



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:42 AM UTC

PDB ID : 7ERE / pdb_00007ere
Title : Crystal structure of human Biliverdin IX-beta reductase B with Pyranel Pamoate (PPA)
Authors : Griesinger, C.; Lee, D.; Ryu, K.S.; Kim, M.; Ha, J.H.
Deposited on : 2021-05-06
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

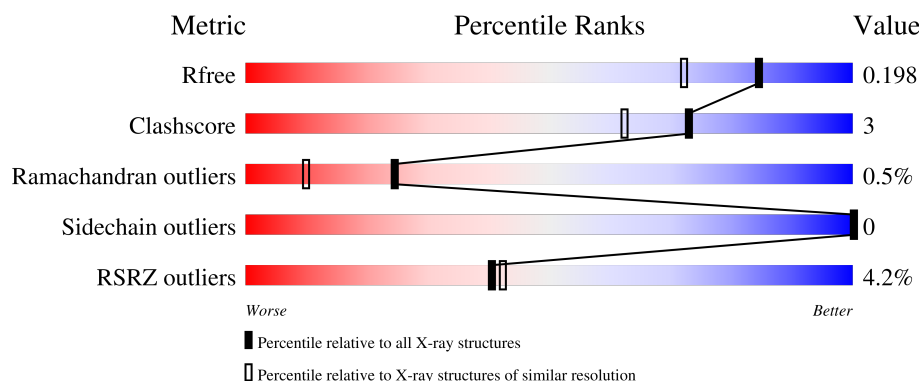
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	207	4% 96% .
1	B	207	5% 92% 8%
1	C	207	3% 92% 8%
1	D	207	5% 93% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7467 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 Flavin reductase (NADPH).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	4	0
			1585	994	283	300	8			
1	B	206	Total	C	N	O	S	0	2	0
			1565	982	280	295	8			
1	C	207	Total	C	N	O	S	0	6	0
			1598	1002	286	302	8			
1	D	206	Total	C	N	O	S	0	5	0
			1584	994	284	298	8			

There are 4 discrepancies between the modelled and reference sequences:

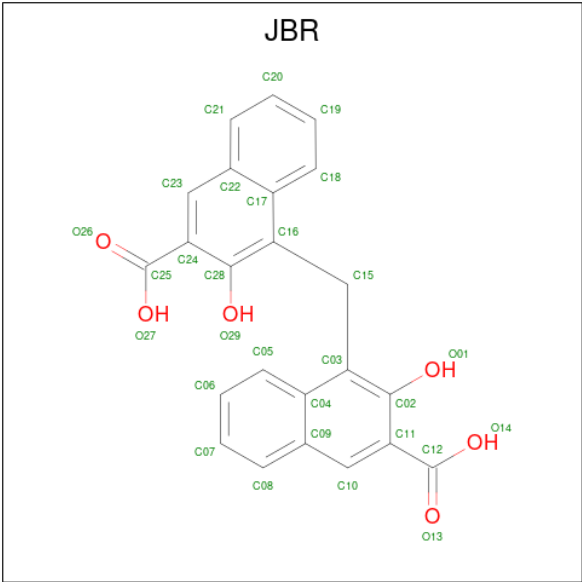
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P30043
B	0	HIS	-	expression tag	UNP P30043
C	0	HIS	-	expression tag	UNP P30043
D	0	HIS	-	expression tag	UNP P30043

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



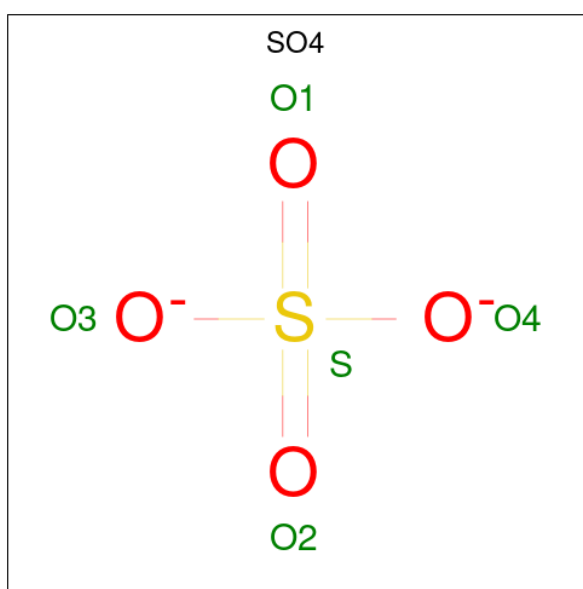
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 4-[(3-carboxy-2-oxidanyl-naphthalen-1-yl)methyl]-3-oxidanyl-naphthalene-2-carboxylic acid (CCD ID: JBR) (formula: C₂₃H₁₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			29	23	6		
3	A	1	Total	C	O	0	0
			29	23	6		
3	C	1	Total	C	O	0	0
			29	23	6		
3	D	1	Total	C	O	0	0
			29	23	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total 227	O 227	0	0
5	B	159	Total 159	O 159	0	0
5	C	215	Total 215	O 215	0	0
5	D	191	Total 191	O 191	0	0

3 Residue-property plots [i](#)

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

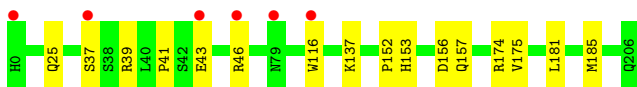
- Molecule 1: Flavin reductase (NADPH)



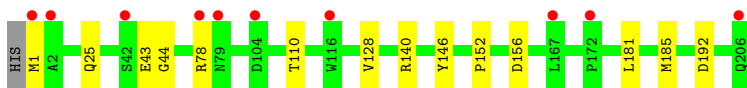
- Molecule 1: Flavin reductase (NADPH)



- Molecule 1: Flavin reductase (NADPH)



- Molecule 1: Flavin reductase (NADPH)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.98Å 117.38Å 81.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 1.60 47.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.72-1.60) 99.6 (47.72-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.171 , 0.198 0.171 , 0.198	Depositor DCC
R_{free} test set	2001 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2865e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: JBR, NAP, SO4

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	0.39	0/1629	0.56	0/2218
1	B	0.30	0/1602	0.52	0/2181
1	C	0.41	0/1648	0.58	0/2243
1	D	0.33	0/1630	0.52	0/2218
All	All	0.36	0/6509	0.54	0/8860

There are no bond length outliers.

There are no bond angle outliers.

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	1585	0	1601	6	0
1	B	1565	0	1586	13	0
1	C	1598	0	1618	13	0
1	D	1584	0	1611	11	0
2	A	48	0	25	1	0
2	B	48	0	23	2	0
2	C	48	0	24	1	0
2	D	48	0	25	1	0
3	A	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	29	0	0	3	0
3	D	29	0	0	0	0
4	A	5	0	0	1	0
4	B	10	0	0	0	0
4	C	5	0	0	1	0
4	D	15	0	0	1	0
5	A	227	0	0	0	1
5	B	159	0	0	4	2
5	C	215	0	0	2	5
5	D	191	0	0	5	4
All	All	7467	0	6513	42	6

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 (42) 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:A:170:ARG:NH1	4:A:404:SO4:O1	2.11	0.81
1:B:126[B]:GLN:OE1	5:B:501:HOH:O	2.12	0.67
1:C:157:GLN:HE22	1:C:175:VAL:HG21	1.62	0.63
1:D:25[B]:GLN:OE1	5:D:501:HOH:O	2.17	0.58
1:B:187:ARG:NH2	5:B:506:HOH:O	2.32	0.58
4:D:403:SO4:O2	5:D:503:HOH:O	2.17	0.58
1:B:112:ALA:O	1:B:116:TRP:HD1	1.92	0.53
1:B:168:ASP:HA	1:B:198:SER:OG	2.09	0.52
1:B:140:ARG:NH1	5:B:503:HOH:O	2.29	0.52
1:D:43:GLU:CD	1:D:44:GLY:H	2.18	0.51
1:C:156[A]:ASP:OD2	5:C:501:HOH:O	2.19	0.51
1:D:78[B]:ARG:NH1	5:D:502:HOH:O	2.17	0.50
1:B:168:ASP:HA	1:B:198:SER:HG	1.77	0.50
1:C:116:TRP:HH2	3:C:402:JBR:C06	2.25	0.49
1:D:78[B]:ARG:NH2	5:D:506:HOH:O	2.30	0.49
1:C:137:LYS:HE2	1:D:156:ASP:OD1	2.13	0.48
1:D:181:LEU:O	1:D:185:MET:HG2	2.13	0.48
1:D:128:VAL:HG23	5:D:558:HOH:O	2.14	0.48
1:C:153:HIS:HB2	3:C:402:JBR:O01	2.14	0.48
1:A:153:HIS:HB2	3:A:402:JBR:O29	2.13	0.47
1:B:173:SER:HB2	1:B:202:SER:HB2	1.96	0.47
1:A:181:LEU:O	1:A:185:MET:HG2	2.15	0.46
1:B:78:ARG:HG2	2:B:401:NAP:O1A	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLY:O	2:A:401:NAP:H8A	2.16	0.46
1:B:76:GLY:O	2:B:401:NAP:H8A	2.16	0.45
1:C:41:PRO:HB2	1:C:43:GLU:HG2	2.00	0.44
1:A:41:PRO:O	1:A:46:ARG:NH2	2.51	0.44
1:B:181:LEU:O	1:B:185:MET:HG2	2.17	0.44
1:A:137:LYS:HE2	1:B:156:ASP:OD1	2.18	0.43
1:B:77:THR:HG22	1:C:37:SER:CB	2.49	0.43
1:C:174:ARG:HG3	4:C:403:SO4:O2	2.19	0.43
1:B:126[B]:GLN:NE2	5:B:514:HOH:O	2.47	0.42
1:D:110:THR:O	2:D:401:NAP:H6N	2.19	0.42
1:D:140:ARG:HG2	1:D:146:TYR:HE2	1.85	0.42
1:C:181:LEU:O	1:C:185:MET:HG2	2.20	0.42
1:C:46:ARG:NE	1:C:46:ARG:HA	2.36	0.41
1:D:140:ARG:HG2	1:D:146:TYR:CE2	2.56	0.41
1:C:25[B]:GLN:HG2	5:C:574:HOH:O	2.20	0.41
1:C:39[B]:ARG:HE	1:C:39[B]:ARG:HB3	1.58	0.41
1:C:116:TRP:CH2	3:C:402:JBR:C06	3.04	0.40
1:D:1:MET:HE2	1:D:192[B]:ASP:OD2	2.21	0.40
2:C:401:NAP:H2D	2:C:401:NAP:H2N	1.87	0.40

All (6) 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)
5:C:667:HOH:O	5:D:625:HOH:O[3_544]	2.00	0.20
5:C:562:HOH:O	5:D:676:HOH:O[4_545]	2.08	0.12
5:C:630:HOH:O	5:D:676:HOH:O[4_545]	2.09	0.11
5:B:521:HOH:O	5:C:554:HOH:O[4_445]	2.11	0.09
5:A:713:HOH:O	5:B:608:HOH:O[3_555]	2.12	0.08
5:C:684:HOH:O	5:D:648:HOH:O[3_544]	2.16	0.04

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	209/207 (101%)	205 (98%)	3 (1%)	1 (0%)	24	10
1	B	206/207 (100%)	202 (98%)	3 (2%)	1 (0%)	24	10
1	C	211/207 (102%)	206 (98%)	4 (2%)	1 (0%)	24	10
1	D	209/207 (101%)	205 (98%)	3 (1%)	1 (0%)	24	10
All	All	835/828 (101%)	818 (98%)	13 (2%)	4 (0%)	24	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	C	152	PRO
1	B	152	PRO
1	D	152	PRO

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	174/170 (102%)	174 (100%)	0	100	100
1	B	171/170 (101%)	171 (100%)	0	100	100
1	C	176/170 (104%)	176 (100%)	0	100	100
1	D	174/170 (102%)	174 (100%)	0	100	100
All	All	695/680 (102%)	695 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	206	GLN
1	C	153	HIS

