



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 7Q3A / pdb_00007q3a
Title : Crystal structure of MAB_4324 a tandem repeat GNAT from Mycobacterium abscessus
Authors : Blaise, M.; Alsarraf, M.A.B.
Deposited on : 2021-10-27
Resolution : 2.00 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

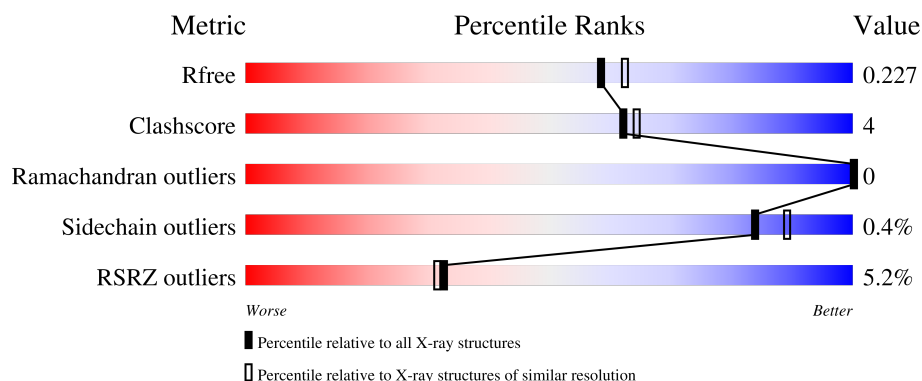
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	352	4% 91% 5%
1	B	352	6% 87% 10%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 6620 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.

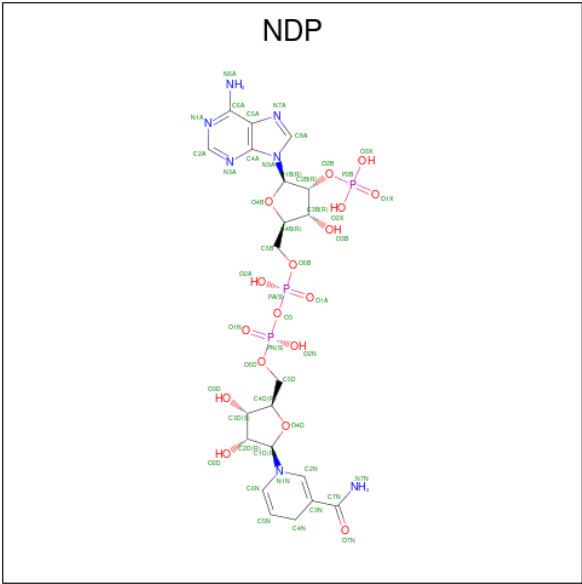
- Molecule 1 is a protein called Putative acetyltransferase, GNAT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	4	0
			2723	1710	481	529	3			
1	B	340	Total	C	N	O	S	0	3	0
			2714	1707	476	528	3			

There are 2 discrepancies between the modelled and reference sequences:

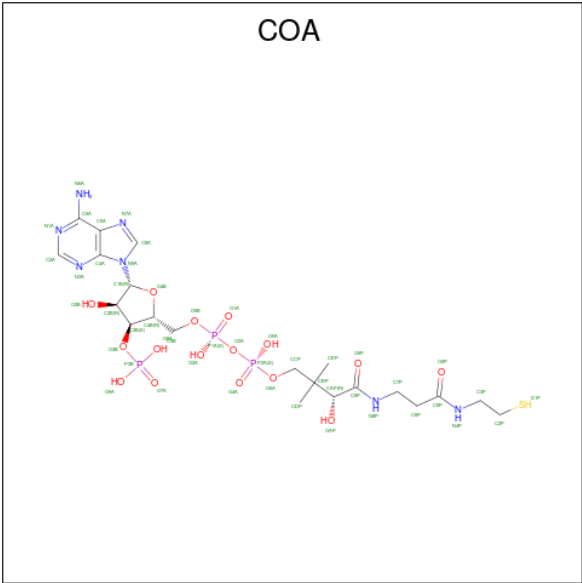
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B1MJN9
B	1	GLY	-	expression tag	UNP B1MJN9

