:B:140:ASN:HA	1:B:142:VAL:N	2.32	0.44
1:C:323:MET:HE2	1:C:323:MET:HB2	1.91	0.44
1:A:187:VAL:HA	1:A:208:VAL:HG12	2.00	0.44
1:C:294:ARG:HG2	1:C:304:THR:HG23	1.99	0.43
1:A:16:ASN:HA	1:A:17:PRO:HD3	1.91	0.43
1:B:314:GLU:O	1:B:318:GLN:HG2	2.18	0.43
1:C:114:ARG:HD3	5:C:571:HOH:O	2.19	0.43
1:D:187:VAL:HA	1:D:208:VAL:HG12	2.00	0.43
1:C:30:LEU:CD1	1:C:52:LEU:HB3	2.49	0.42
1:C:282:MET:HE2	1:C:282:MET:HB2	1.88	0.42
1:A:282:MET:HE1	1:A:304:THR:CG2	2.50	0.42
1:B:161:ILE:HD11	1:B:300:GLY:HA2	2.02	0.42
1:B:29:GLY:O	1:B:97:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD23	1:C:298:GLU:HB2	2.01	0.41
1:A:30:LEU:HD13	1:A:52:LEU:HB3	2.02	0.41
1:C:30:LEU:HD13	1:C:52:LEU:HB3	2.01	0.41
1:B:52:LEU:HD11	1:B:79:ILE:HD11	2.03	0.41
1:B:59:LYS:O	1:B:63:GLU:HG2	2.19	0.41
1:B:98:ALA:O	1:B:139:THR:OG1	2.36	0.41
1:B:270:GLU:HG3	1:B:297:SER:HB2	2.03	0.41
1:B:323:MET:HE2	1:B:323:MET:HB2	2.01	0.41
1:D:23:ARG:HD3	1:D:266:LEU:HD22	2.02	0.41
1:D:282:MET:HE3	1:D:282:MET:HB2	1.94	0.40
1:A:24:LYS:HG3	1:A:49:GLU:HG3	2.02	0.40
1:C:16:ASN:HA	1:C:17:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/337 (97%)	317 (97%)	11 (3%)	0	100	100
1	B	327/337 (97%)	315 (96%)	12 (4%)	0	100	100
1	C	329/337 (98%)	319 (97%)	10 (3%)	0	100	100
1	D	327/337 (97%)	316 (97%)	11 (3%)	0	100	100
All	All	1311/1348 (97%)	1267 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/288 (95%)	265 (97%)	9 (3%)	33	59
1	B	265/288 (92%)	255 (96%)	10 (4%)	29	54
1	C	272/288 (94%)	268 (98%)	4 (2%)	57	79
1	D	270/288 (94%)	268 (99%)	2 (1%)	76	89
All	All	1081/1152 (94%)	1056 (98%)	25 (2%)	44	69

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	86	ASN
1	A	102	GLN
1	A	113	GLU
1	A	142	VAL
1	A	223	GLU
1	A	250	THR
1	A	262	VAL
1	A	286	GLU
1	B	20	LEU
1	B	30	LEU
1	B	49	GLU
1	B	113	GLU
1	B	178	LYS
1	B	208	VAL
1	B	212	LYS
1	B	216	ASN
1	B	221	LEU
1	B	292	ILE
1	C	30	LEU
1	C	250	THR
1	C	286	GLU
1	C	302	ILE
1	D	250	THR
1	D	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	102	GLN
1	A	318	GLN
1	B	207	ASN
1	B	216	ASN
1	C	32	GLN
1	C	318	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OXM	A	401	-	5,5,5	2.15	2 (40%)	2,6,6	0.42	0
4	NAI	B	402	-	47,48,48	0.25	0	64,73,73	0.44	0
4	NAI	A	403	-	47,48,48	0.27	0	64,73,73	0.50	0
4	NAI	D	402	-	47,48,48	0.28	0	64,73,73	0.52	0
2	OXM	C	401	-	5,5,5	0.31	0	2,6,6	0.60	0
3	FBP	C	403	-	18,20,20	0.73	0	21,32,32	0.63	0
2	OXM	B	401	-	5,5,5	2.21	2 (40%)	2,6,6	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FBP	A	402	-	18,20,20	0.64	0	21,32,32	0.65	0
4	NAI	C	402	-	47,48,48	0.25	0	64,73,73	0.59	0
2	OXM	D	401	-	5,5,5	0.23	0	2,6,6	0.78	0

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
2	OXM	A	401	-	-	0/4/4/4	-
4	NAI	B	402	-	-	10/29/72/72	0/5/5/5
4	NAI	A	403	-	-	10/29/72/72	0/5/5/5
4	NAI	D	402	-	-	17/29/72/72	0/5/5/5
2	OXM	C	401	-	-	0/4/4/4	-
3	FBP	C	403	-	-	0/13/32/32	0/1/1/1
2	OXM	B	401	-	-	0/4/4/4	-
3	FBP	A	402	-	-	3/13/32/32	0/1/1/1
4	NAI	C	402	-	-	4/29/72/72	0/5/5/5
2	OXM	D	401	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	OXM	O2-C2	3.87	1.32	1.22
2	B	401	OXM	O2-C2	3.78	1.31	1.22
2	B	401	OXM	O3-C2	-3.08	1.22	1.30
2	A	401	OXM	O3-C2	-2.76	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	FBP	C1-O1-P1-O1P
4	A	403	NAI	C5B-O5B-PA-O1A
4	A	403	NAI	C5B-O5B-PA-O3
4	B	402	NAI	C5B-O5B-PA-O1A
4	B	402	NAI	C5B-O5B-PA-O3
4	B	402	NAI	C2N-C3N-C7N-O7N