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 ⓘ

15 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	NAP	A	401	-	50,52,52	3.00	15 (30%)	71,80,80	1.74	13 (18%)
2	NAP	D	401	-	50,52,52	3.62	17 (34%)	71,80,80	1.76	19 (26%)
4	SO4	D	404	-	4,4,4	0.24	0	6,6,6	0.09	0
3	JBR	D	402	-	32,32,32	1.17	3 (9%)	47,47,47	1.26	6 (12%)
2	NAP	B	401	-	50,52,52	3.68	17 (34%)	71,80,80	1.81	16 (22%)
4	SO4	D	405	-	4,4,4	0.24	0	6,6,6	0.10	0
3	JBR	C	402	-	32,32,32	1.20	2 (6%)	47,47,47	1.12	4 (8%)
4	SO4	D	403	-	4,4,4	0.31	0	6,6,6	0.24	0
4	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	B	403	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	A	404	-	4,4,4	0.21	0	6,6,6	0.24	0
3	JBR	A	402	-	32,32,32	1.12	2 (6%)	47,47,47	1.13	3 (6%)
2	NAP	C	401	-	50,52,52	3.05	13 (26%)	71,80,80	1.65	14 (19%)
3	JBR	A	403	-	32,32,32	1.15	2 (6%)	47,47,47	1.23	3 (6%)
4	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.15	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	NAP	A	401	-	-	4/35/67/67	0/5/5/5
2	NAP	D	401	-	-	5/35/67/67	0/5/5/5
3	JBR	D	402	-	-	4/12/12/12	0/4/4/4
2	NAP	B	401	-	-	5/35/67/67	0/5/5/5
3	JBR	C	402	-	-	4/12/12/12	0/4/4/4
3	JBR	A	402	-	-	4/12/12/12	0/4/4/4
2	NAP	C	401	-	-	6/35/67/67	0/5/5/5
3	JBR	A	403	-	-	6/12/12/12	0/4/4/4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	O4D-C1D	15.76	1.61	1.40
2	D	401	NAP	O4D-C1D	15.43	1.61	1.40
2	A	401	NAP	O4D-C1D	12.71	1.57	1.40
2	C	401	NAP	O4D-C1D	12.23	1.56	1.40
2	D	401	NAP	C2B-C1B	-8.38	1.32	1.53
2	B	401	NAP	C2B-C1B	-8.27	1.32	1.53
2	D	401	NAP	O4B-C1B	8.00	1.60	1.42
2	B	401	NAP	O4B-C1B	7.95	1.60	1.42
2	D	401	NAP	C7N-N7N	7.92	1.47	1.33
2	C	401	NAP	C7N-N7N	7.76	1.47	1.33
2	B	401	NAP	C7N-N7N	7.63	1.47	1.33
2	A	401	NAP	C7N-N7N	7.48	1.46	1.33
2	B	401	NAP	PA-O3	6.88	1.66	1.59
2	C	401	NAP	C2B-C1B	-6.70	1.36	1.53
2	A	401	NAP	C2B-C1B	-6.44	1.37	1.53
2	D	401	NAP	PA-O3	6.37	1.66	1.59
2	C	401	NAP	O4B-C1B	6.12	1.56	1.42
2	C	401	NAP	PA-O3	5.85	1.65	1.59
2	A	401	NAP	O4B-C1B	5.27	1.54	1.42
2	B	401	NAP	O4D-C4D	-5.26	1.33	1.45
2	B	401	NAP	O4B-C4B	-5.22	1.33	1.45
2	D	401	NAP	O4B-C4B	-5.15	1.33	1.45
2	D	401	NAP	O4D-C4D	-5.03	1.33	1.45
2	A	401	NAP	P2B-O2B	4.79	1.67	1.59
2	A	401	NAP	O4D-C4D	-4.72	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	P2B-O2B	4.68	1.67	1.59
2	C	401	NAP	O4D-C4D	-4.59	1.34	1.45
2	D	401	NAP	P2B-O2B	4.57	1.67	1.59
2	B	401	NAP	PN-O3	4.47	1.64	1.59
2	C	401	NAP	O4B-C4B	-4.26	1.35	1.45
2	D	401	NAP	PN-O3	3.96	1.63	1.59
2	C	401	NAP	P2B-O2B	3.86	1.66	1.59
2	A	401	NAP	PA-O3	3.73	1.63	1.59
2	A	401	NAP	O4B-C4B	-3.72	1.36	1.45
2	A	401	NAP	PN-O3	3.14	1.62	1.59
2	A	401	NAP	C8A-N7A	3.10	1.37	1.31
2	C	401	NAP	C2A-N3A	3.07	1.39	1.33
2	D	401	NAP	C6A-N6A	2.98	1.41	1.34
2	B	401	NAP	C6A-N6A	2.87	1.41	1.34
2	D	401	NAP	C8A-N7A	2.76	1.37	1.31
2	B	401	NAP	C8A-N7A	2.72	1.36	1.31
2	C	401	NAP	C6A-N6A	2.69	1.41	1.34
2	B	401	NAP	O3B-C3B	-2.68	1.36	1.43
3	C	402	JBR	C04-C09	-2.64	1.38	1.43
2	B	401	NAP	O3D-C3D	-2.62	1.36	1.43
2	B	401	NAP	C4N-C3N	-2.59	1.35	1.39
2	C	401	NAP	O3B-C3B	-2.59	1.36	1.43
2	D	401	NAP	C4N-C3N	-2.52	1.35	1.39
2	C	401	NAP	C4N-C3N	-2.47	1.35	1.39
2	B	401	NAP	C5A-C4A	-2.44	1.34	1.39
3	C	402	JBR	C17-C22	-2.40	1.38	1.43
2	D	401	NAP	O3B-C3B	-2.38	1.37	1.43
3	A	403	JBR	C04-C09	-2.38	1.38	1.43
2	D	401	NAP	O3D-C3D	-2.37	1.37	1.43
2	A	401	NAP	C2N-C3N	2.37	1.42	1.39
2	A	401	NAP	C2A-N3A	2.32	1.38	1.33
3	A	402	JBR	C04-C09	-2.31	1.38	1.43
2	D	401	NAP	C2A-N3A	2.30	1.38	1.33
3	D	402	JBR	C04-C09	-2.30	1.38	1.43
3	A	402	JBR	C17-C22	-2.28	1.38	1.43
3	A	403	JBR	C17-C22	-2.25	1.38	1.43
2	A	401	NAP	C6A-N6A	2.22	1.39	1.34
2	A	401	NAP	C5A-C4A	-2.18	1.35	1.39
2	B	401	NAP	C2A-N3A	2.17	1.37	1.33
3	D	402	JBR	C17-C22	-2.16	1.39	1.43
2	D	401	NAP	C5A-C4A	-2.14	1.35	1.39
2	B	401	NAP	O7N-C7N	-2.14	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O3B-C3B	-2.10	1.37	1.43
2	C	401	NAP	C8A-N7A	2.05	1.35	1.31
2	D	401	NAP	O2D-C2D	2.05	1.48	1.43
3	D	402	JBR	C24-C25	2.02	1.54	1.49

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	N3A-C2A-N1A	-6.16	119.26	128.58
2	B	401	NAP	N3A-C2A-N1A	-5.95	119.58	128.58
2	D	401	NAP	N3A-C2A-N1A	-5.76	119.87	128.58
2	C	401	NAP	N3A-C2A-N1A	-5.66	120.02	128.58
2	B	401	NAP	C5A-C4A-N3A	-4.90	119.97	126.72
2	D	401	NAP	C5A-C4A-N3A	-4.89	119.98	126.72
2	B	401	NAP	N6A-C6A-N1A	-4.33	108.73	118.38
2	C	401	NAP	C5A-C4A-N3A	-4.33	120.75	126.72
2	D	401	NAP	N6A-C6A-N1A	-4.01	109.45	118.38
2	A	401	NAP	C5A-C4A-N3A	-4.00	121.20	126.72
2	D	401	NAP	N9A-C8A-N7A	-3.97	108.30	113.94
2	A	401	NAP	O4B-C1B-C2B	-3.82	100.01	106.59
2	B	401	NAP	N9A-C8A-N7A	-3.81	108.54	113.94
2	A	401	NAP	N9A-C8A-N7A	-3.76	108.60	113.94
2	D	401	NAP	N3A-C4A-N9A	3.62	133.32	127.17
2	B	401	NAP	N3A-C4A-N9A	3.53	133.18	127.17
2	A	401	NAP	N6A-C6A-N1A	-3.51	110.55	118.38
2	B	401	NAP	C4A-N9A-C1B	-3.41	118.65	126.63
2	B	401	NAP	C2A-N3A-C4A	3.39	120.12	111.83
2	C	401	NAP	N3A-C4A-N9A	3.38	132.92	127.17
2	C	401	NAP	N6A-C6A-N1A	-3.34	110.94	118.38
2	D	401	NAP	C2A-N3A-C4A	3.26	119.79	111.83
2	A	401	NAP	C4D-O4D-C1D	-3.20	106.99	109.92
2	A	401	NAP	N3A-C4A-N9A	3.17	132.56	127.17
2	C	401	NAP	O4B-C1B-C2B	-3.14	101.19	106.59
2	A	401	NAP	C6N-N1N-C2N	-3.11	119.23	121.88
2	A	401	NAP	C4A-N9A-C8A	3.10	108.99	105.74
2	A	401	NAP	C4A-N9A-C1B	-3.02	119.56	126.63
2	A	401	NAP	C2A-N3A-C4A	3.01	119.17	111.83
2	B	401	NAP	C6N-N1N-C2N	-3.00	119.33	121.88
2	C	401	NAP	C4D-O4D-C1D	-2.99	107.19	109.92
2	D	401	NAP	C5A-C6A-N6A	2.97	130.65	123.29
2	B	401	NAP	C5A-C6A-N6A	2.96	130.61	123.29
3	A	403	JBR	C15-C03-C02	2.91	122.78	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	JBR	C15-C03-C02	2.91	122.78	119.50
2	D	401	NAP	C2B-C1B-N9A	-2.89	109.00	113.75
2	C	401	NAP	C6N-N1N-C2N	-2.86	119.44	121.88
2	D	401	NAP	C4A-N9A-C1B	-2.86	119.94	126.63
2	A	401	NAP	C2N-C3N-C4N	2.83	121.55	118.26
2	B	401	NAP	C2N-C3N-C4N	2.80	121.51	118.26
2	C	401	NAP	C4A-N9A-C1B	-2.74	120.22	126.63
2	B	401	NAP	C1B-N9A-C8A	2.69	133.07	127.09
2	B	401	NAP	C4D-O4D-C1D	-2.69	107.46	109.92
2	C	401	NAP	C2A-N3A-C4A	2.66	118.33	111.83
2	C	401	NAP	N9A-C8A-N7A	-2.60	110.25	113.94
2	D	401	NAP	C6N-N1N-C2N	-2.55	119.71	121.88
3	D	402	JBR	O14-C12-C11	2.55	122.53	115.28
2	C	401	NAP	C5A-C6A-N6A	2.54	129.57	123.29
3	C	402	JBR	C28-C24-C25	2.48	122.64	119.86
2	A	401	NAP	C5A-C6A-N6A	2.48	129.41	123.29
2	D	401	NAP	C4A-N9A-C8A	2.44	108.30	105.74
3	C	402	JBR	C16-C15-C03	-2.44	111.37	116.07
2	D	401	NAP	C4D-O4D-C1D	-2.43	107.70	109.92
2	C	401	NAP	C6A-C5A-C4A	2.43	120.49	117.18
3	A	402	JBR	C08-C09-C10	-2.41	117.86	122.00
3	A	402	JBR	C16-C15-C03	-2.38	111.49	116.07
2	B	401	NAP	C4A-N9A-C8A	2.38	108.23	105.74
2	D	401	NAP	O4B-C1B-C2B	-2.36	102.53	106.59
2	C	401	NAP	C1B-N9A-C8A	2.32	132.24	127.09
3	A	402	JBR	O14-C12-C11	2.30	121.82	115.28
2	D	401	NAP	C2N-C3N-C4N	2.29	120.93	118.26
2	D	401	NAP	C5A-N7A-C8A	2.27	107.02	103.45
2	D	401	NAP	C6A-C5A-C4A	2.19	120.17	117.18
2	C	401	NAP	C2B-C1B-N9A	-2.18	110.16	113.75
2	B	401	NAP	C2B-C1B-N9A	-2.16	110.20	113.75
2	B	401	NAP	C5A-N7A-C8A	2.16	106.84	103.45
3	A	403	JBR	C15-C03-C04	-2.13	118.79	121.67
2	D	401	NAP	C3N-C7N-N7N	2.13	120.37	117.74
3	A	403	JBR	O01-C02-C03	2.13	121.65	118.74
2	B	401	NAP	C3N-C7N-N7N	2.12	120.36	117.74
3	D	402	JBR	C10-C11-C02	2.12	120.80	119.11
3	D	402	JBR	O27-C25-C24	2.09	121.22	115.28
2	D	401	NAP	C1B-N9A-C8A	2.09	131.72	127.09
3	C	402	JBR	O27-C25-O26	-2.08	118.89	123.35
3	D	402	JBR	C15-C03-C04	-2.07	118.88	121.67
2	D	401	NAP	O2A-PA-O3	2.07	112.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	JBR	O27-C25-O26	-2.01	119.03	123.35
3	C	402	JBR	C21-C22-C23	-2.00	118.56	122.00

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2D-C1D-N1N-C2N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	B	401	NAP	O4D-C1D-N1N-C2N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	C2D-C1D-N1N-C2N
2	B	401	NAP	C2D-C1D-N1N-C6N
2	C	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	C2D-C1D-N1N-C2N
2	C	401	NAP	C2D-C1D-N1N-C6N
2	D	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	C2D-C1D-N1N-C2N
2	D	401	NAP	C2D-C1D-N1N-C6N
3	C	402	JBR	C02-C11-C12-O13
3	C	402	JBR	C02-C11-C12-O14
3	D	402	JBR	C04-C03-C15-C16
3	A	403	JBR	C02-C03-C15-C16
3	A	403	JBR	C04-C03-C15-C16
3	D	402	JBR	C02-C03-C15-C16
3	A	402	JBR	C28-C24-C25-O26
3	A	403	JBR	C02-C11-C12-O13
3	A	402	JBR	C28-C24-C25-O27
3	A	403	JBR	C02-C11-C12-O14
3	D	402	JBR	C02-C11-C12-O14
3	D	402	JBR	C02-C11-C12-O13
3	C	402	JBR	C10-C11-C12-O13
3	C	402	JBR	C10-C11-C12-O14
2	B	401	NAP	C2B-O2B-P2B-O1X
3	A	402	JBR	C23-C24-C25-O27
3	A	403	JBR	C10-C11-C12-O14
3	A	402	JBR	C23-C24-C25-O26
3	A	403	JBR	C10-C11-C12-O13

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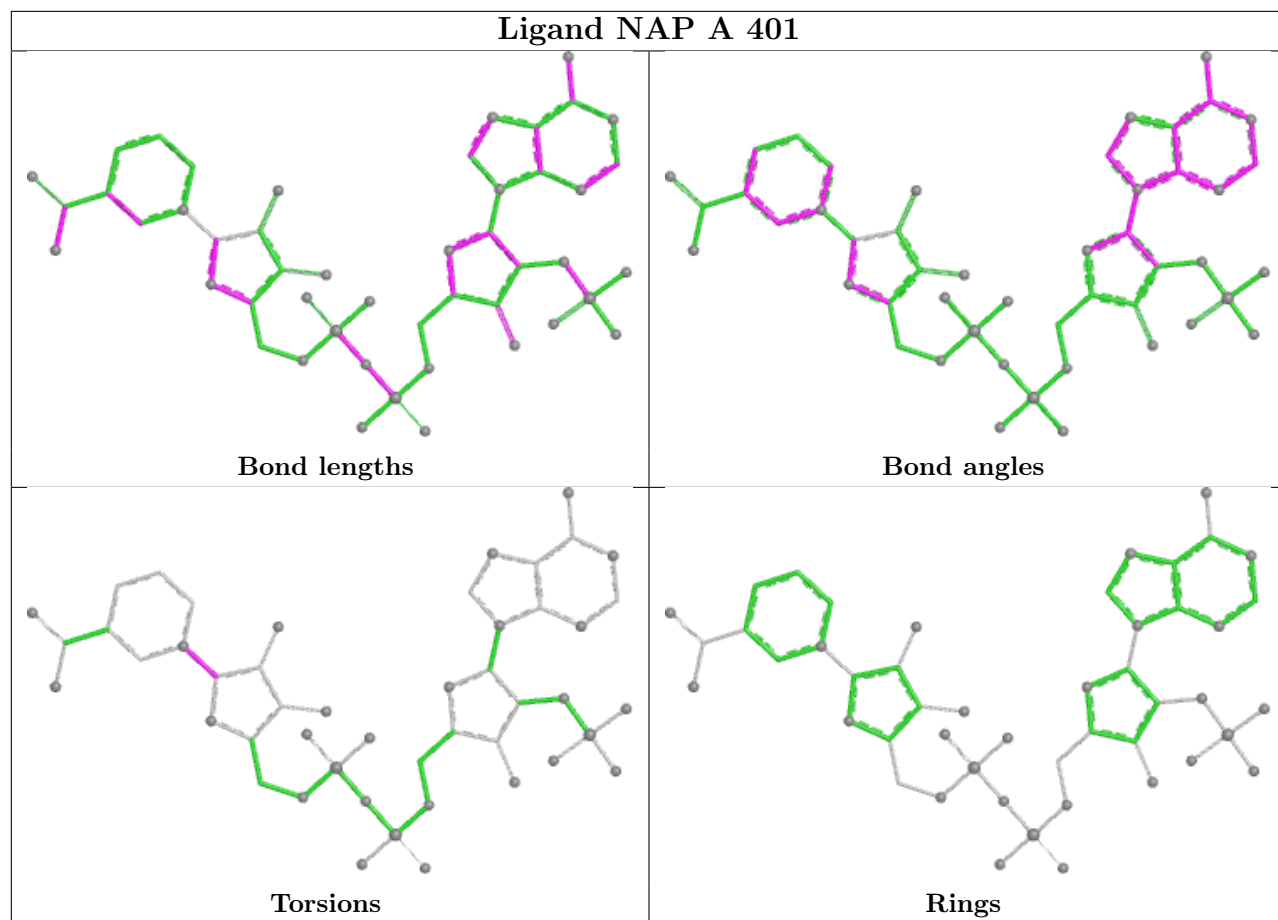
Mol	Chain	Res	Type	Atoms
2	D	401	NAP	C2B-O2B-P2B-O3X
2	C	401	NAP	C2B-O2B-P2B-O1X
2	C	401	NAP	O4B-C4B-C5B-O5B