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



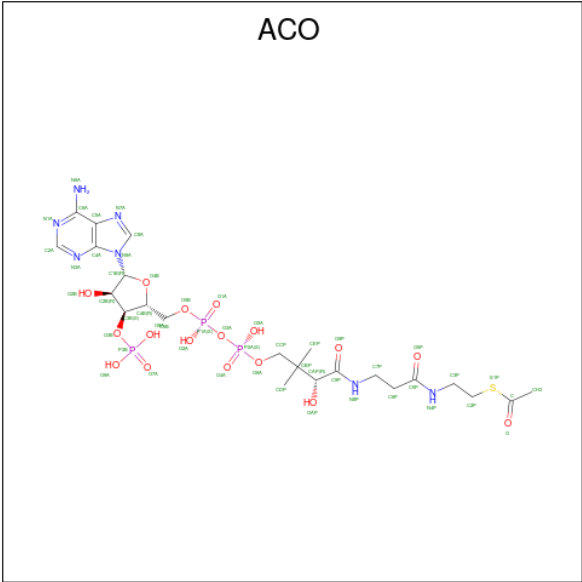
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



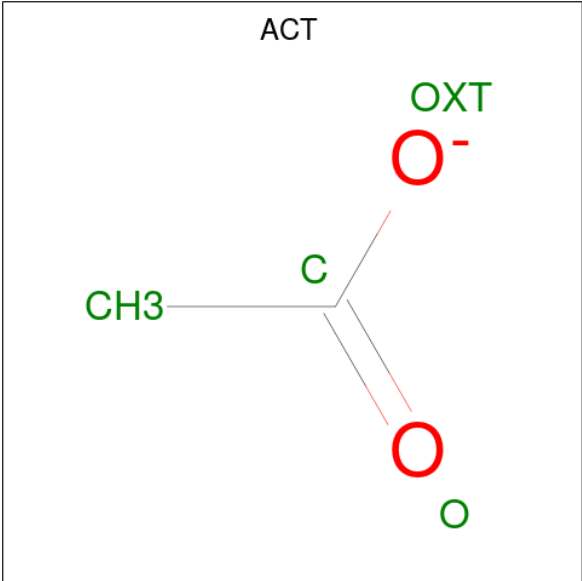
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			48	21	7	16	3		
3	B	1	Total	C	N	O	P	0	1
			48	21	7	16	3		

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	1
			51	23	7	17	3	1		
4	B	1	Total	C	N	O	P	S	0	1
			51	23	7	17	3	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂) (labeled as "Ligand of Interest" by depositor).



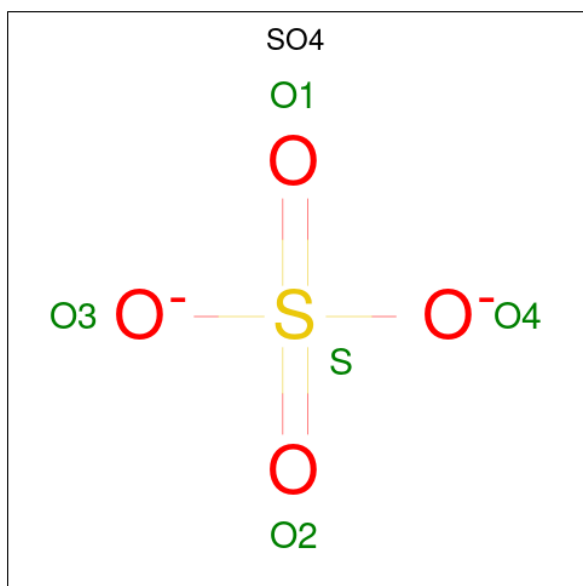
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			4	2	2		

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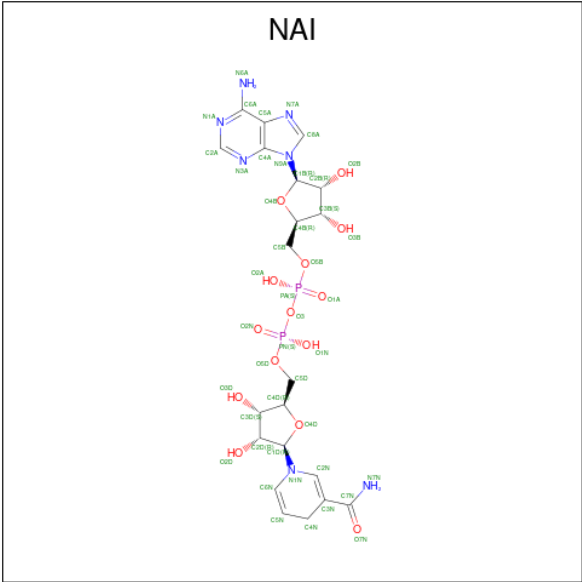
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	1
			4	2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