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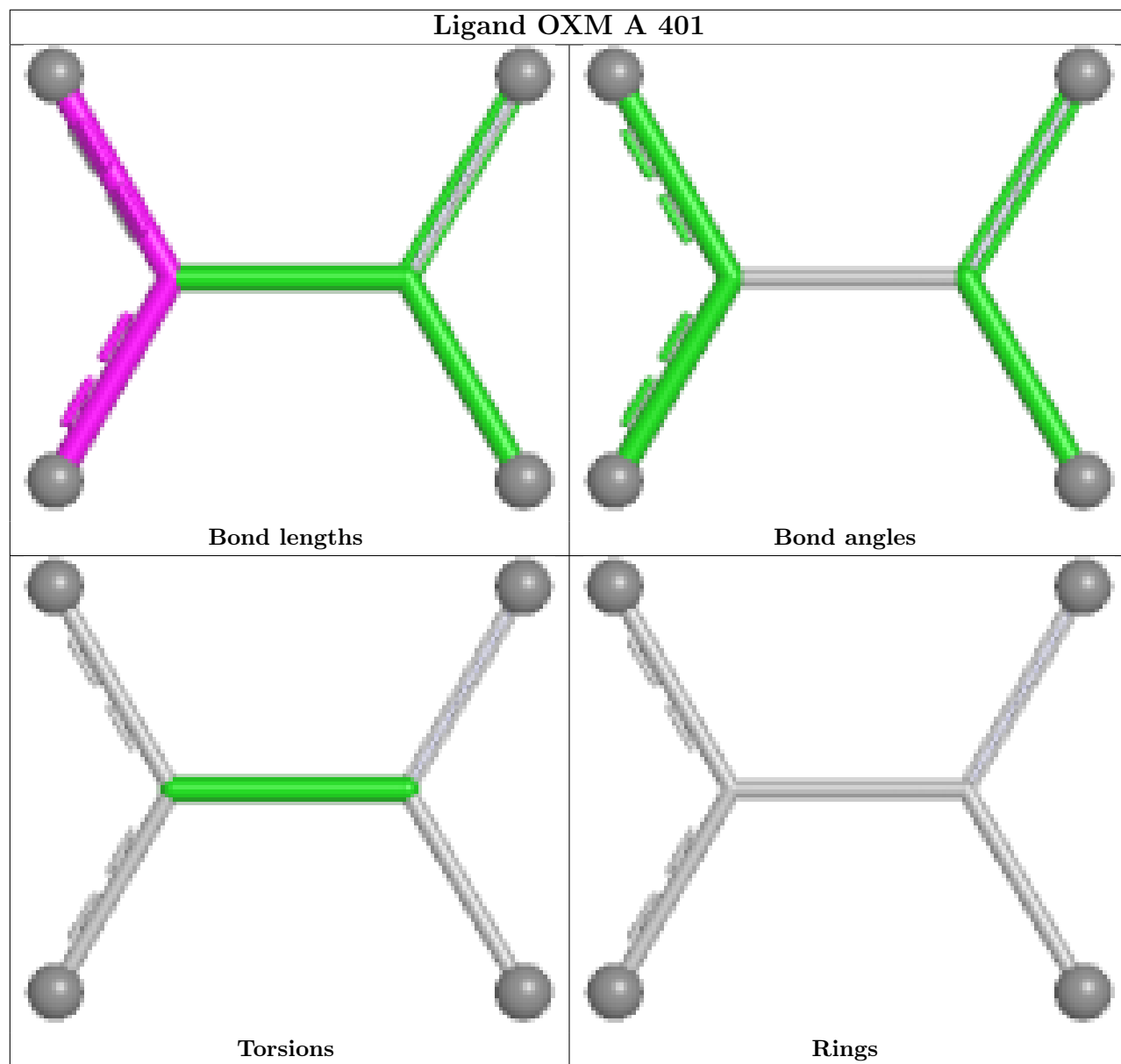
Mol	Chain	Res	Type	Atoms
4	D	402	NAI	C5B-O5B-PA-O1A
4	D	402	NAI	C5B-O5B-PA-O3
4	D	402	NAI	PN-O3-PA-O5B
4	D	402	NAI	C5D-O5D-PN-O3
4	D	402	NAI	C5D-O5D-PN-O2N
4	D	402	NAI	O4D-C4D-C5D-O5D
4	D	402	NAI	C3D-C4D-C5D-O5D
4	B	402	NAI	O4B-C4B-C5B-O5B
4	B	402	NAI	C2N-C3N-C7N-N7N
4	A	403	NAI	PN-O3-PA-O5B
4	B	402	NAI	PN-O3-PA-O5B
3	A	402	FBP	C1-O1-P1-O2P
4	A	403	NAI	PA-O3-PN-O2N
4	D	402	NAI	PA-O3-PN-O2N
4	D	402	NAI	C2D-C1D-N1N-C2N
4	D	402	NAI	C2D-C1D-N1N-C6N
4	D	402	NAI	O4B-C4B-C5B-O5B
4	A	403	NAI	C5B-O5B-PA-O2A
4	B	402	NAI	C5B-O5B-PA-O2A
4	D	402	NAI	C5B-O5B-PA-O2A
4	D	402	NAI	C5D-O5D-PN-O1N
4	D	402	NAI	O4D-C1D-N1N-C6N
4	D	402	NAI	O4D-C1D-N1N-C2N
4	A	403	NAI	O4B-C4B-C5B-O5B
4	A	403	NAI	O4D-C1D-N1N-C2N
4	B	402	NAI	O4D-C1D-N1N-C2N
4	C	402	NAI	O4D-C1D-N1N-C2N
4	B	402	NAI	C3B-C4B-C5B-O5B
4	A	403	NAI	C2D-C1D-N1N-C2N
4	C	402	NAI	C2D-C1D-N1N-C2N
4	A	403	NAI	PA-O3-PN-O1N
4	B	402	NAI	PA-O3-PN-O1N
4	D	402	NAI	PA-O3-PN-O1N
4	C	402	NAI	O4B-C4B-C5B-O5B
4	C	402	NAI	O4D-C1D-N1N-C6N
3	A	402	FBP	O1-C1-C2-O2
4	D	402	NAI	C3B-C4B-C5B-O5B
4	A	403	NAI	O4D-C1D-N1N-C6N

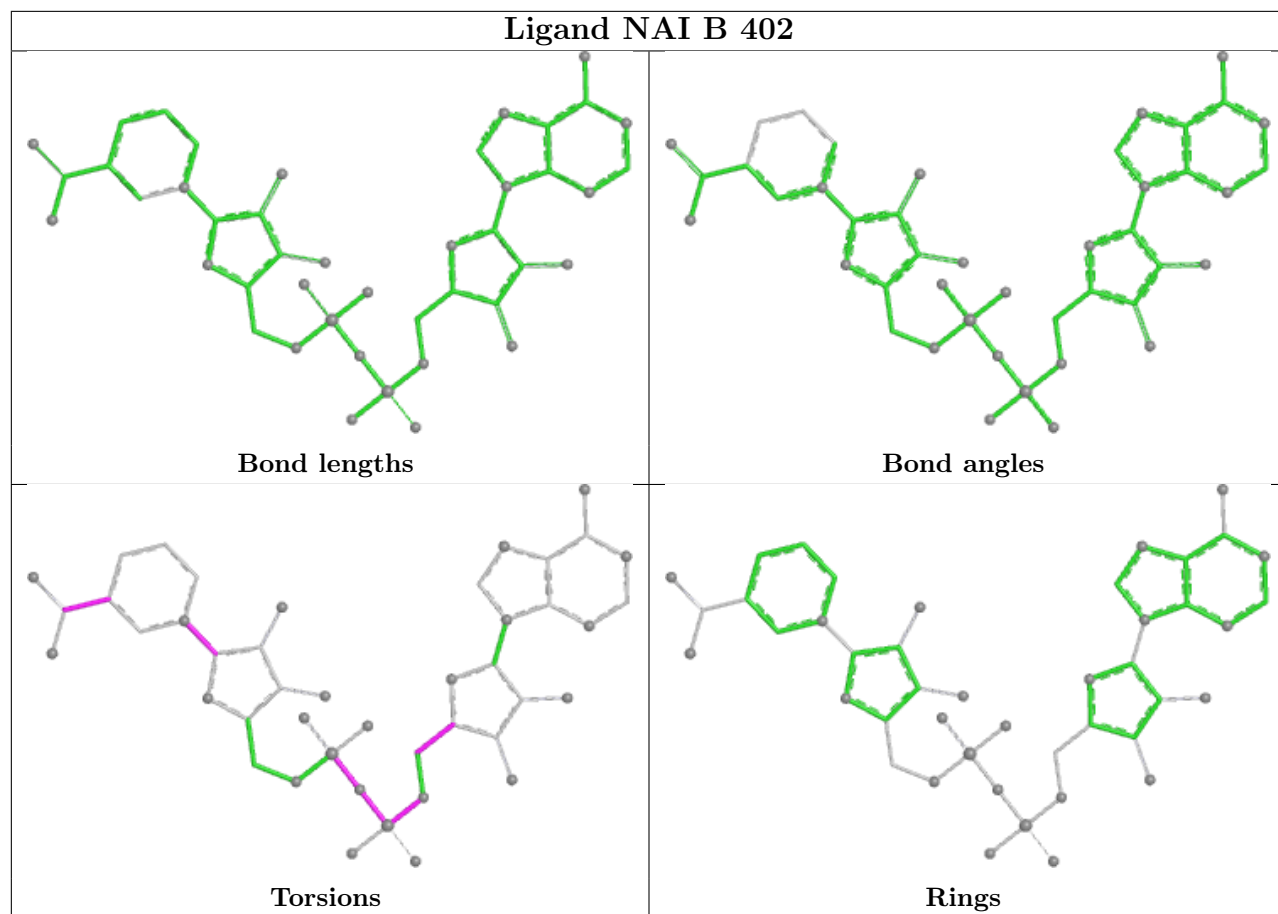
There are no ring outliers.