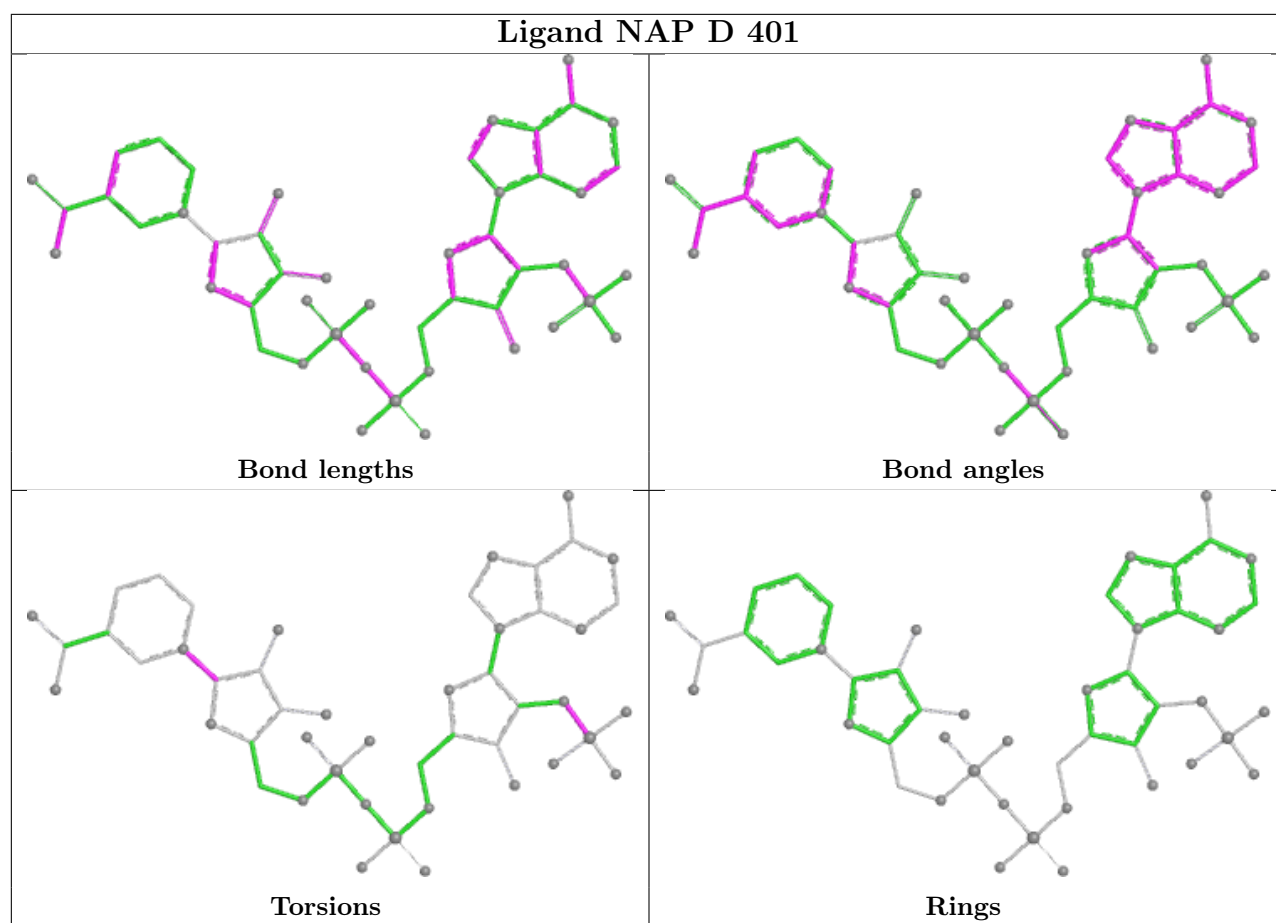
There are no ring outliers.

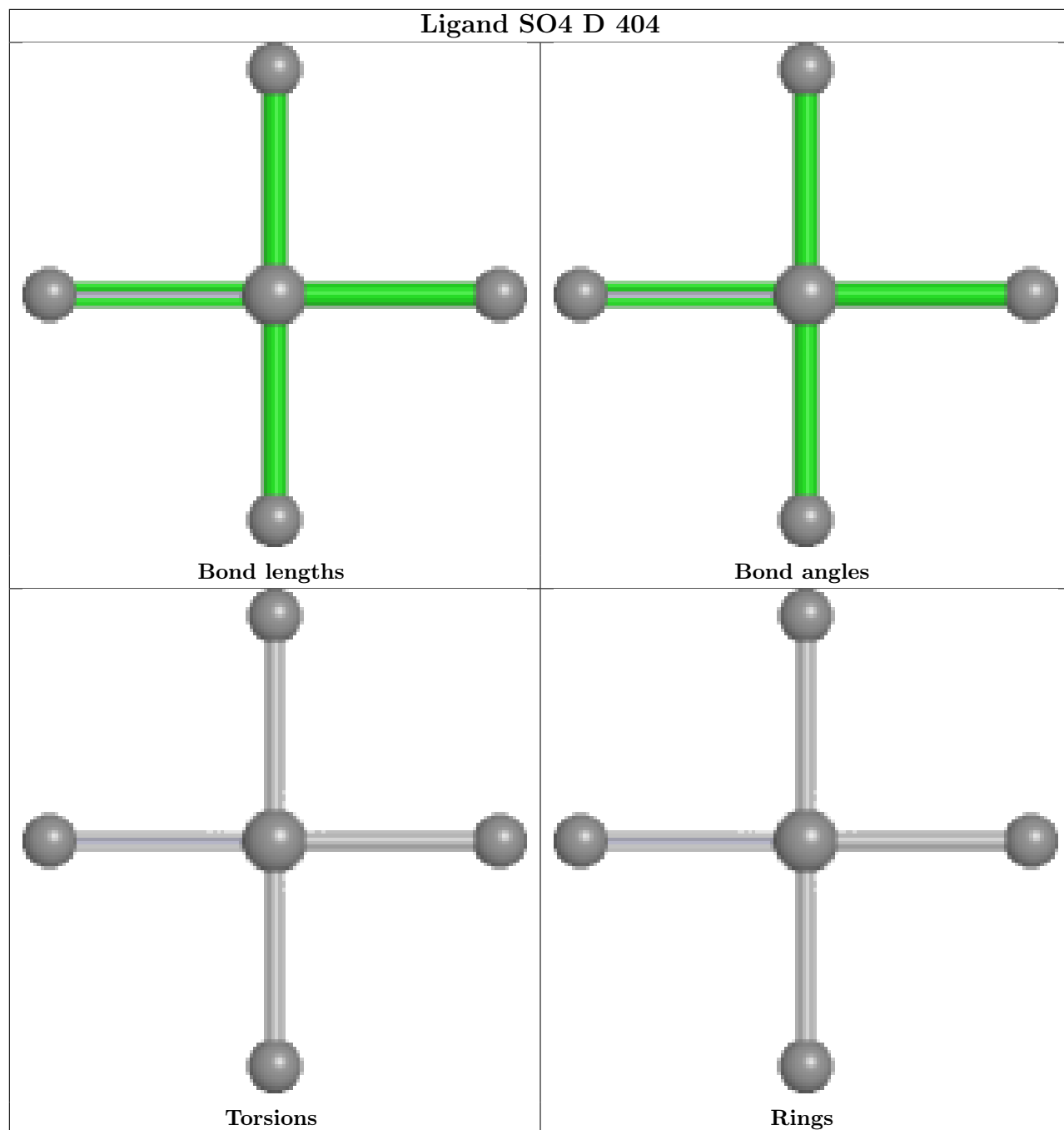
9 monomers are involved in 12 short contacts:

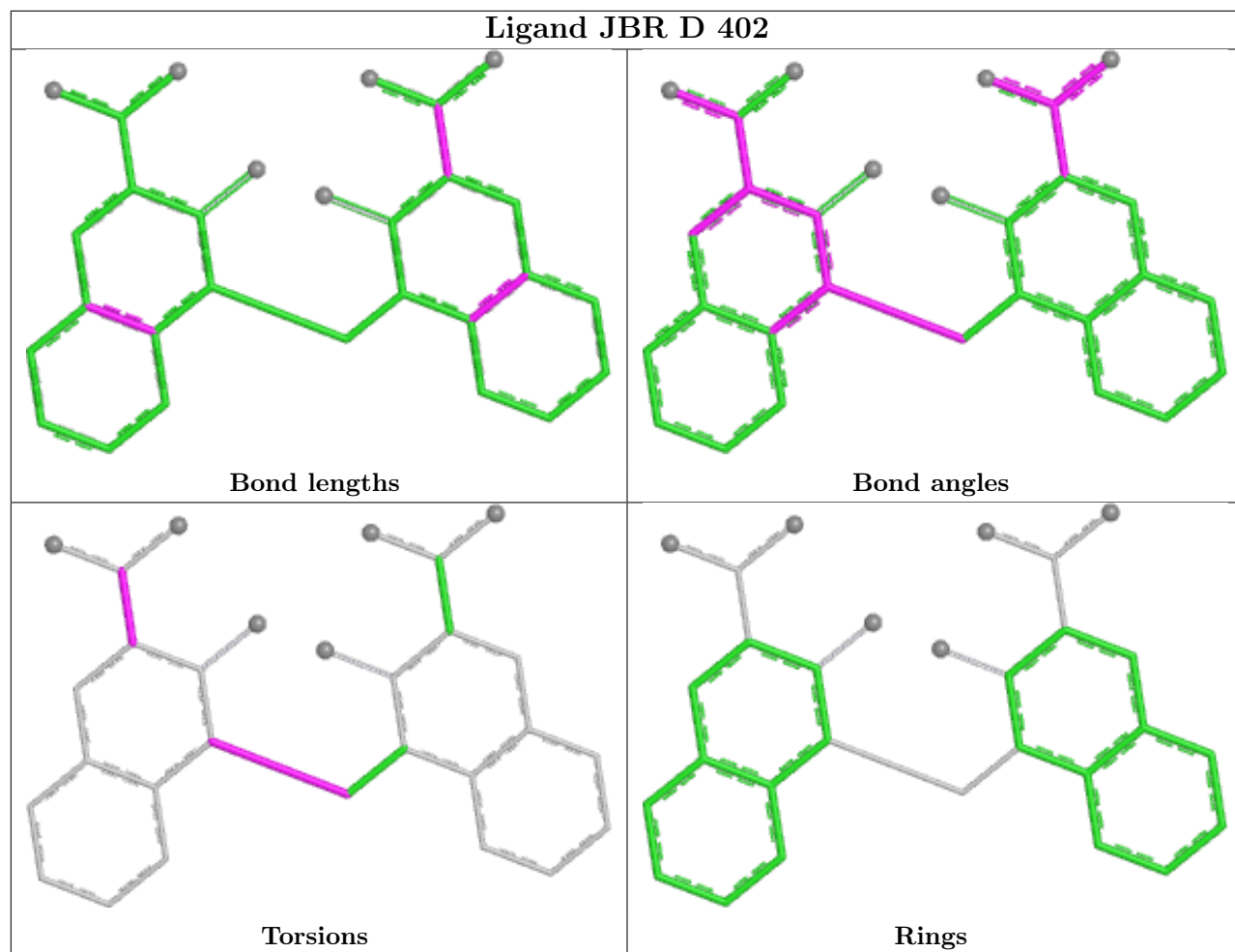
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	1	0
2	D	401	NAP	1	0
2	B	401	NAP	2	0
3	C	402	JBR	3	0
4	D	403	SO4	1	0
4	C	403	SO4	1	0
4	A	404	SO4	1	0
3	A	402	JBR	1	0
2	C	401	NAP	1	0

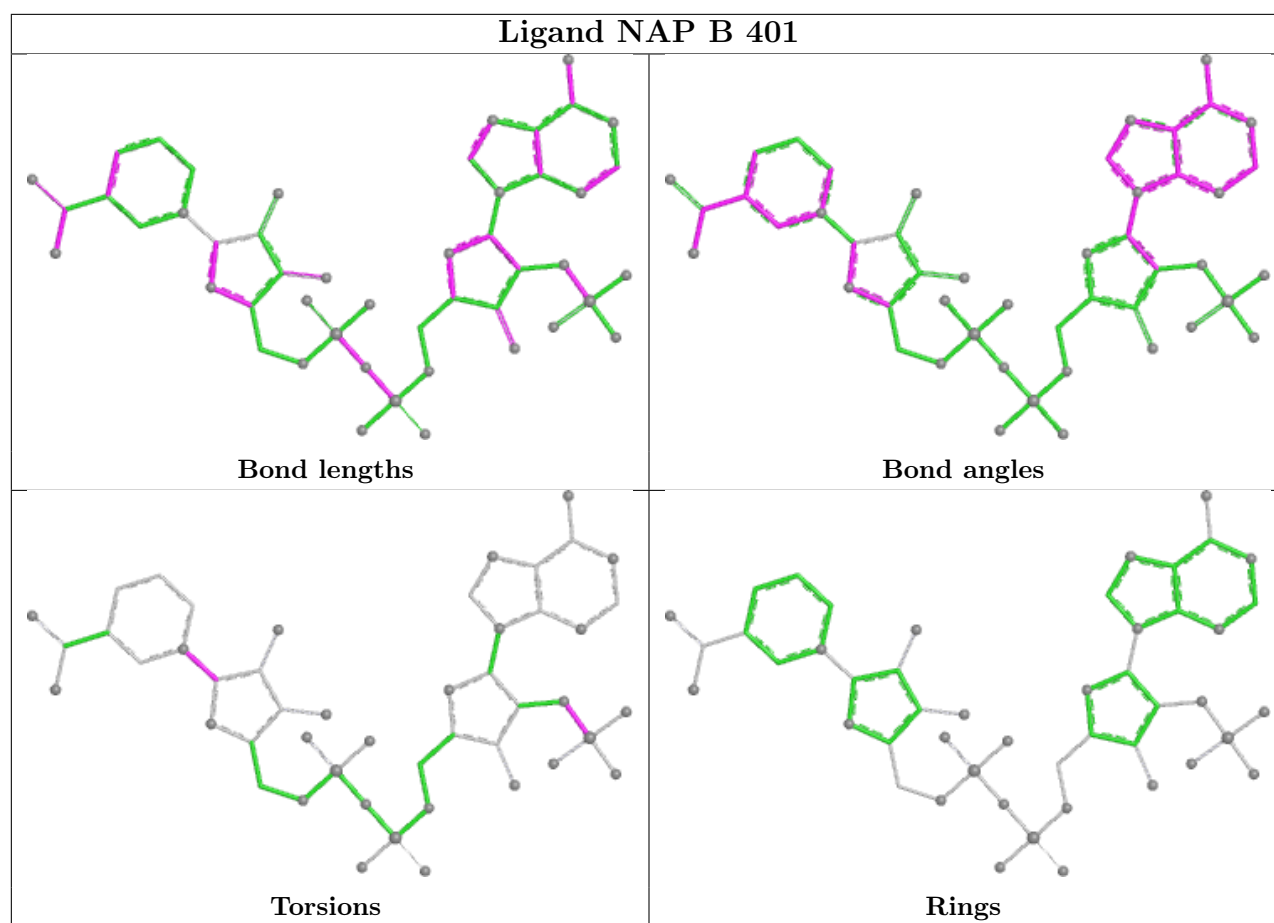
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