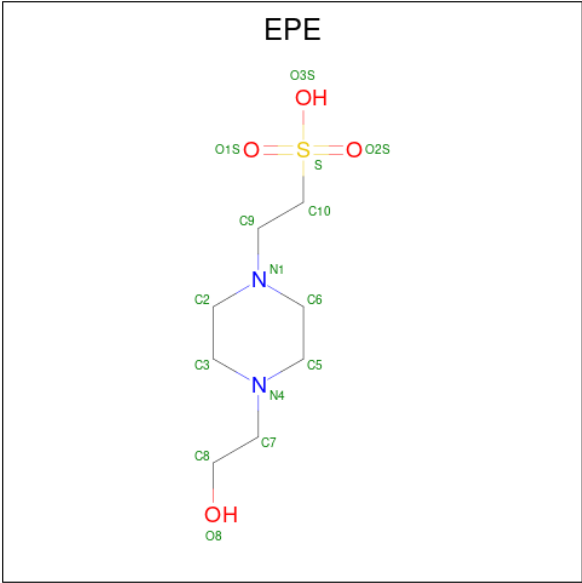
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	453	Total 453	O 453	0	0
9	B	407	Total 407	O 407	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.96Å 149.96Å 183.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.00 49.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.09-2.00) 98.3 (49.09-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.05 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.186 , 0.226 0.187 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6620	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4, EPE, ACO, NAI, COA, NDP

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	0.35	0/2792	0.51	0/3804
1	B	0.35	0/2785	0.49	0/3795
All	All	0.35	0/5577	0.50	0/7599

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

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	2723	0	2560	17	0
1	B	2714	0	2560	21	0
2	A	48	0	26	0	0
3	A	48	0	32	2	0
3	B	48	0	32	1	0
4	A	51	0	34	2	0
4	B	51	0	34	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	44	0	27	3	0
8	B	15	0	17	2	0
9	A	453	0	0	7	2
9	B	407	0	0	7	2
All	All	6620	0	5328	46	2

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 4.

All (46) 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:147:CYS:SG	9:A:932:HOH:O	2.48	0.72
1:A:254:ASP:OD1	1:A:258:GLN:HB2	1.93	0.68
1:B:287:LEU:HD22	1:B:303[B]:LEU:HD21	1.75	0.67
4:B:503[B]:ACO:H8A	4:B:503[B]:ACO:H52A	1.75	0.67
6:A:505:SO4:O4	9:A:601:HOH:O	2.14	0.66
1:A:253:ARG:HG2	9:A:727:HOH:O	1.96	0.65
1:B:73:ASP:OD2	1:B:101:LYS:NZ	2.27	0.65
8:B:505:EPE:H82	8:B:505:EPE:H22	1.83	0.60
1:B:66:GLU:O	1:B:70:GLU:HG3	2.02	0.60
7:B:501:NAI:H8A	9:B:832:HOH:O	2.04	0.57
4:A:503[B]:ACO:H21	9:A:709:HOH:O	2.04	0.56
1:B:99:THR:HG21	9:B:956:HOH:O	2.06	0.56
1:B:237:HIS:HD2	9:B:685:HOH:O	1.88	0.56
1:A:39:LYS:HG3	9:A:900:HOH:O	2.07	0.55
1:B:12:SER:O	1:B:16:ARG:HB2	2.07	0.55
1:B:28:ALA:HB2	1:B:128:SER:OG	2.08	0.54
7:B:501:NAI:H3B	9:B:640:HOH:O	2.06	0.53
1:A:99[A]:THR:HG21	9:A:879:HOH:O	2.08	0.53
1:B:195:PRO:HB2	1:B:198:ILE:HD12	1.91	0.51
1:B:135:GLN:HG3	9:B:691:HOH:O	2.11	0.51
1:B:165:GLU:O	1:B:169:ARG:HG3	2.12	0.49
1:A:295:GLY:N	4:A:503[B]:ACO:O5A	2.32	0.48
1:A:297:LYS:HA	3:A:502[A]:COA:O2A	2.14	0.48
1:B:271:GLU:HA	1:B:274:TRP:CE2	2.51	0.46
1:A:320:LEU:HD12	1:A:320:LEU:C	2.40	0.45
1:B:139:GLN:O	1:B:143:GLU:HG3	2.16	0.45
1:A:25:ILE:HG23	1:A:26:PRO:HD2	1.98	0.45
7:B:501:NAI:H52A	9:B:667:HOH:O	2.17	0.45
1:B:25:ILE:HG23	1:B:26:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:CG	1:A:317:ARG:HG2	2.52	0.44
1:B:279:TYR:CG	1:B:317:ARG:HG3	2.52	0.43
1:B:297:LYS:HA	3:B:502[A]:COA:O2A	2.18	0.43
8:B:505:EPE:H22	8:B:505:EPE:C8	2.48	0.43
1:A:274:TRP:CG	1:A:280:SER:HA	2.54	0.43
1:A:265:LEU:C	1:A:265:LEU:HD23	2.44	0.43
1:A:39:LYS:HB2	1:A:39:LYS:HE3	1.68	0.42
1:B:274:TRP:CG	1:B:280:SER:HA	2.54	0.42
1:A:317:ARG:NH1	9:A:615:HOH:O	2.47	0.41
1:B:265:LEU:C	1:B:265:LEU:HD23	2.45	0.41
1:A:332:ALA:HB3	3:A:502[A]:COA:H8A	2.02	0.41
1:A:254:ASP:OD1	1:A:258:GLN:CB	2.65	0.41
1:B:254:ASP:O	1:B:255:ALA:C	2.64	0.41
1:B:146:GLU:OE1	9:B:601:HOH:O	2.22	0.41
1:B:175:VAL:HG21	1:B:349:ILE:HD12	2.03	0.41
1:A:325:ASP:O	1:A:326:SER:C	2.63	0.41
1:B:320:LEU:C	1:B:320:LEU:HD12	2.46	0.40