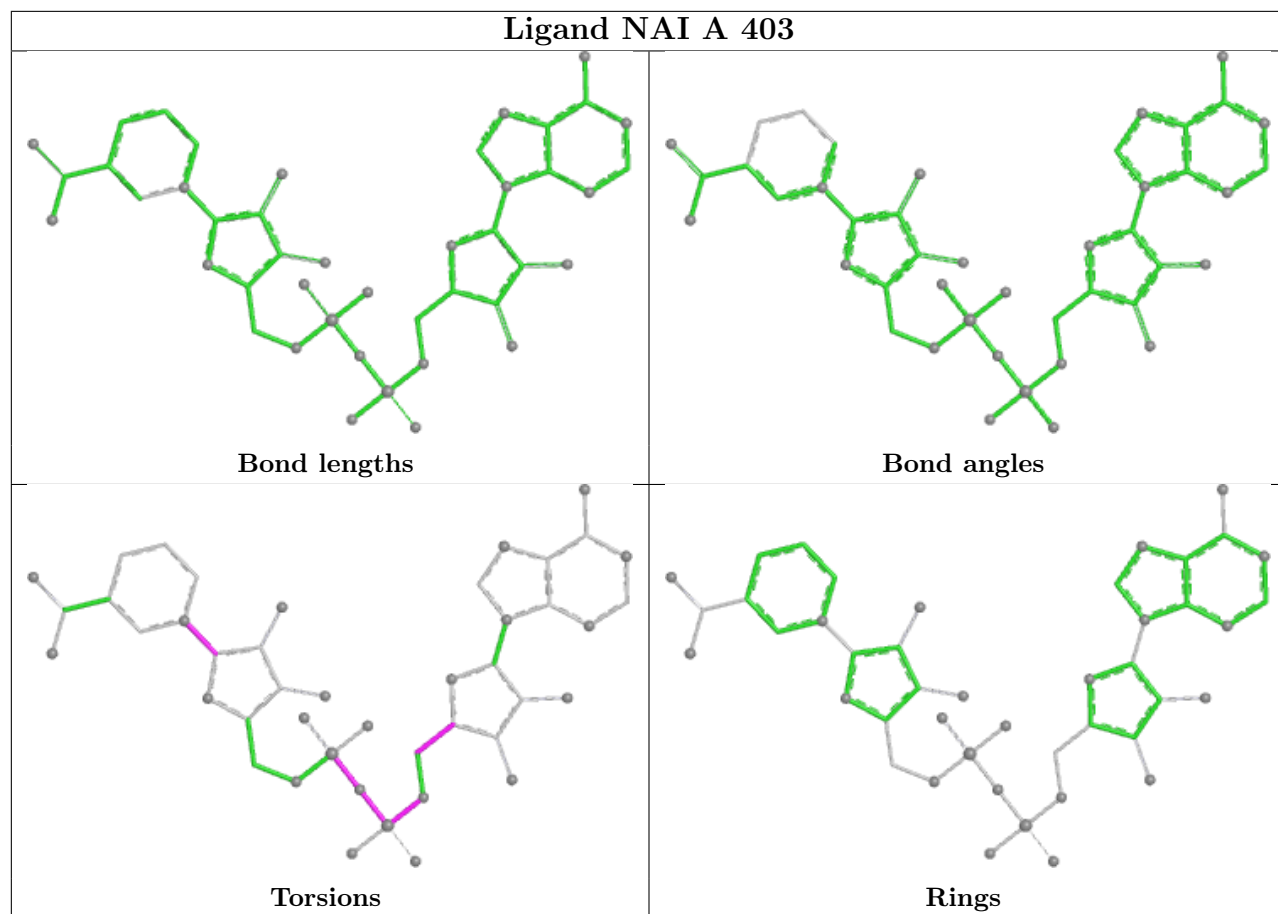
2 monomers are involved in 2 short contacts:

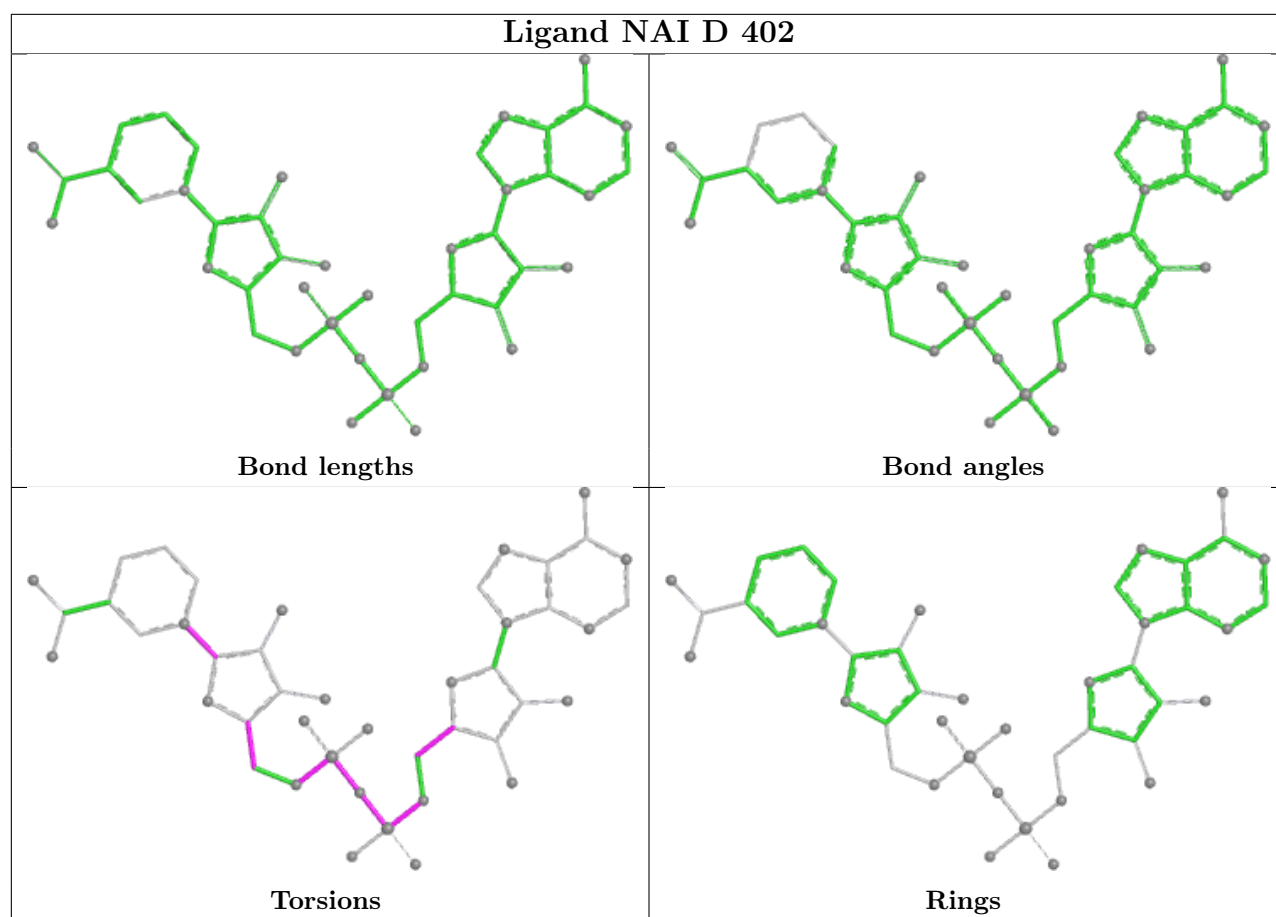
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	NAI	1	0
4	D	402	NAI	1	0

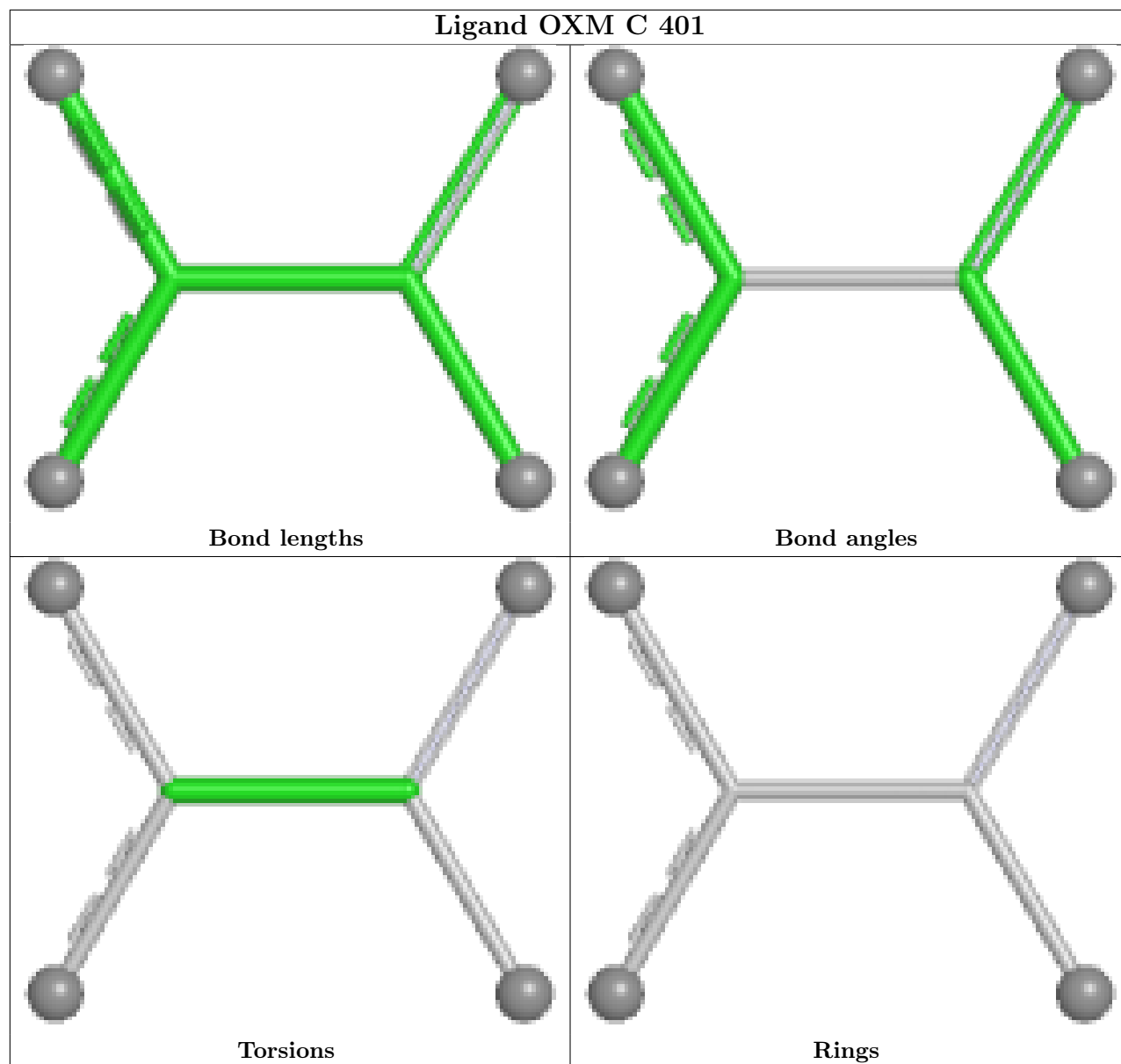
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