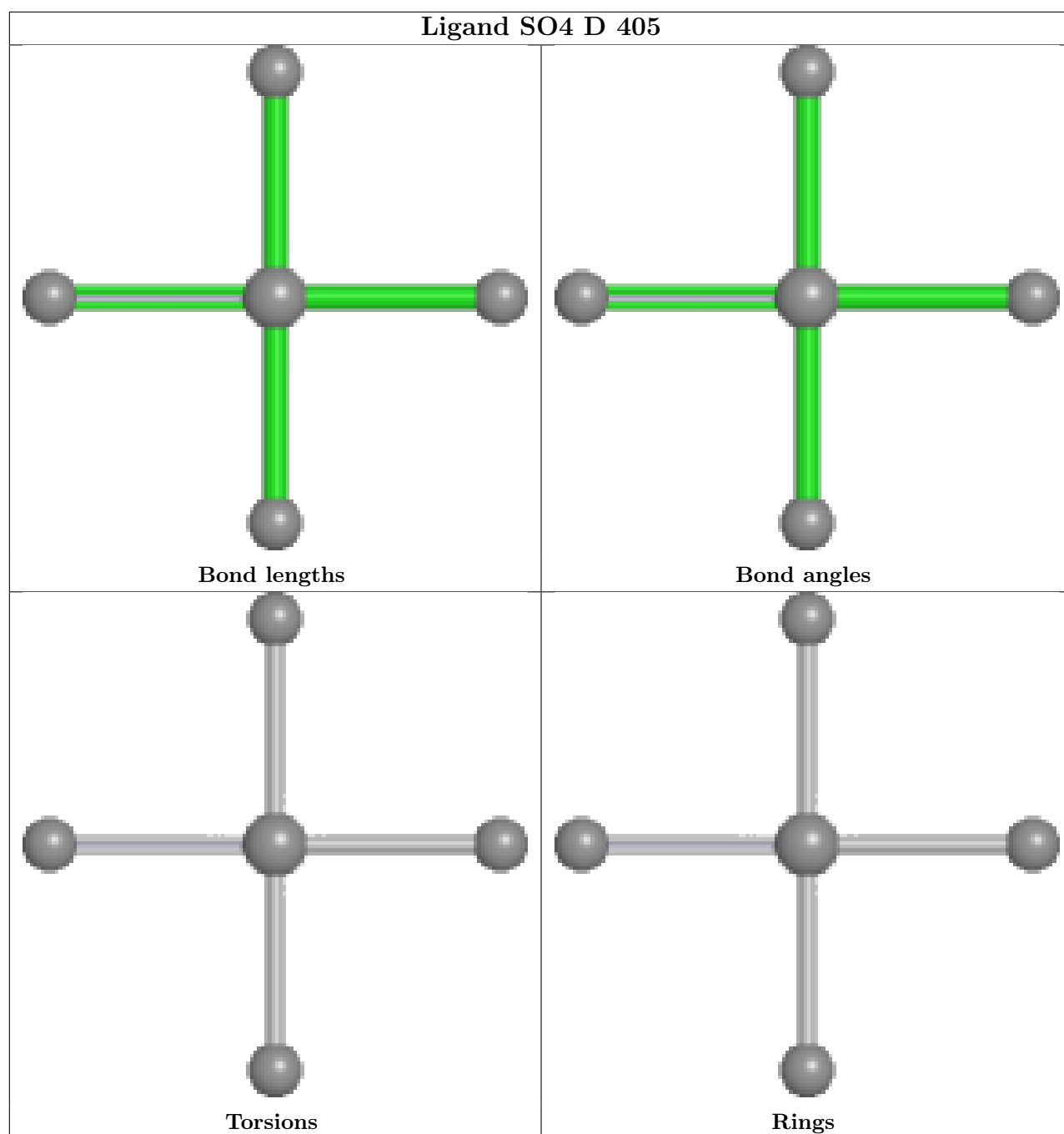


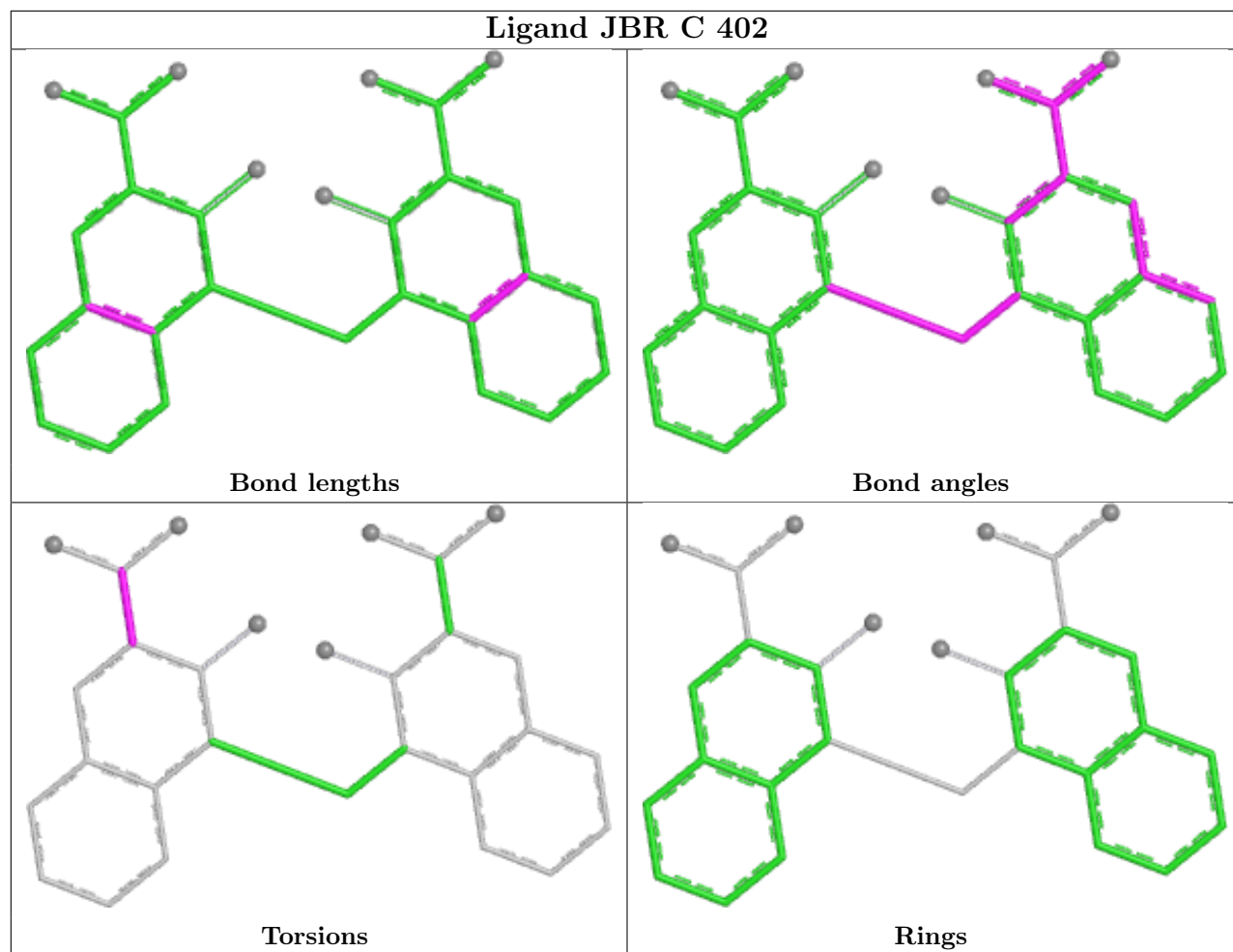


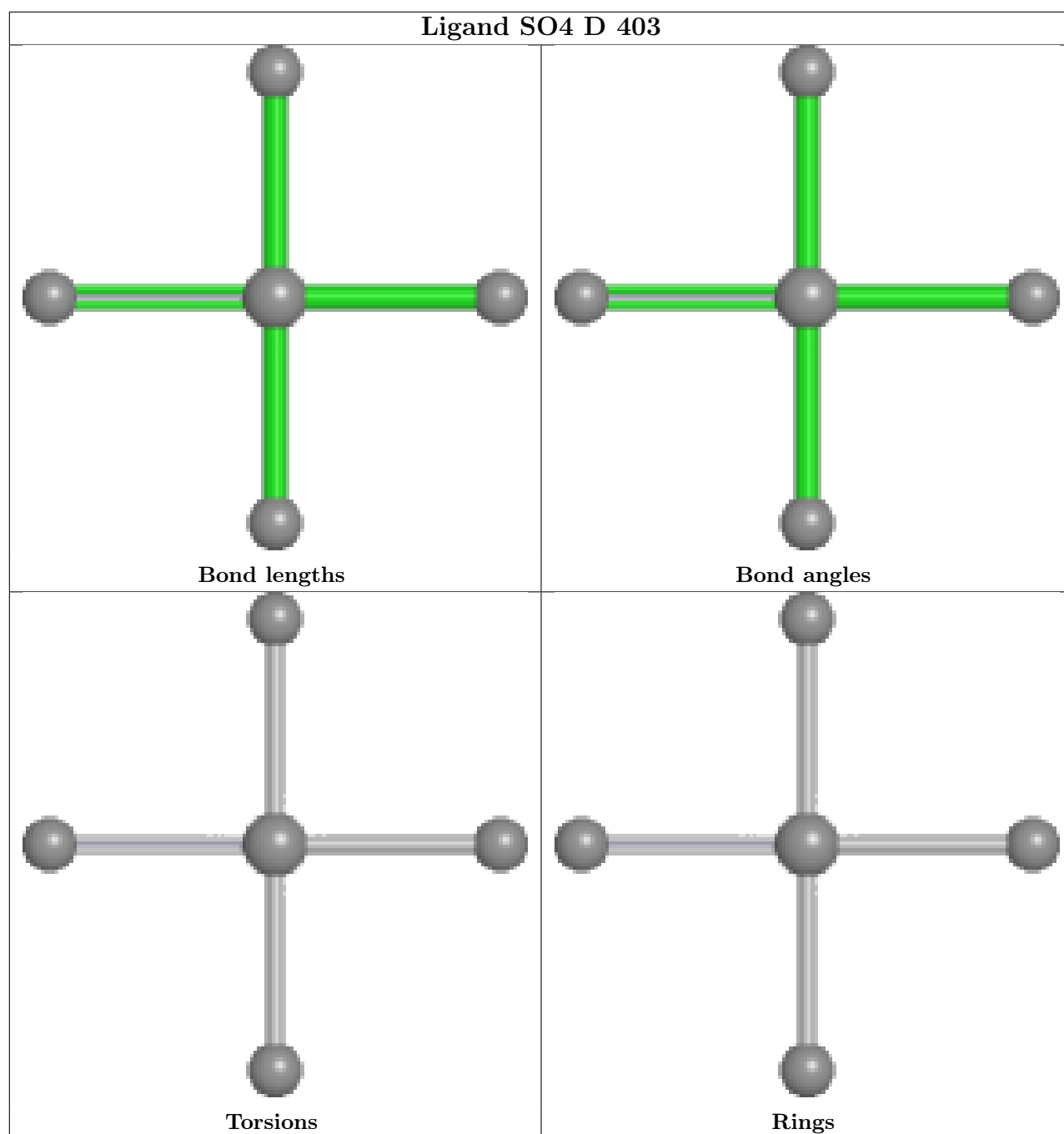


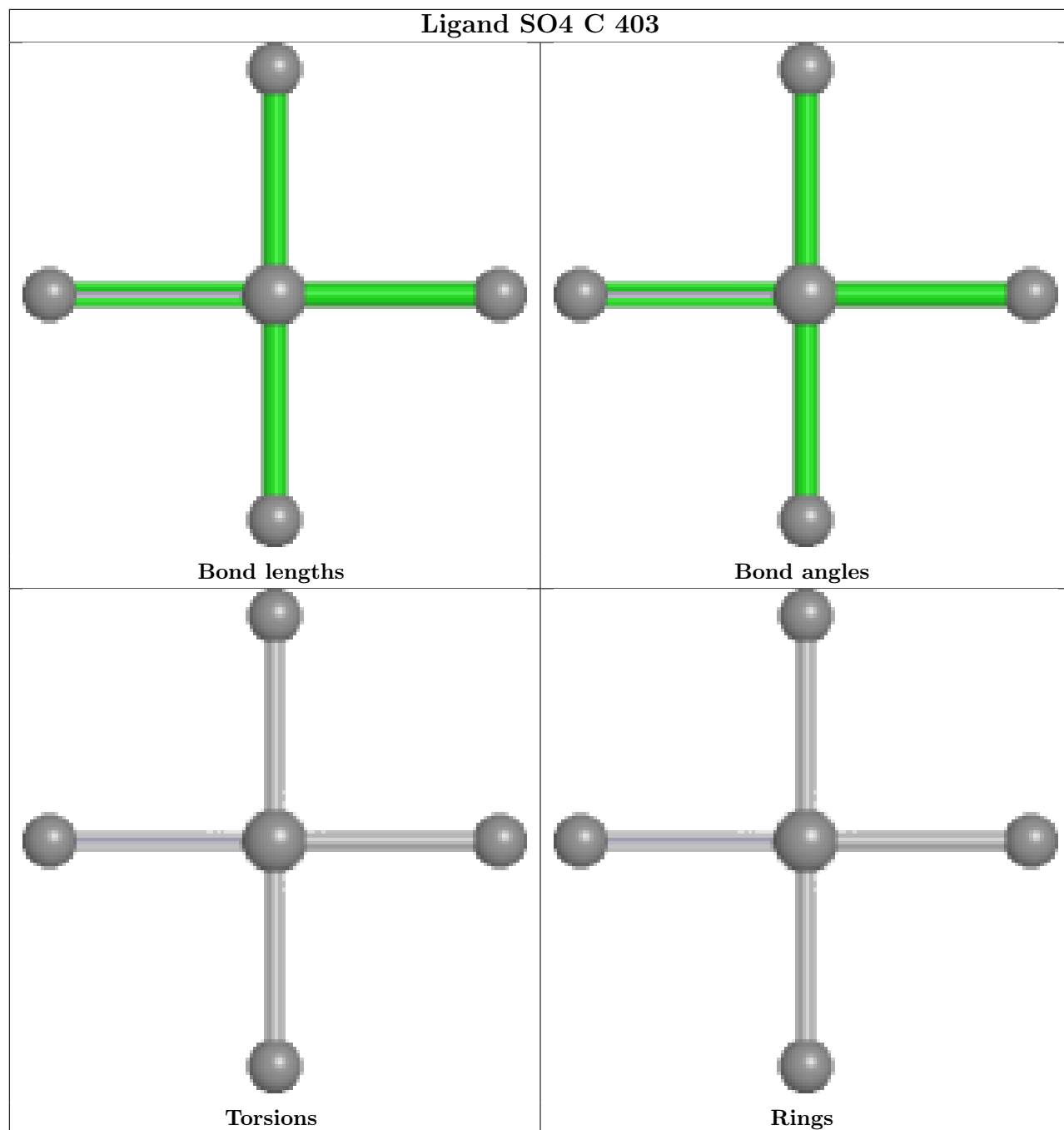


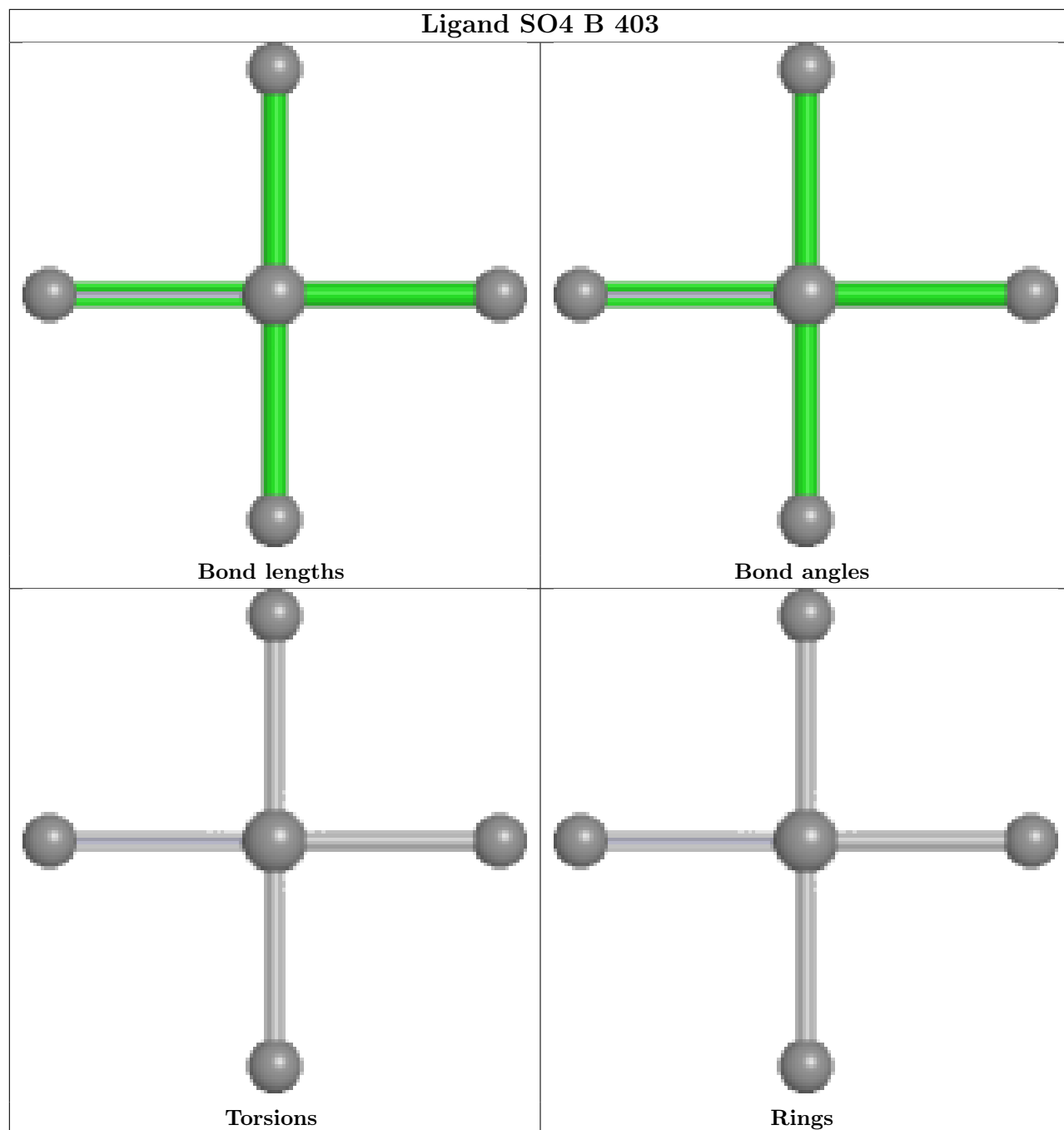


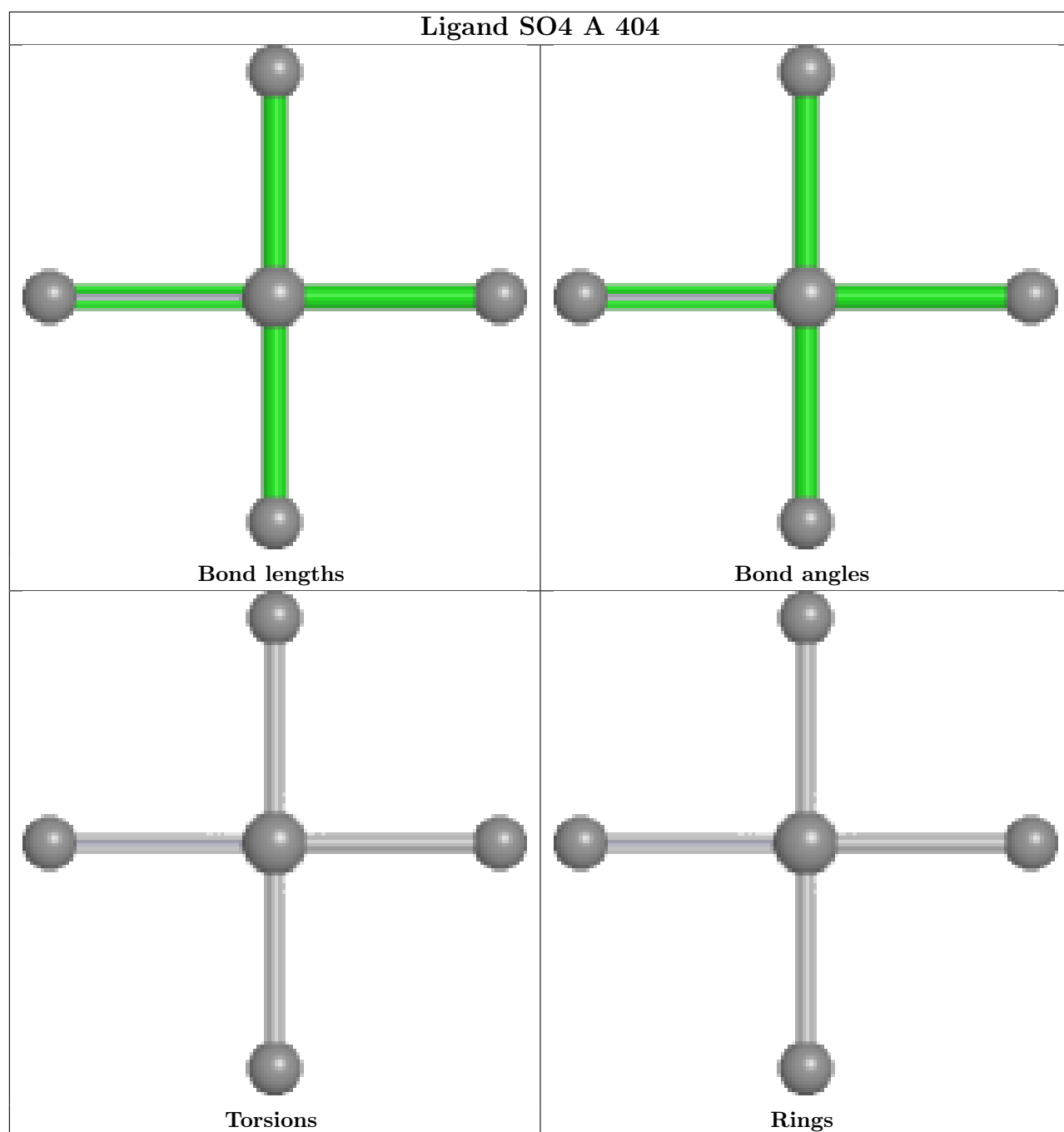


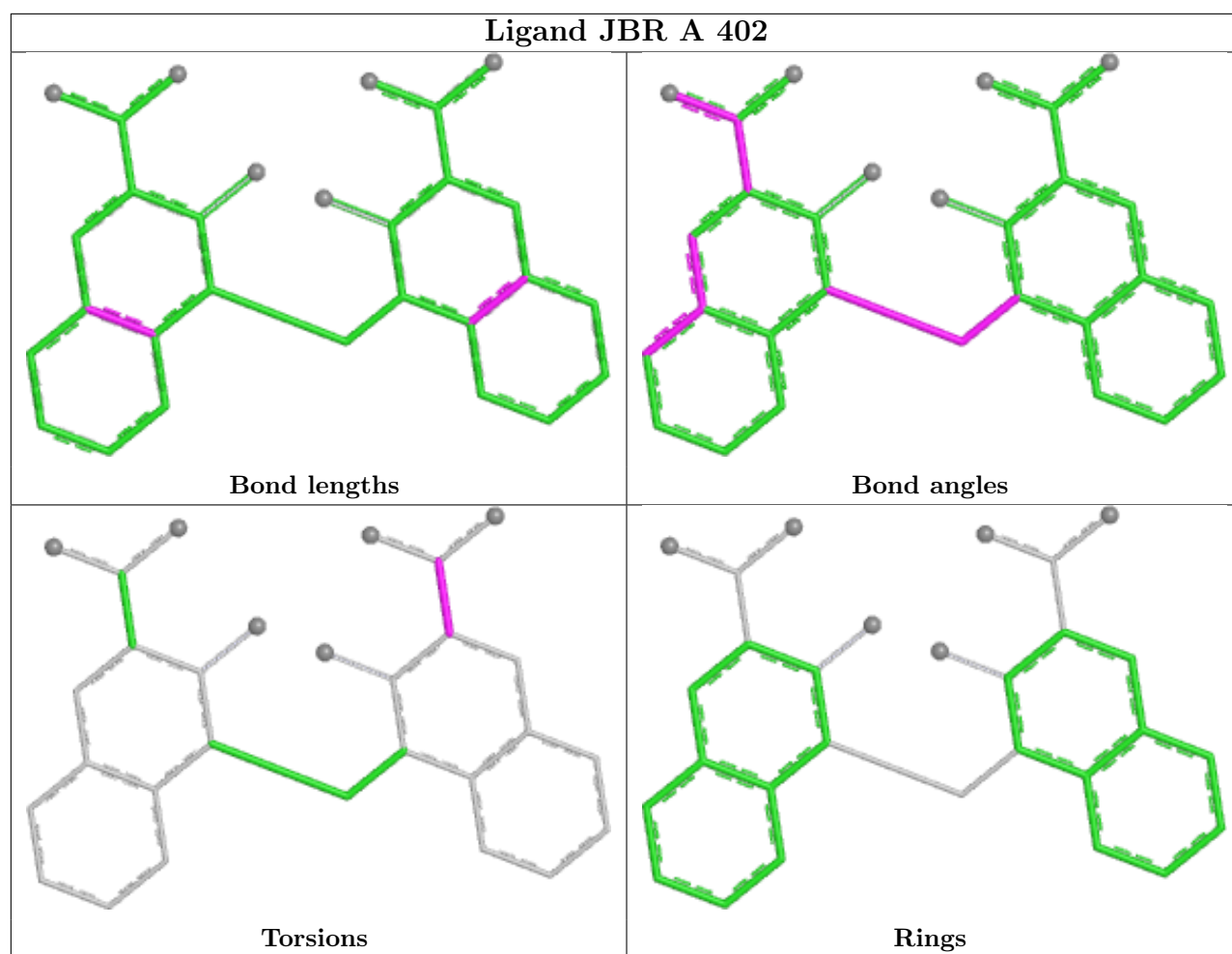


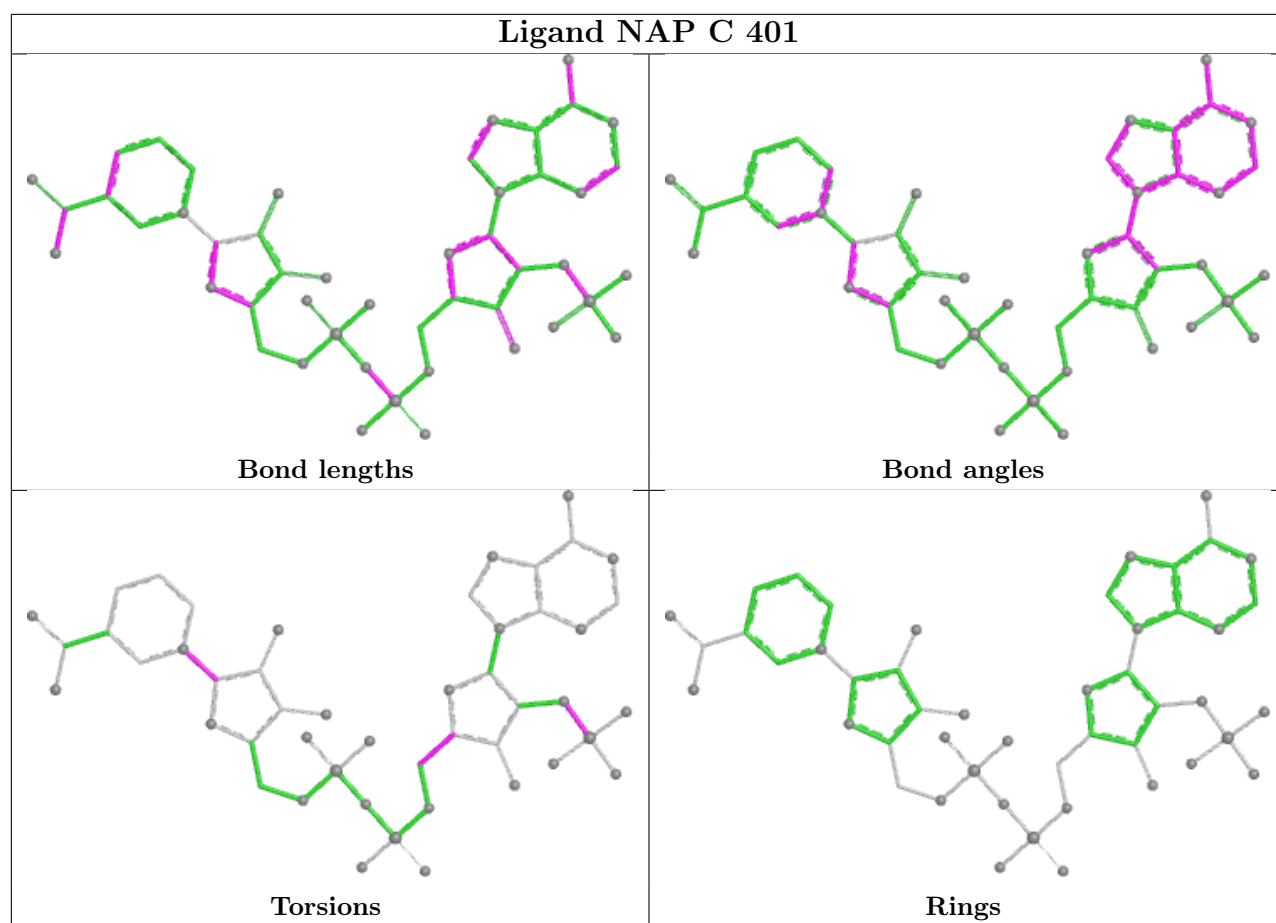


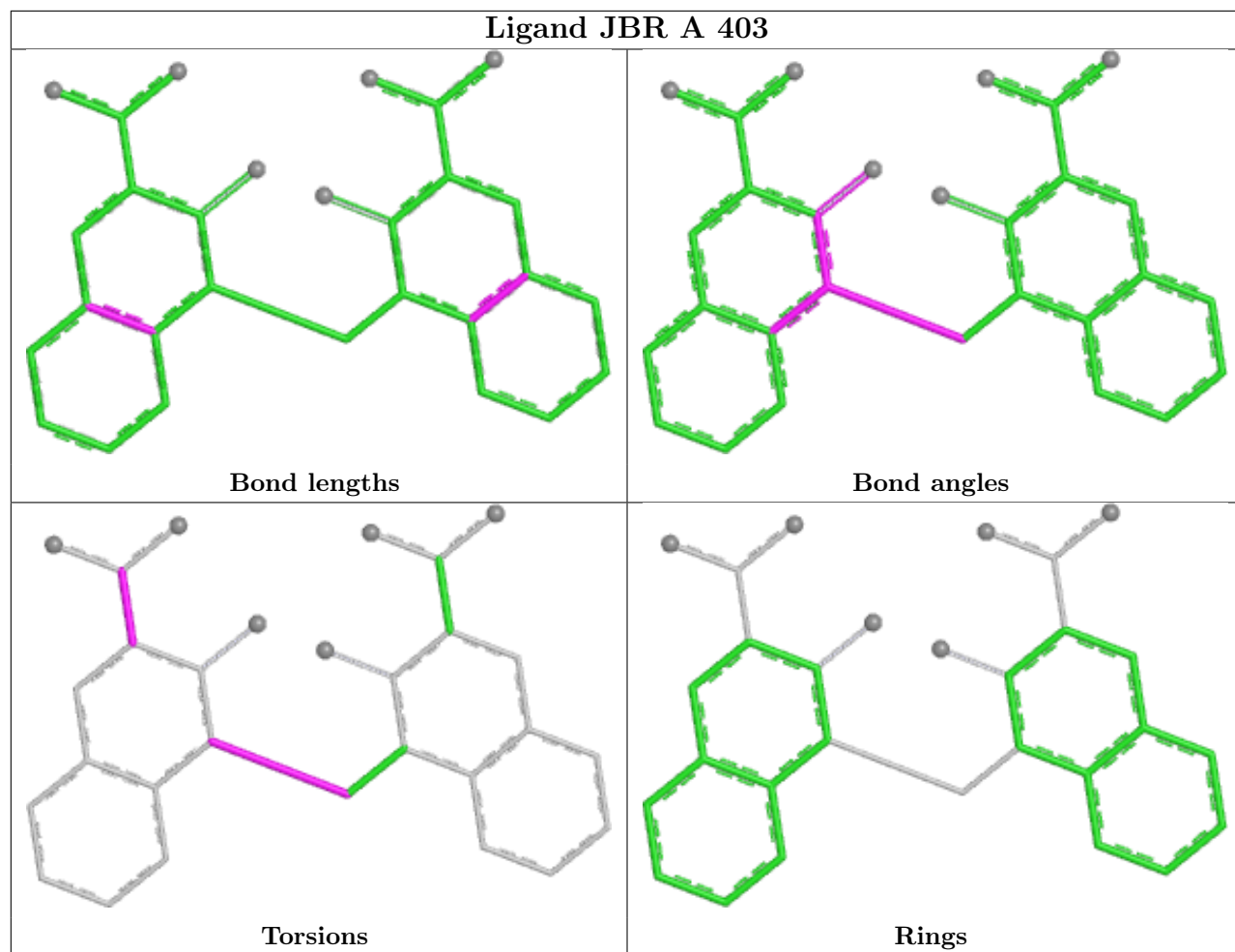


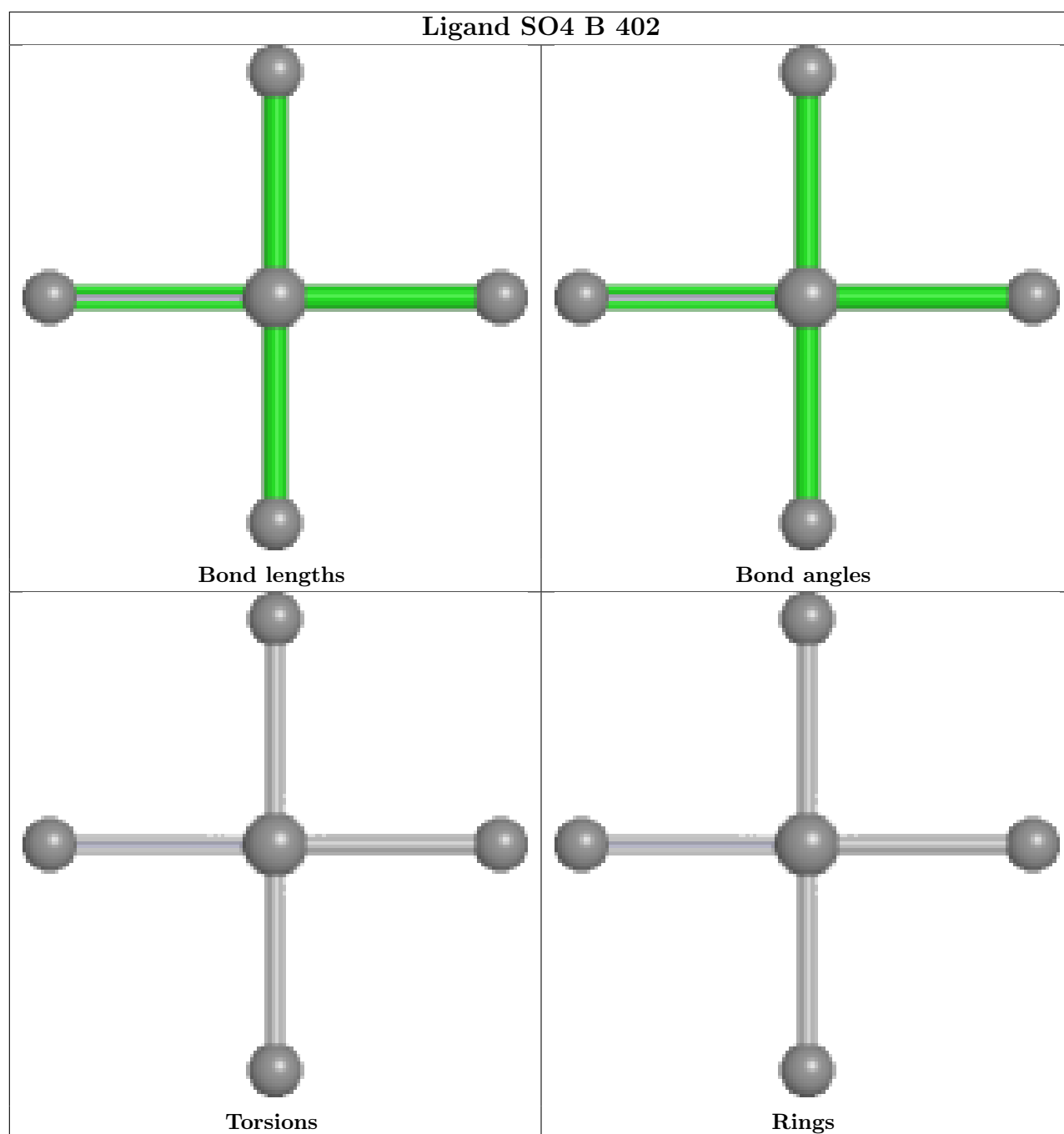












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	207/207 (100%)	-0.38	8 (3%)	43	45	8, 14, 35, 76	4 (1%)
1	B	206/207 (99%)	0.33	11 (5%)	32	33	12, 24, 48, 89	2 (0%)
1	C	207/207 (100%)	-0.43	6 (2%)	53	56	8, 13, 36, 63	6 (2%)
1	D	206/207 (99%)	0.05	10 (4%)	35	36	9, 21, 42, 88	5 (2%)