All (2) 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)
9:A:804:HOH:O	9:B:901:HOH:O[12_564]	2.10	0.10
9:A:926:HOH:O	9:B:852:HOH:O[3_565]	2.15	0.05

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	339/352 (96%)	336 (99%)	3 (1%)	0	100	100
1	B	339/352 (96%)	333 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	678/704 (96%)	669 (99%)	9 (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	281/285 (99%)	280 (100%)	1 (0%)	84	89
1	B	280/285 (98%)	279 (100%)	1 (0%)	84	89
All	All	561/570 (98%)	559 (100%)	2 (0%)	84	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	ARG
1	B	15	GLU

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	312	HIS
1	B	351	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
5	ACT	B	504[A]	-	3,3,3	0.89	0	3,3,3	0.65	0
3	COA	B	502[A]	-	47,50,50	1.94	5 (10%)	69,75,75	1.87	8 (11%)
4	ACO	A	503[B]	-	51,53,53	1.33	3 (5%)	73,79,79	1.25	7 (9%)
2	NDP	A	501	-	51,52,52	1.37	3 (5%)	71,80,80	1.22	5 (7%)
5	ACT	A	504[A]	-	3,3,3	0.75	0	3,3,3	0.91	0
7	NAI	B	501	-	47,48,48	1.04	3 (6%)	64,73,73	1.18	4 (6%)
8	EPE	B	505	-	15,15,15	1.03	1 (6%)	19,20,20	1.08	0
4	ACO	B	503[B]	-	51,53,53	1.23	3 (5%)	73,79,79	1.19	7 (9%)
6	SO4	B	506	-	4,4,4	0.22	0	6,6,6	0.19	0
6	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.22	0
3	COA	A	502[A]	-	47,50,50	1.91	6 (12%)	69,75,75	1.97	9 (13%)

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	COA	B	502[A]	-	-	5/48/64/64	0/3/3/3
4	ACO	A	503[B]	-	-	14/51/67/67	0/3/3/3
2	NDP	A	501	-	-	3/34/77/77	0/5/5/5
7	NAI	B	501	-	-	11/29/72/72	0/5/5/5
8	EPE	B	505	-	-	2/9/19/19	0/1/1/1
4	ACO	B	503[B]	-	-	9/51/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	502[A]	-	-	6/48/64/64	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	COA	C8A-N9A	-8.83	1.22	1.37
3	B	502[A]	COA	C8A-N9A	-8.69	1.22	1.37
2	A	501	NDP	C2B-C1B	-6.72	1.36	1.53
4	A	503[B]	ACO	P2A-O3A	5.96	1.65	1.59
3	A	502[A]	COA	P1A-O3A	5.94	1.65	1.59
3	B	502[A]	COA	P1A-O3A	5.77	1.65	1.59
4	B	503[B]	ACO	P2A-O3A	5.50	1.65	1.59
4	A	503[B]	ACO	P1A-O3A	5.11	1.65	1.59
4	B	503[B]	ACO	P1A-O3A	4.28	1.64	1.59
2	A	501	NDP	PN-O3	4.05	1.63	1.59
3	B	502[A]	COA	P2A-O3A	3.94	1.63	1.59
7	B	501	NAI	PN-O3	3.67	1.63	1.59
3	B	502[A]	COA	C4A-N9A	3.47	1.44	1.37
3	A	502[A]	COA	C4A-N9A	3.33	1.44	1.37
3	A	502[A]	COA	P2A-O3A	2.89	1.62	1.59
7	B	501	NAI	PA-O3	2.83	1.62	1.59
3	B	502[A]	COA	C5A-N7A	2.81	1.44	1.39
3	A	502[A]	COA	C5A-N7A	2.55	1.43	1.39
2	A	501	NDP	C5A-N7A	-2.33	1.34	1.39
7	B	501	NAI	C8A-N7A	2.24	1.36	1.31
4	A	503[B]	ACO	C4A-N9A	-2.12	1.33	1.37
4	B	503[B]	ACO	C4A-N9A	-2.05	1.33	1.37
8	B	505	EPE	C2-N1	-2.02	1.41	1.46
3	A	502[A]	COA	P1A-O2A	-2.01	1.46	1.55