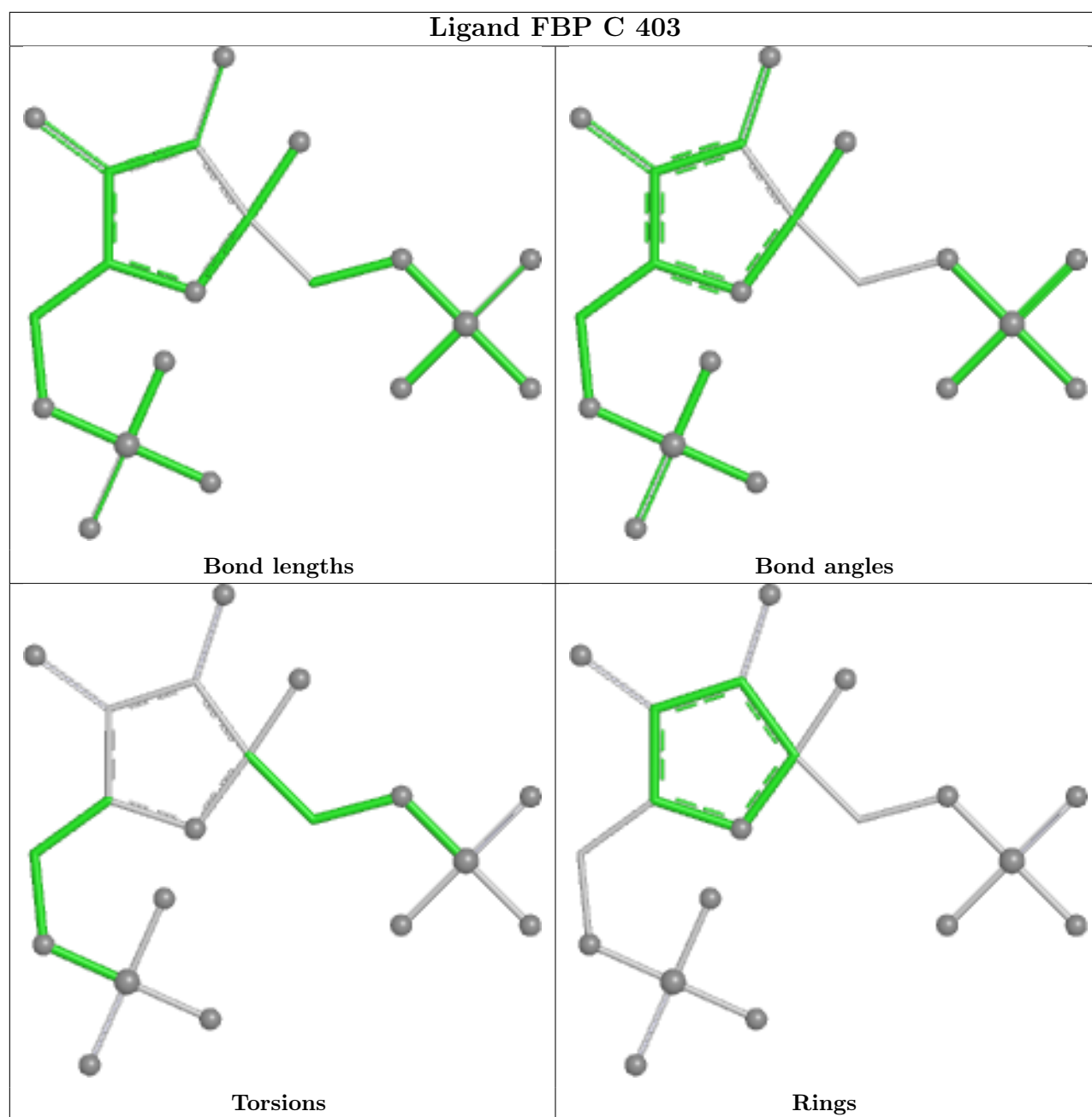


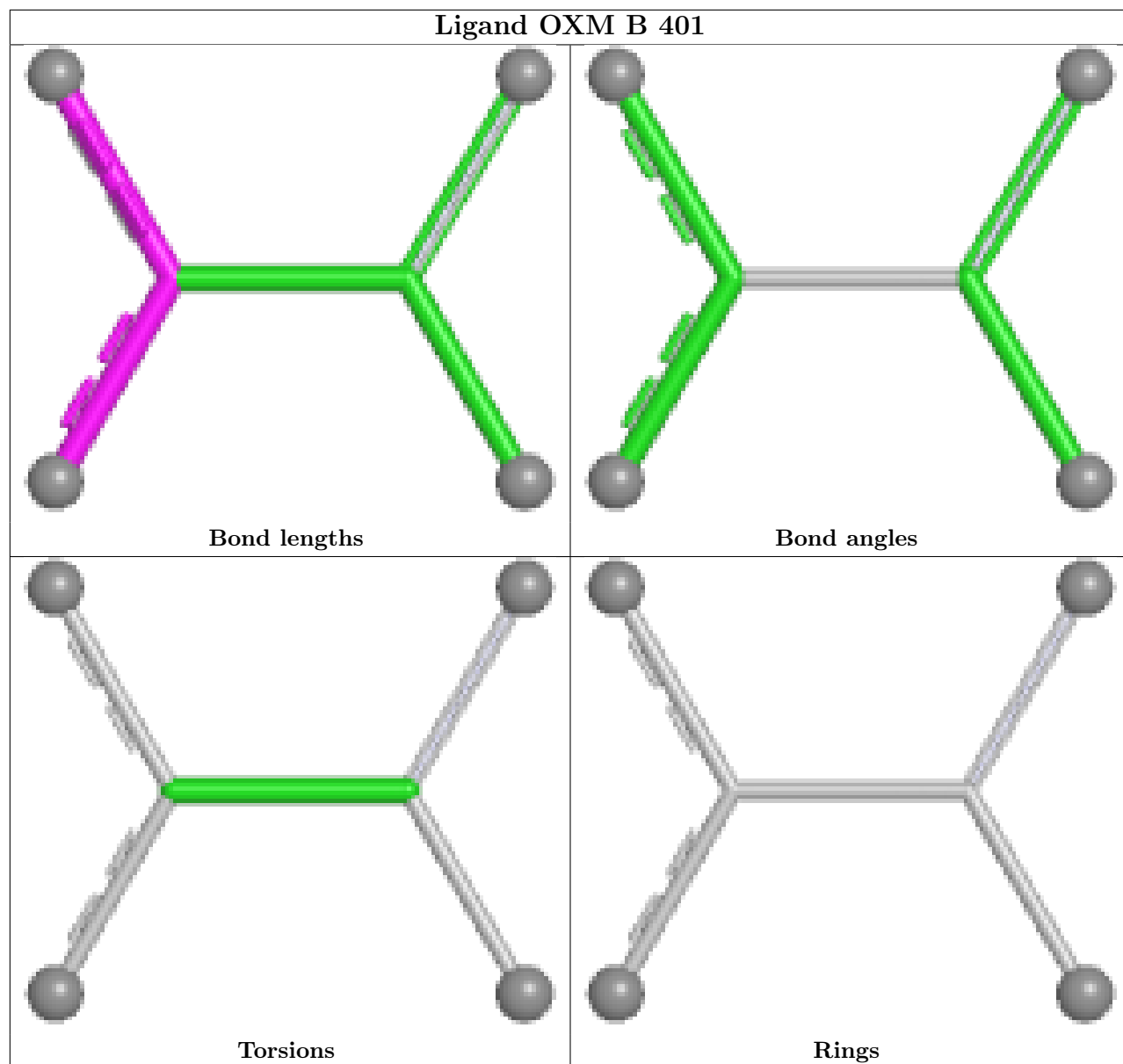


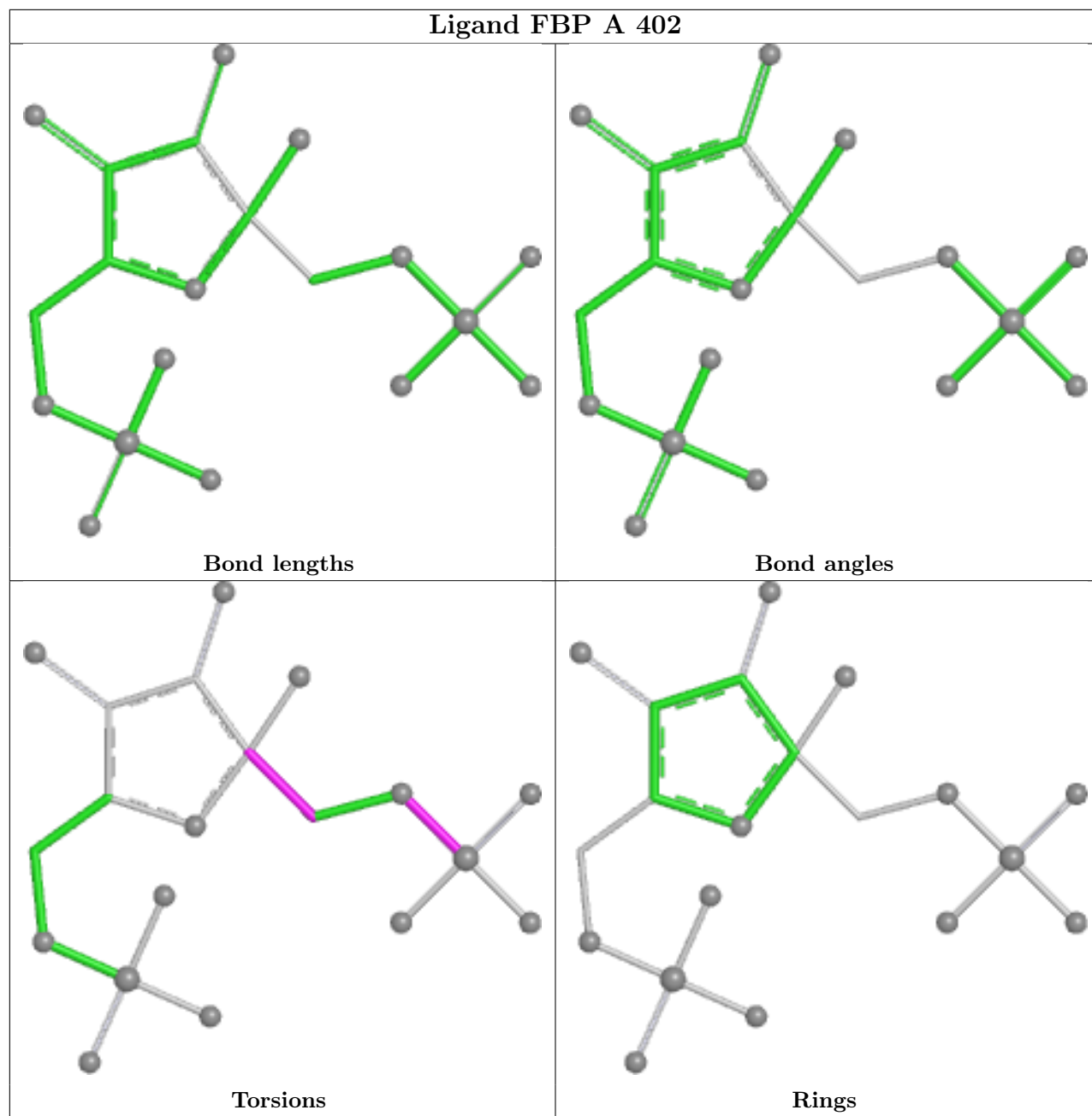


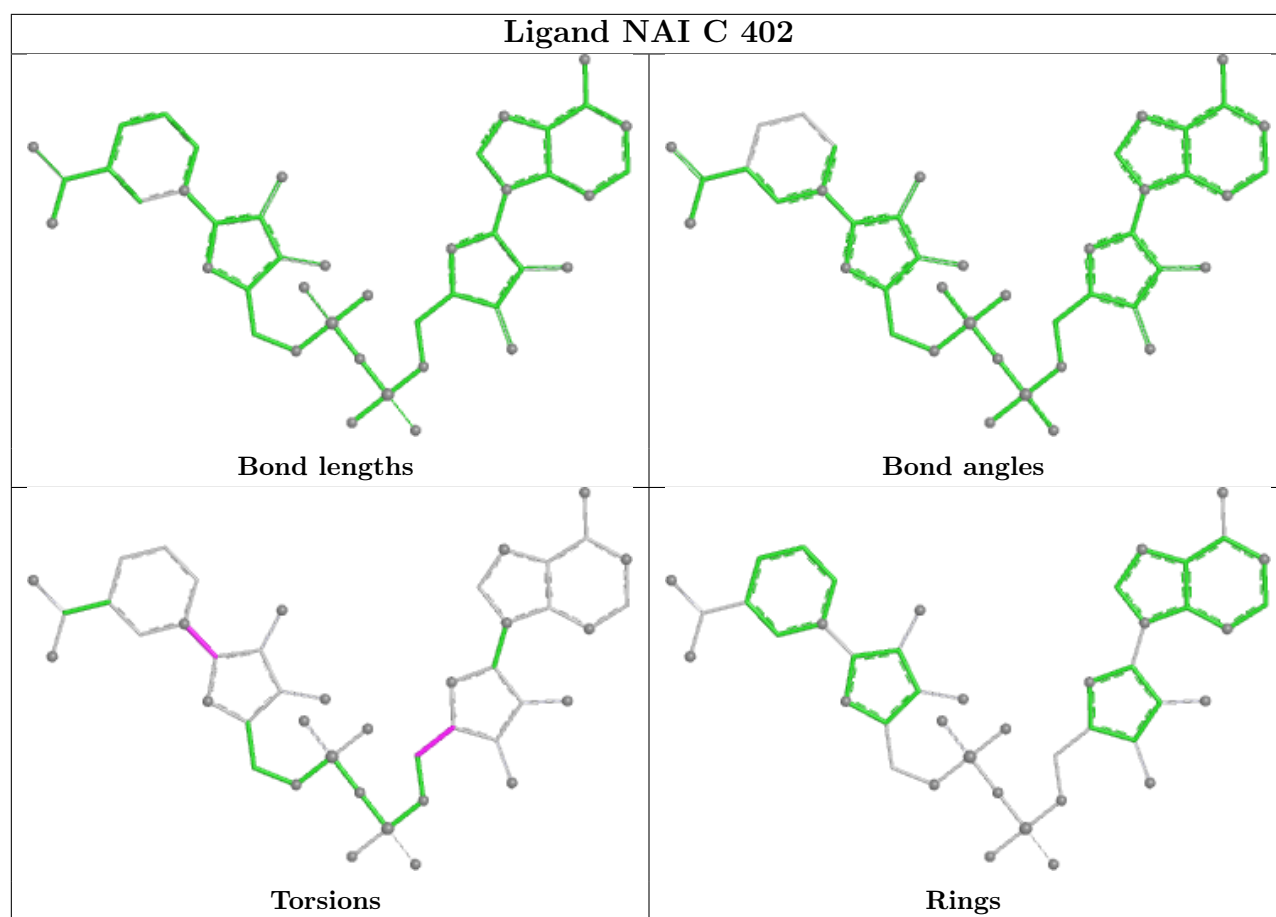


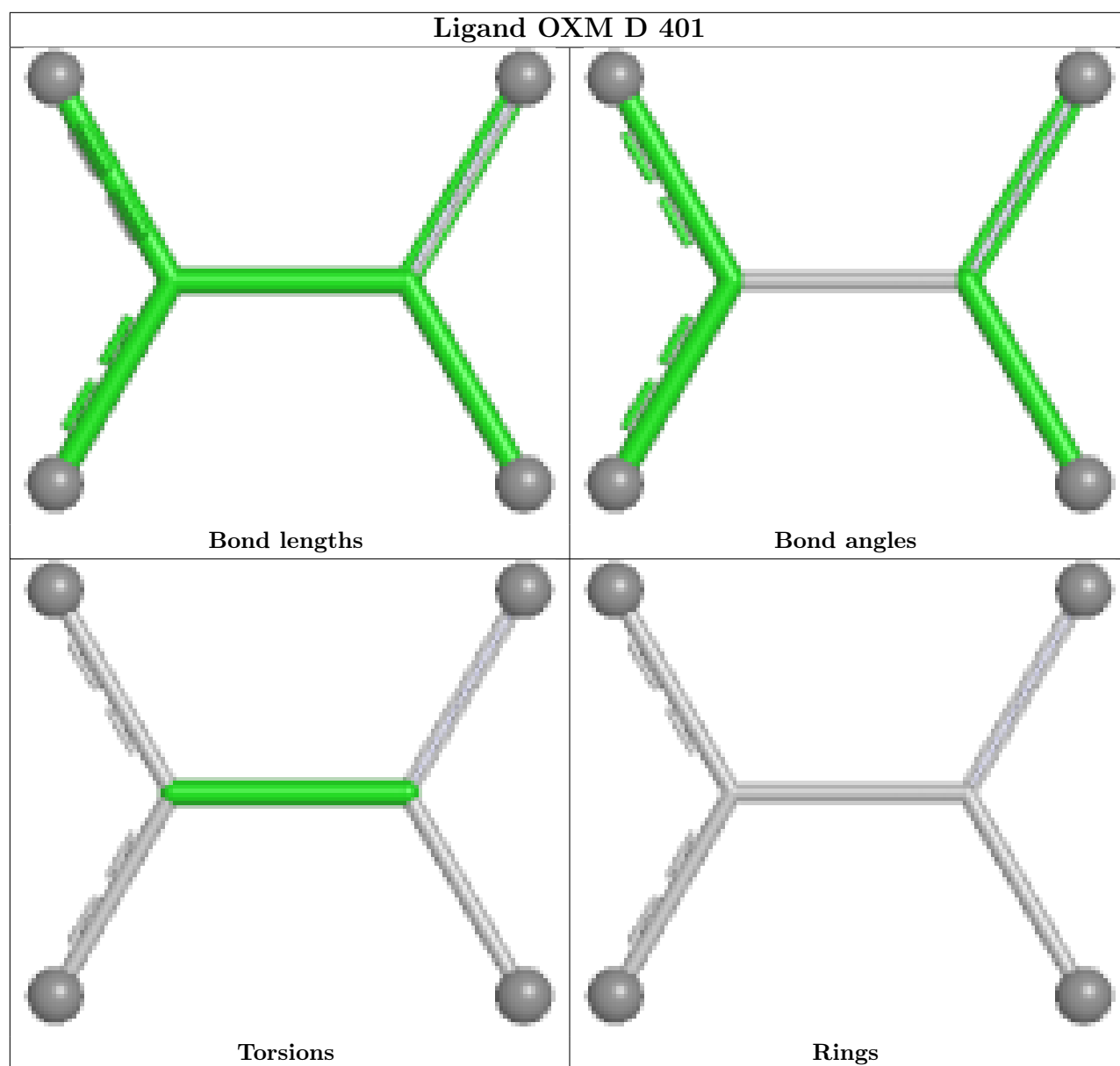












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/337 (97%)	-0.28	0 100 100	22, 36, 59, 74	0
1	B	328/337 (97%)	-0.14	5 (1%) 72 68	19, 40, 66, 79	1 (0%)
1	C	330/337 (97%)	-0.26	3 (0%) 81 78	13, 34, 58, 70	1 (0%)
1	D	328/337 (97%)	-0.24	3 (0%) 81 78	22, 38, 60, 72	1 (0%)