All	All	826/828 (99%)	-0.11	35 (4%)	40	42	8, 18, 42, 89	17 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.1
1	B	2	ALA	4.7
1	D	1	MET	4.2
1	D	2	ALA	4.1
1	A	0	HIS	3.9
1	B	79	ASN	3.8
1	D	78[A]	ARG	3.7
1	B	172	PRO	3.7
1	A	42	SER	3.5
1	C	0	HIS	3.5
1	C	79	ASN	3.4
1	D	172	PRO	3.4
1	C	37	SER	3.3
1	D	167	LEU	3.2
1	A	79	ASN	3.1
1	B	116	TRP	3.0
1	D	116	TRP	3.0
1	B	78	ARG	2.9
1	D	79	ASN	2.8
1	B	77	THR	2.7
1	A	46	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	43	GLU	2.6
1	D	104	ASP	2.5
1	B	104	ASP	2.5
1	C	46	ARG	2.4
1	C	116	TRP	2.4
1	B	46	ARG	2.4
1	A	45	PRO	2.4
1	D	206	GLN	2.3
1	B	167	LEU	2.3
1	D	42	SER	2.3
1	B	206	GLN	2.3
1	A	43	GLU	2.2
1	A	37	SER	2.1
1	A	119	THR	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 [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
4	SO4	A	404	5/5	0.39	0.15	66,76,79,79	0
4	SO4	C	403	5/5	0.71	0.19	87,87,88,88	0
3	JBR	A	403	29/29	0.76	0.16	33,36,47,47	0
4	SO4	D	405	5/5	0.76	0.15	77,78,79,80	0
3	JBR	C	402	29/29	0.78	0.18	33,45,68,70	0
4	SO4	B	402	5/5	0.82	0.16	50,50,51,55	0
4	SO4	B	403	5/5	0.83	0.13	72,73,74,75	0
4	SO4	D	404	5/5	0.84	0.15	74,75,76,76	0
3	JBR	D	402	29/29	0.84	0.13	30,33,40,42	0

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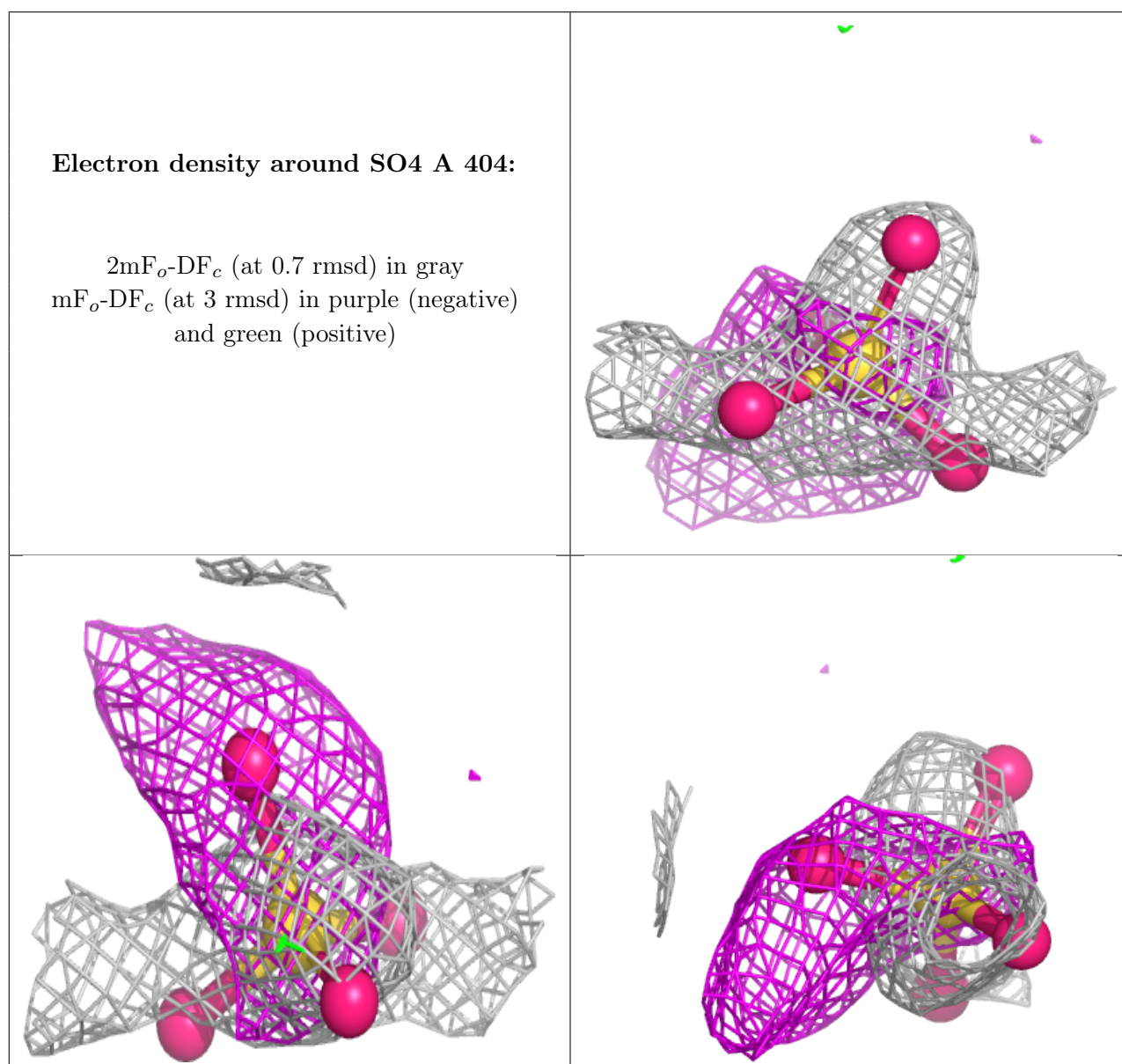
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	JBR	A	402	29/29	0.90	0.12	19,28,57,59	0
4	SO4	D	403	5/5	0.90	0.11	39,39,41,47	0
2	NAP	B	401	48/48	0.94	0.08	18,22,29,33	0
2	NAP	D	401	48/48	0.95	0.08	16,21,24,27	0
2	NAP	A	401	48/48	0.98	0.05	7,10,15,19	0
2	NAP	C	401	48/48	0.99	0.04	7,9,14,21	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.