All	All	1316/1348 (97%)	-0.23	11 (0%) 82 80	13, 37, 62, 79	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	ILE	3.7
1	D	18	SER	3.0
1	B	107	SER	2.6
1	B	109	LEU	2.6
1	B	110	SER	2.6
1	C	17	PRO	2.5
1	D	220	ASP	2.4
1	D	16	ASN	2.3
1	C	104	GLU	2.2
1	B	16	ASN	2.2
1	C	3	MET	2.1

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

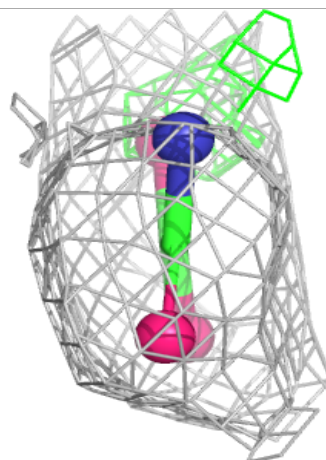
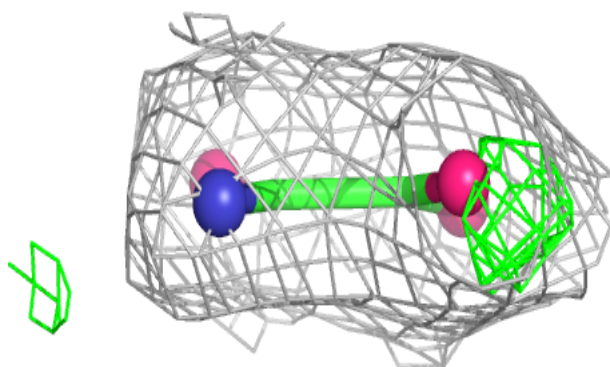
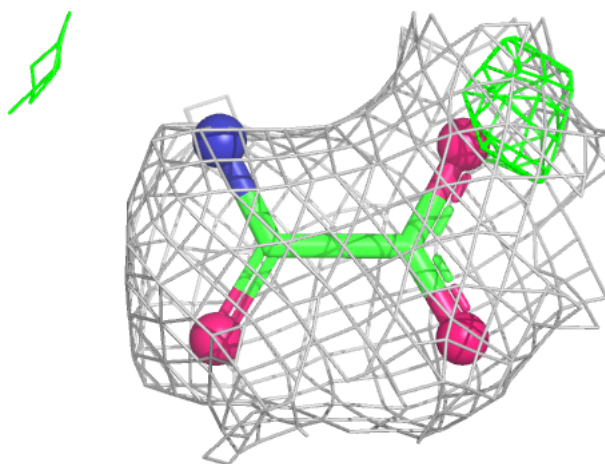
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OXM	D	401	6/6	0.85	0.12	44,45,45,46	0
2	OXM	C	401	6/6	0.92	0.09	41,42,42,43	0
2	OXM	A	401	6/6	0.94	0.07	40,40,41,41	0
2	OXM	B	401	6/6	0.94	0.09	44,44,45,45	0
3	FBP	C	403	20/20	0.94	0.09	37,38,39,40	0
4	NAI	D	402	44/44	0.94	0.09	38,43,48,48	0
4	NAI	B	402	44/44	0.96	0.08	49,50,53,53	0
3	FBP	A	402	20/20	0.96	0.07	39,41,42,42	0
4	NAI	C	402	44/44	0.97	0.06	27,28,29,30	0
4	NAI	A	403	44/44	0.97	0.07	28,30,32,33	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.

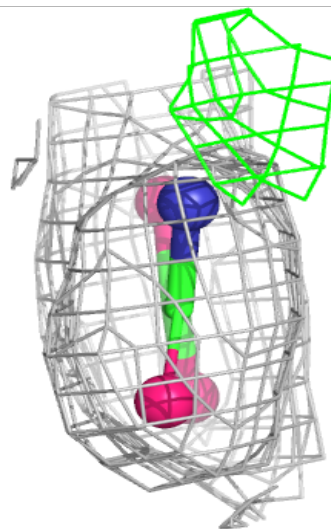
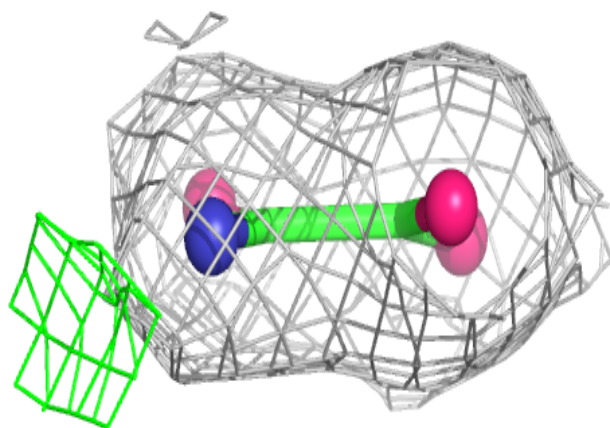
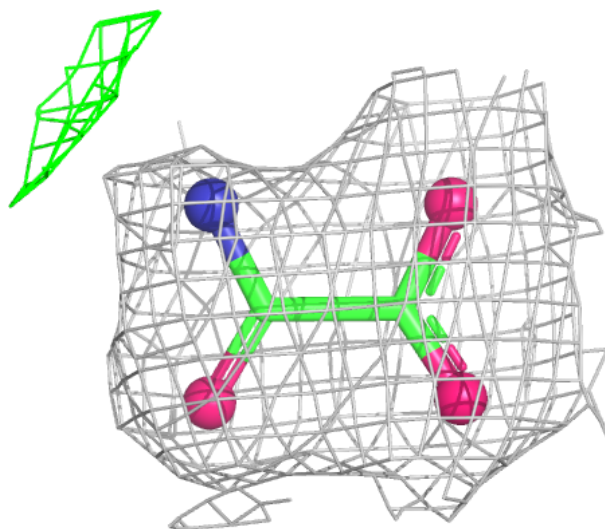
Electron density around OXM D 401:

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



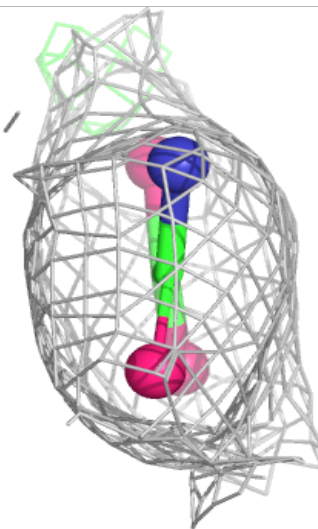
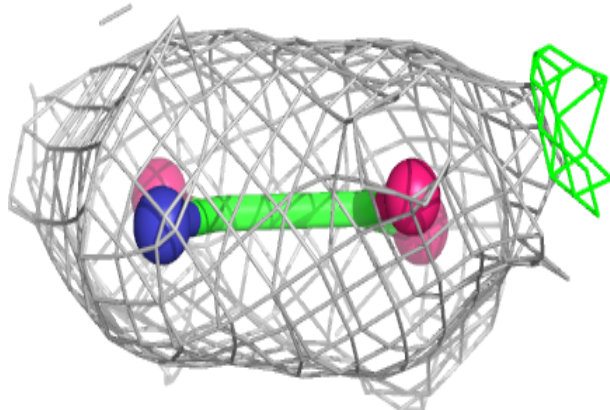
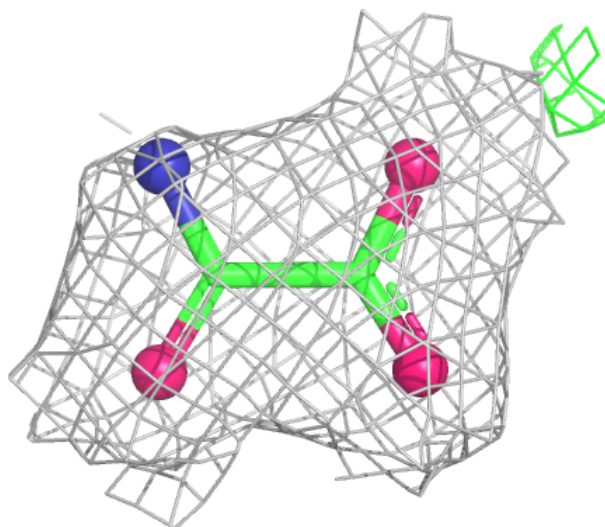
Electron density around OXM C 401:

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



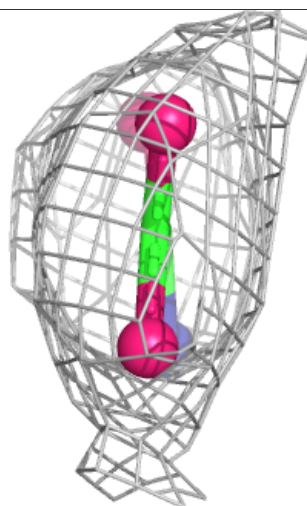
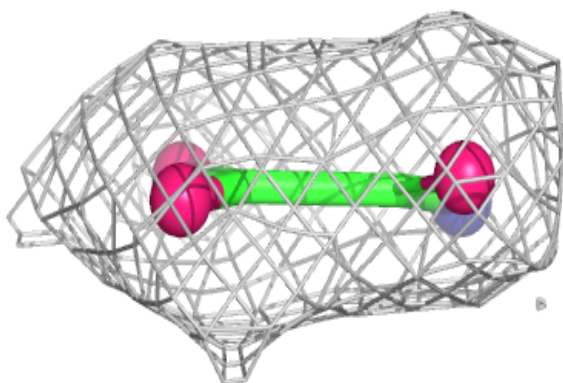
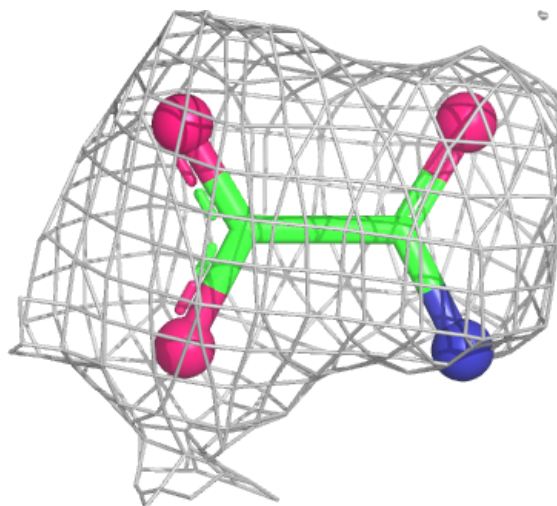
Electron density around OXM A 401:

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



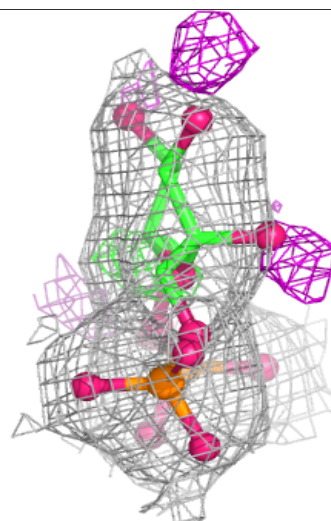
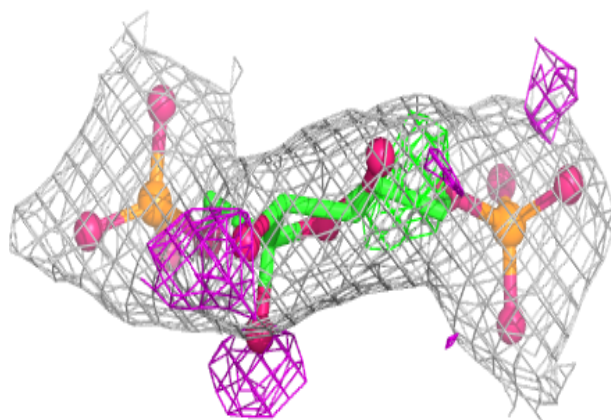
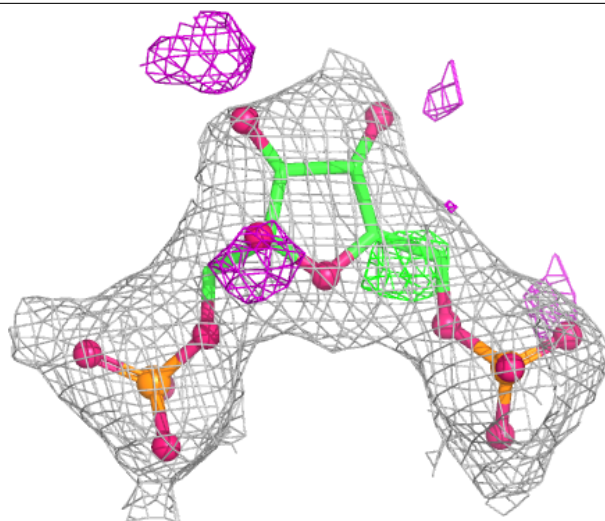
Electron density around OXM B 401:

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



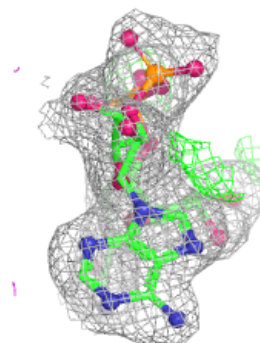
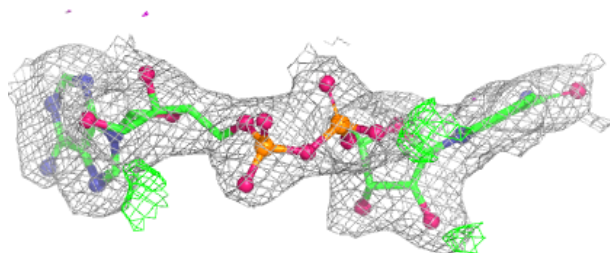
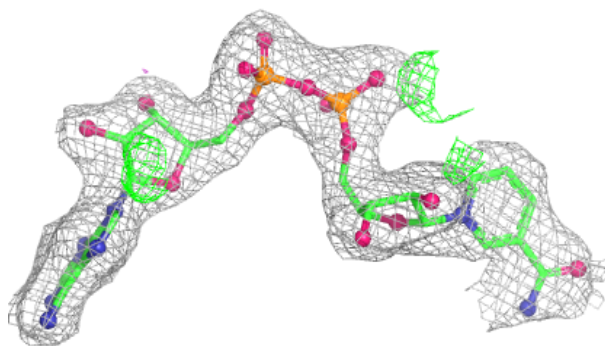
Electron density around FBP C 403:

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

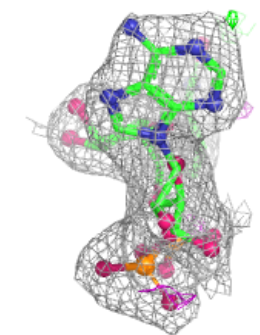
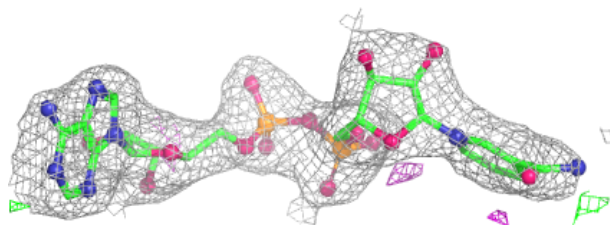
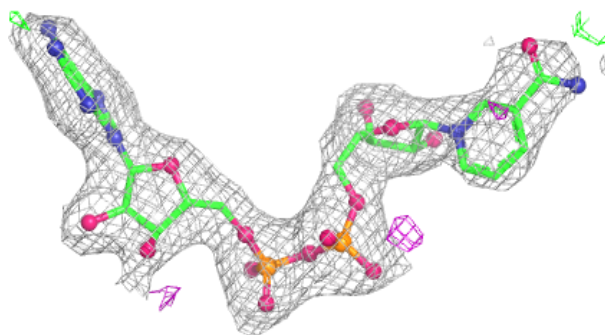


Electron density around NAI D 402:

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

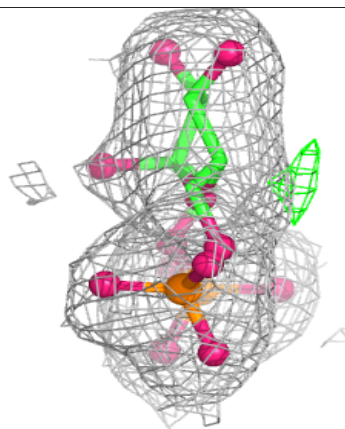
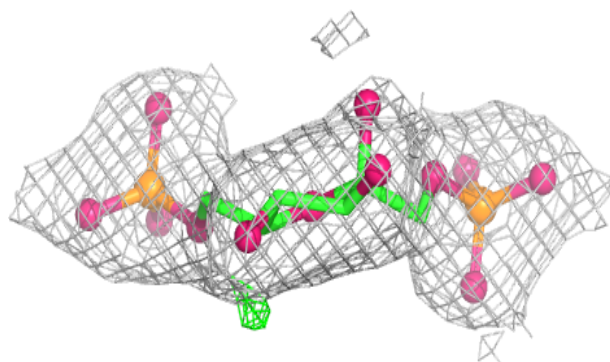
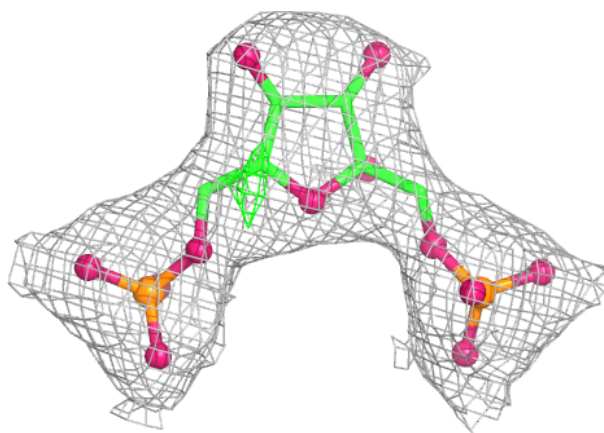
**Electron density around NAI B 402:**

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

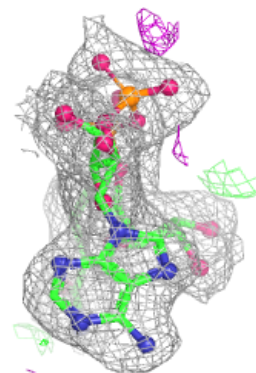
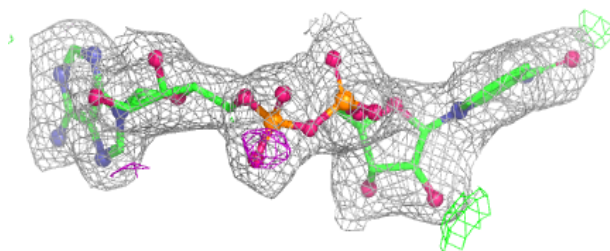
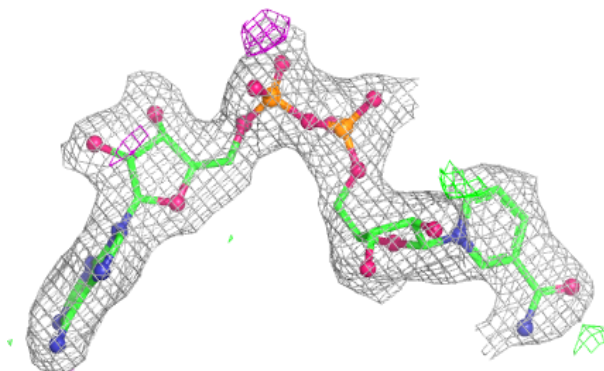


Electron density around FBP A 402:

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

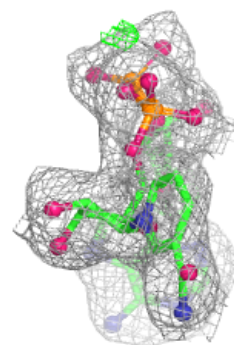
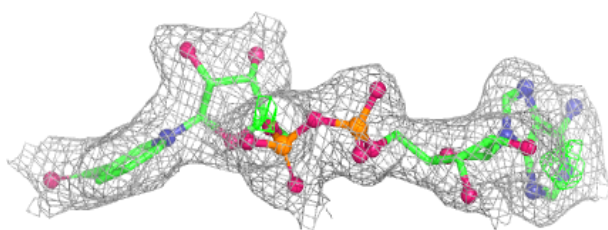
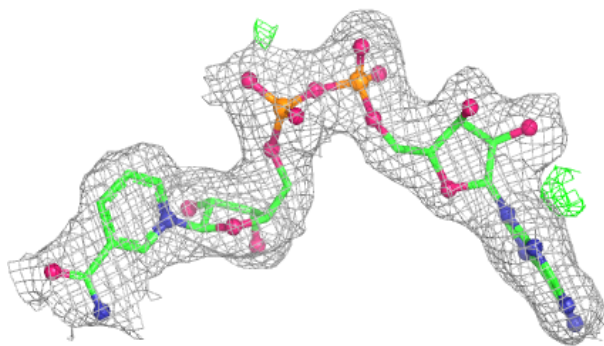
**Electron density around NAI C 402:**

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



Electron density around NAI A 403:

$2mF_o-DF_c$ (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.