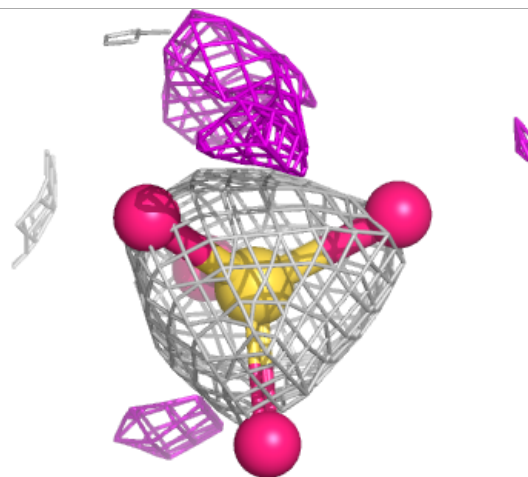
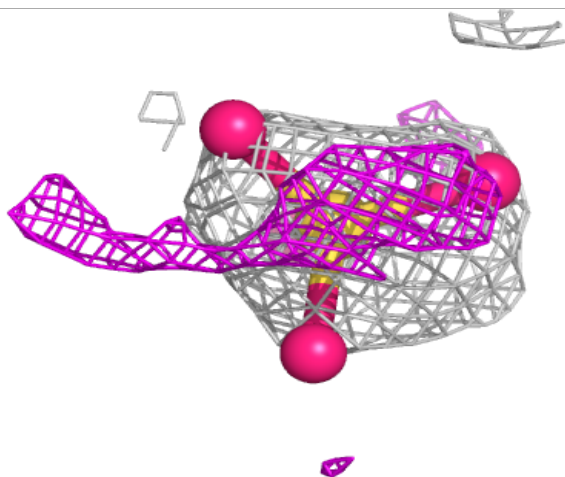
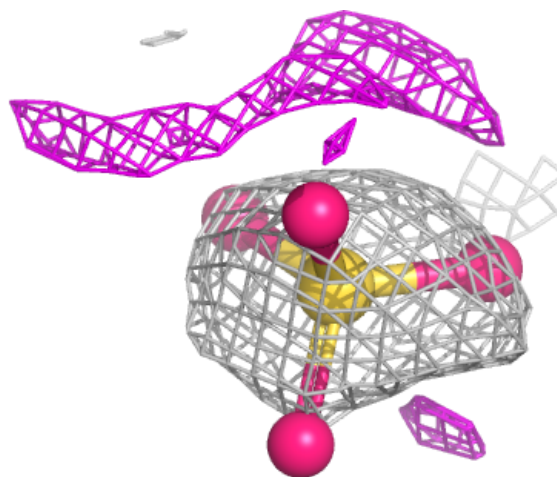
Electron density around SO4 A 404:

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



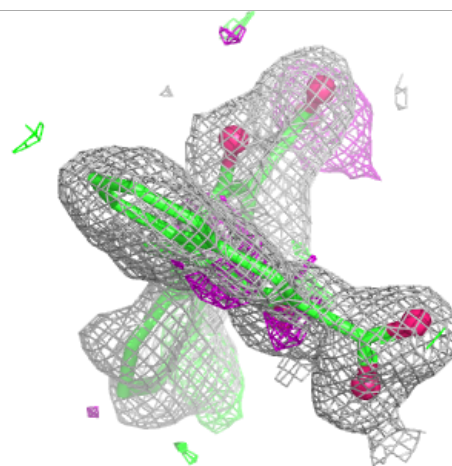
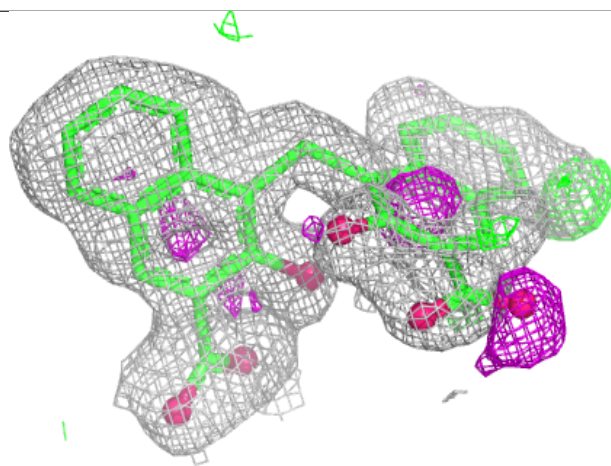
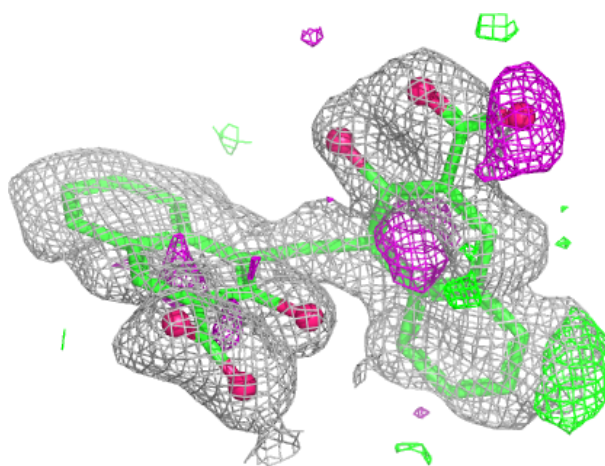
Electron density around SO4 C 403:

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



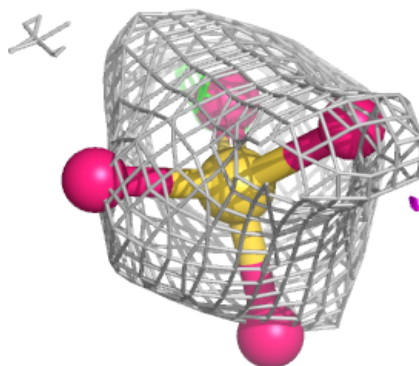
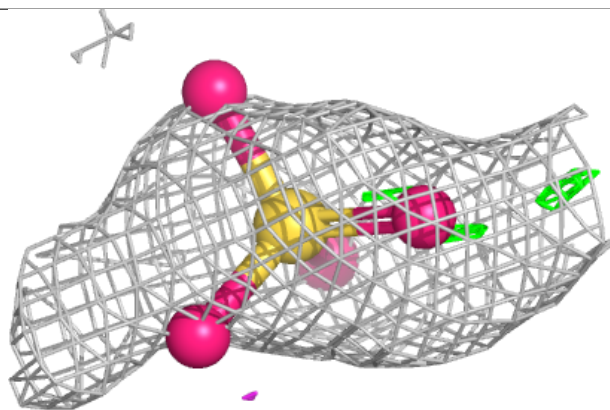
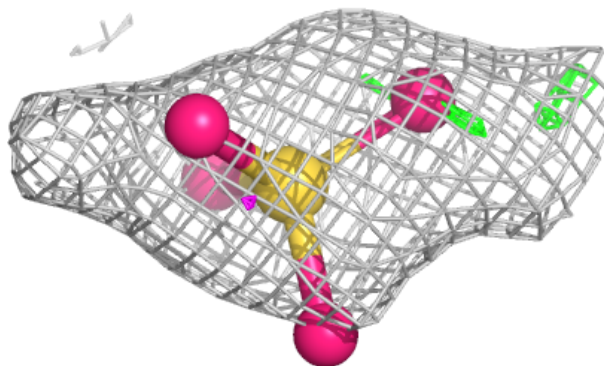
Electron density around JBR A 403:

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

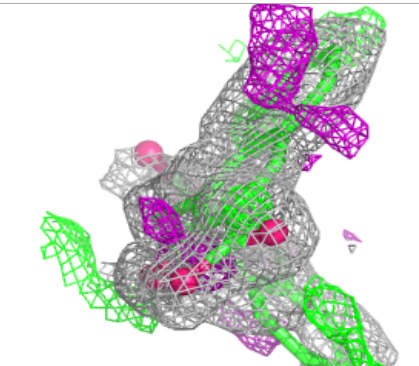
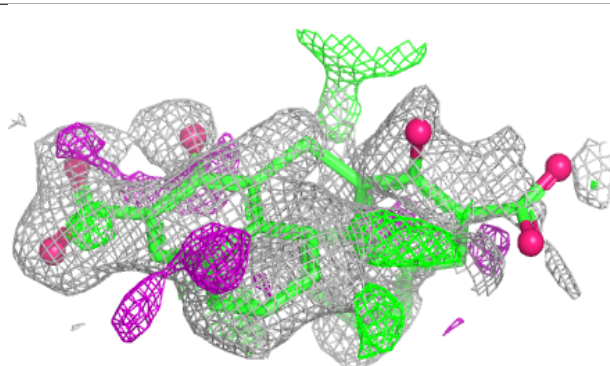
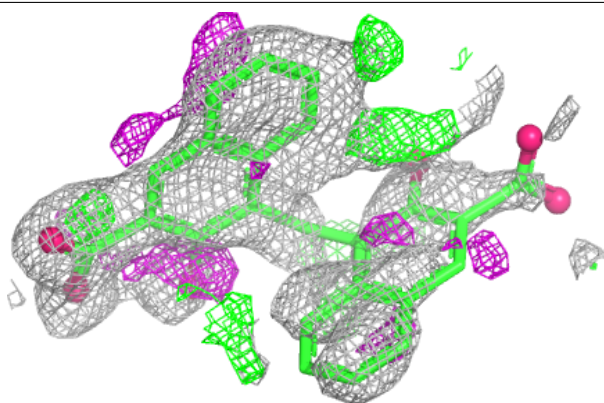


Electron density around SO4 D 405:

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

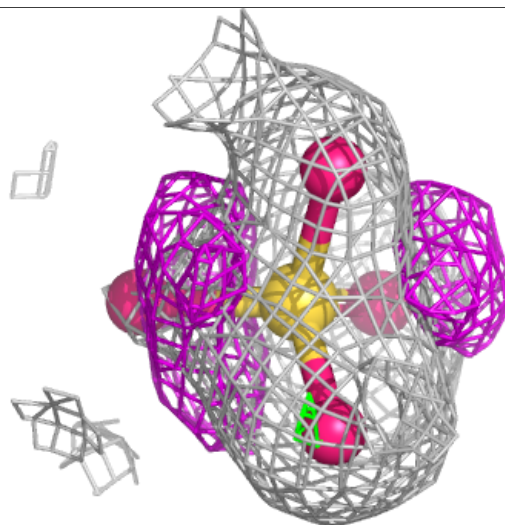
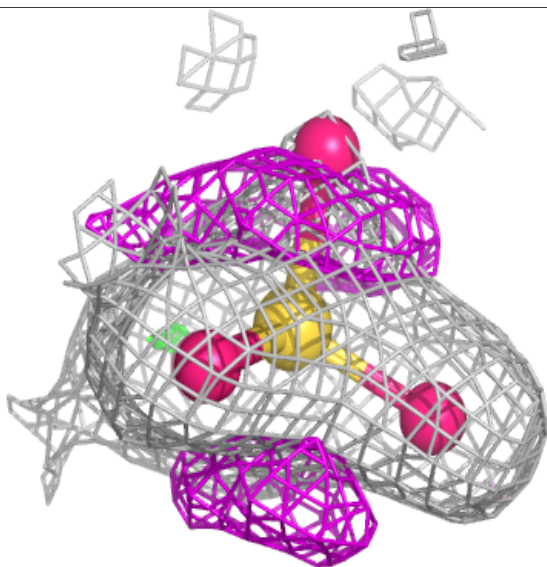
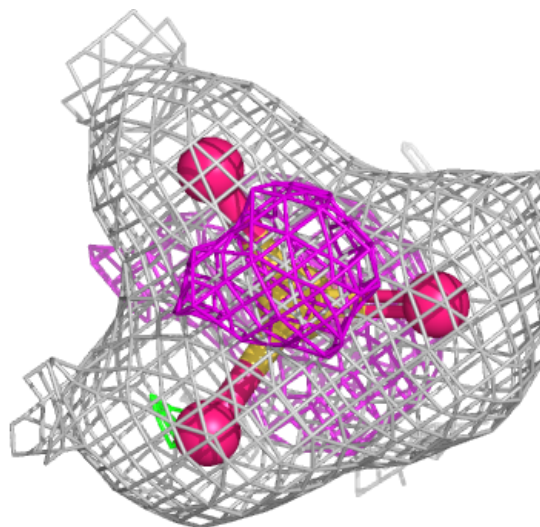
**Electron density around JBR C 402:**

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



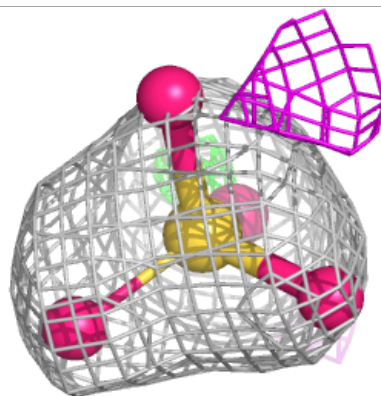
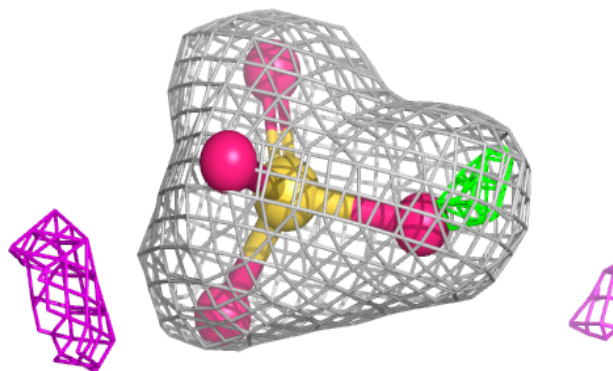
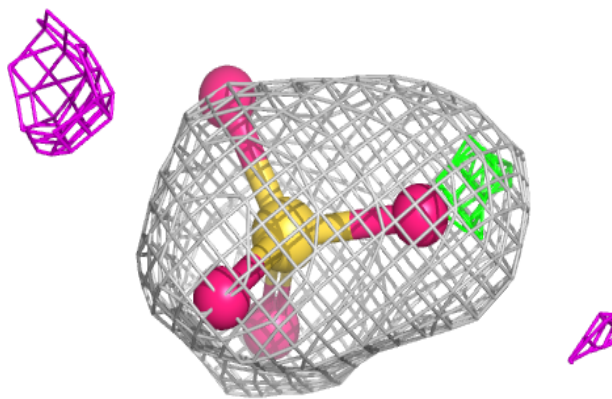
Electron density around SO4 B 402:

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



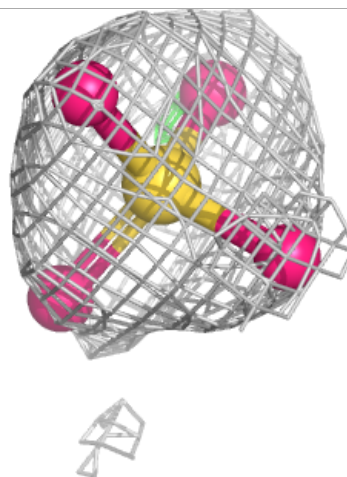
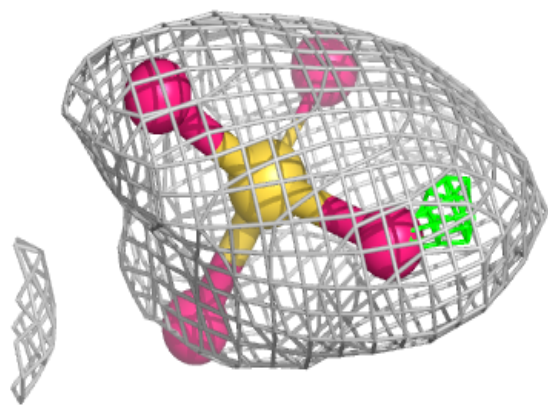
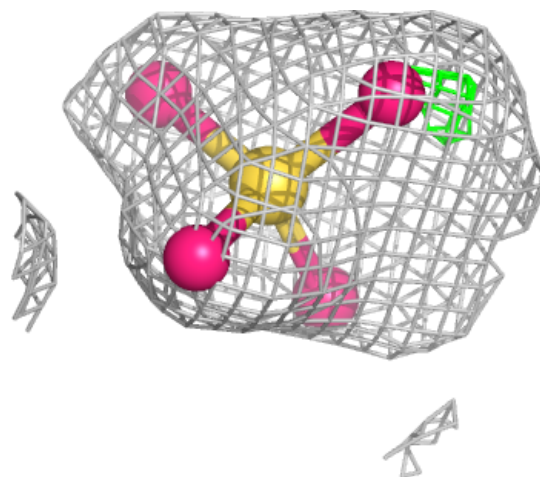
Electron density around SO4 B 403:

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



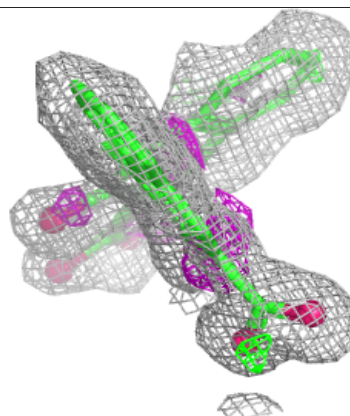
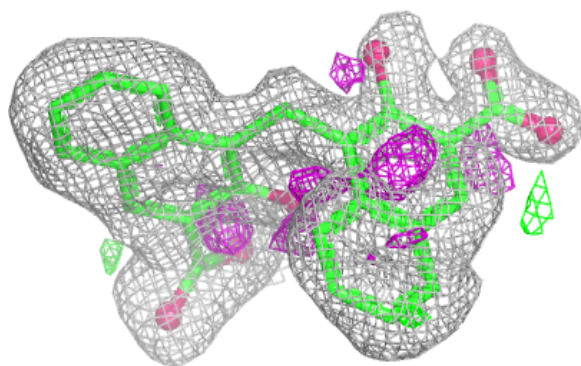
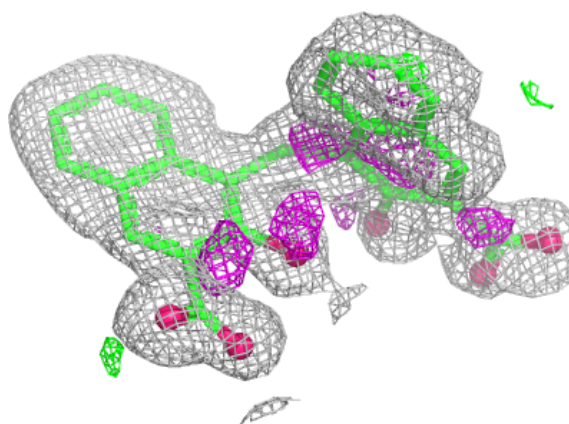
Electron density around SO4 D 404:

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

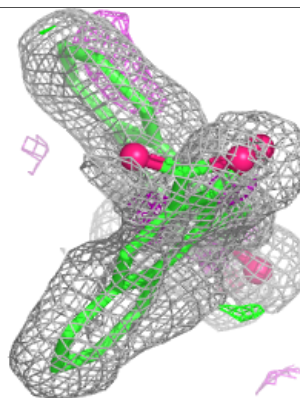
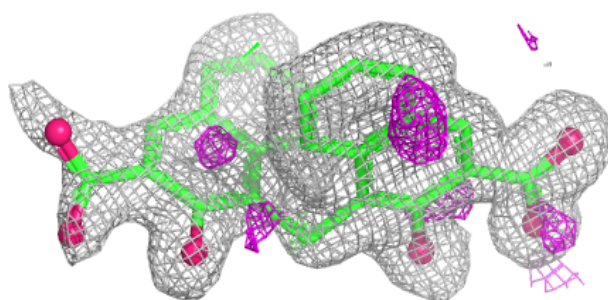
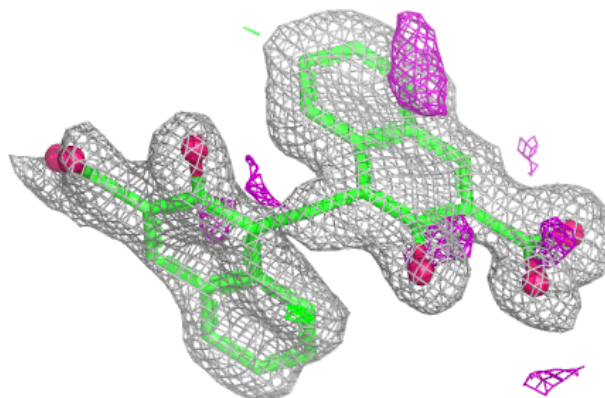


Electron density around JBR D 402:

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

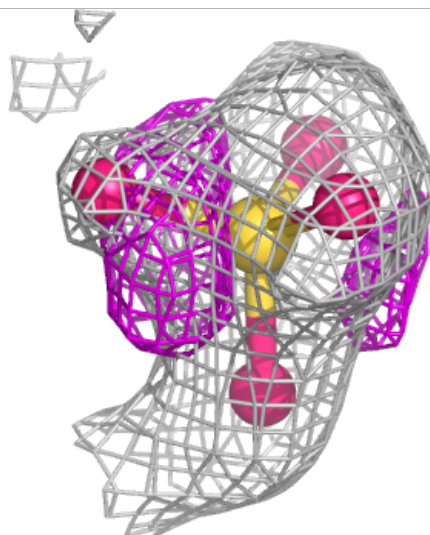
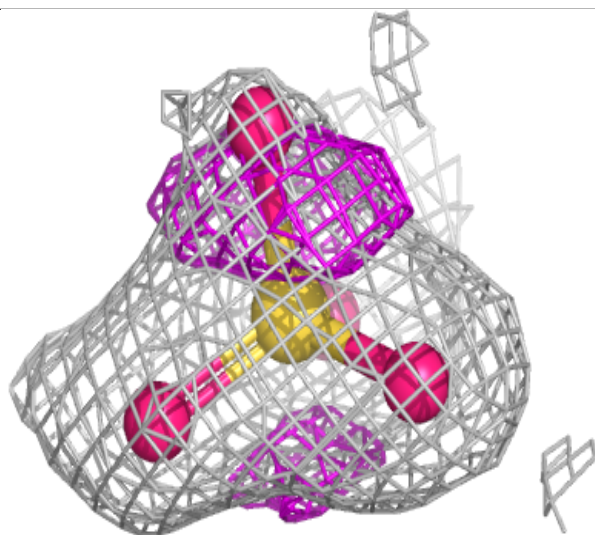
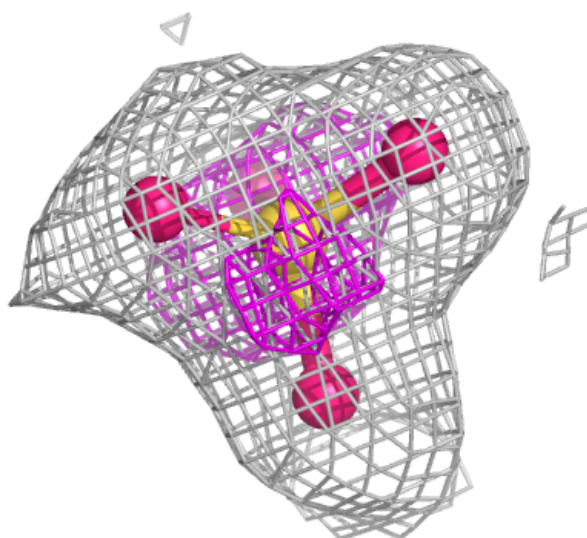
**Electron density around JBR A 402:**

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



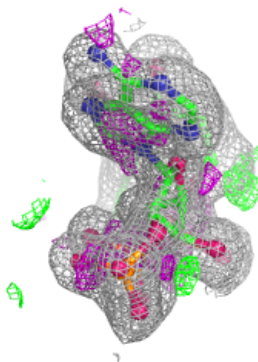
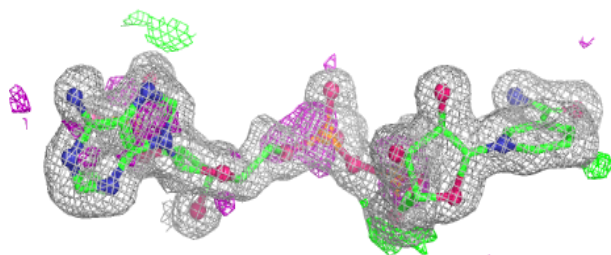
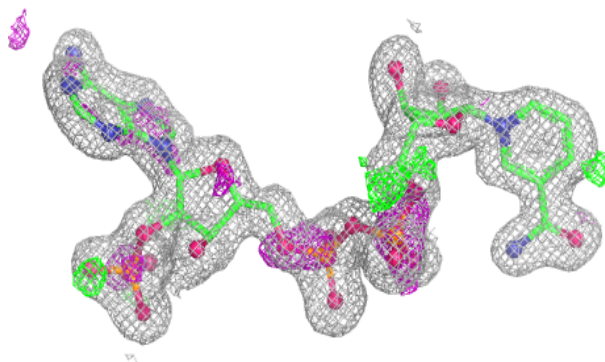
Electron density around SO4 D 403:

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

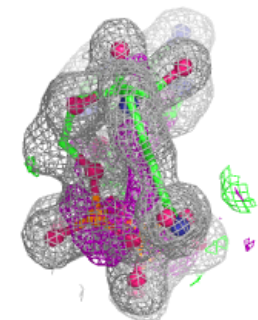
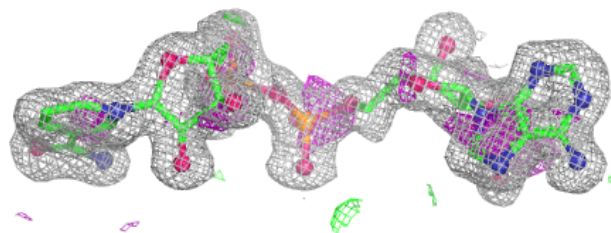
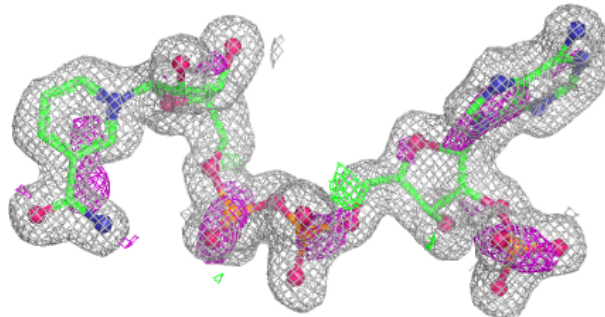


Electron density around NAP B 401:

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

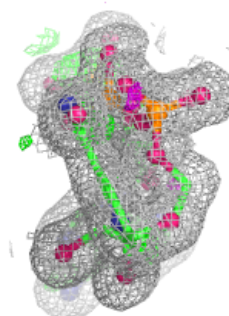
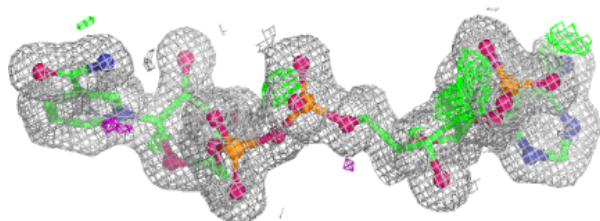
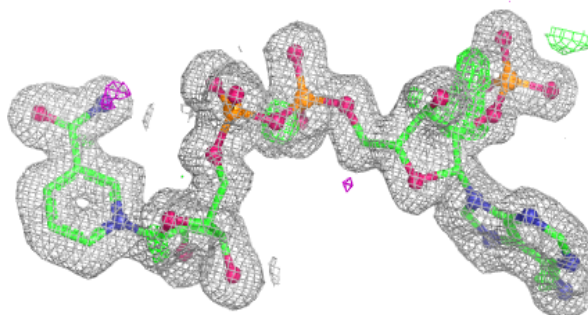
**Electron density around NAP D 401:**

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

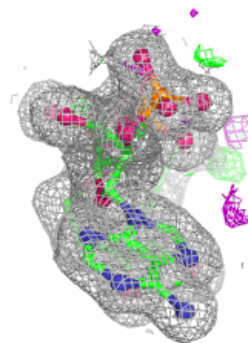
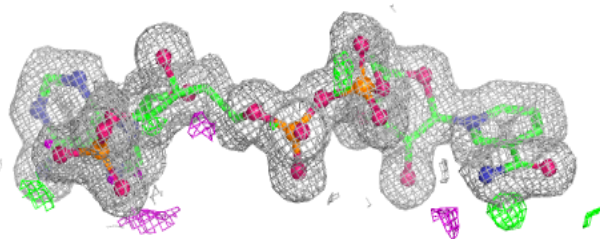
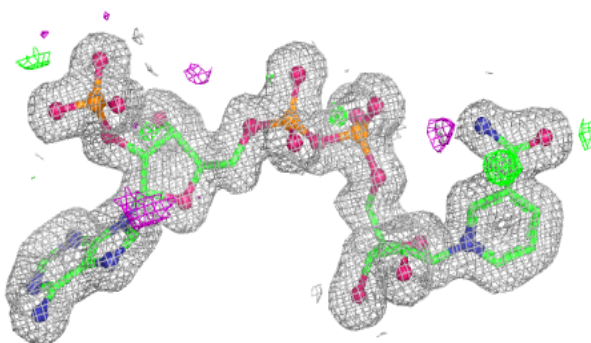


Electron density around NAP A 401:

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

**Electron density around NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.