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[A]	COA	C4A-N9A-C8A	8.56	114.73	105.74
3	B	502[A]	COA	C4A-N9A-C8A	8.48	114.64	105.74
3	A	502[A]	COA	N3A-C4A-N9A	7.17	139.36	127.17
3	B	502[A]	COA	N3A-C4A-N9A	6.88	138.86	127.17
2	A	501	NDP	C5A-C4A-N3A	-5.62	118.97	126.72
3	A	502[A]	COA	C5A-C4A-N9A	-5.26	100.08	105.81
3	B	502[A]	COA	C5A-C4A-N9A	-5.11	100.24	105.81
4	A	503[B]	ACO	C5A-C4A-N3A	-4.91	119.95	126.72
4	B	503[B]	ACO	C5A-C4A-N3A	-4.85	120.04	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	NAI	C5A-C4A-N3A	-4.69	120.26	126.72
3	A	502[A]	COA	C1B-N9A-C8A	-4.67	116.72	127.09
3	A	502[A]	COA	C5A-C4A-N3A	-4.47	120.57	126.72
3	B	502[A]	COA	C1B-N9A-C8A	-4.27	117.61	127.09
3	B	502[A]	COA	C5A-C4A-N3A	-4.23	120.89	126.72
4	A	503[B]	ACO	N3A-C4A-N9A	3.78	133.59	127.17
7	B	501	NAI	N3A-C4A-N9A	3.76	133.56	127.17
4	B	503[B]	ACO	N3A-C4A-N9A	3.59	133.28	127.17
7	B	501	NAI	C4A-N9A-C8A	3.26	109.16	105.74
4	A	503[B]	ACO	C4A-N9A-C8A	3.23	109.13	105.74
4	A	503[B]	ACO	O4B-C1B-N9A	3.18	114.20	108.09
4	B	503[B]	ACO	C4A-N9A-C8A	3.06	108.95	105.74
2	A	501	NDP	N3A-C4A-N9A	2.97	132.22	127.17
2	A	501	NDP	C5A-C4A-N9A	2.75	108.80	105.81
4	A	503[B]	ACO	N9A-C8A-N7A	-2.63	110.20	113.94
4	B	503[B]	ACO	P3B-O3B-C3B	-2.59	116.52	123.43
4	B	503[B]	ACO	N9A-C8A-N7A	-2.58	110.27	113.94
3	A	502[A]	COA	O4B-C1B-N9A	2.48	112.85	108.09
4	B	503[B]	ACO	C2A-N3A-C4A	2.45	117.81	111.83
4	A	503[B]	ACO	C2A-N3A-C4A	2.43	117.76	111.83
7	B	501	NAI	N9A-C8A-N7A	-2.38	110.57	113.94
2	A	501	NDP	C2A-N3A-C4A	2.36	117.60	111.83
2	A	501	NDP	O4B-C1B-N9A	2.32	112.54	108.09
3	B	502[A]	COA	C2A-N3A-C4A	2.27	117.37	111.83
4	B	503[B]	ACO	C4A-C5A-N7A	-2.26	108.00	110.58
3	A	502[A]	COA	N9A-C8A-N7A	-2.26	110.73	113.94
3	B	502[A]	COA	N9A-C8A-N7A	-2.25	110.74	113.94
3	A	502[A]	COA	C2A-N3A-C4A	2.24	117.31	111.83
4	A	503[B]	ACO	C4A-C5A-N7A	-2.11	108.16	110.58
3	A	502[A]	COA	O9A-P3B-O3B	2.07	113.90	105.85
3	B	502[A]	COA	P3B-O3B-C3B	-2.00	118.08	123.43

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	COA	O4B-C1B-N9A-C4A
3	A	502[A]	COA	O4B-C1B-N9A-C8A
4	A	503[B]	ACO	O4B-C1B-N9A-C4A
4	A	503[B]	ACO	O4B-C1B-N9A-C8A
4	A	503[B]	ACO	O4B-C4B-C5B-O5B
4	A	503[B]	ACO	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
4	A	503[B]	ACO	CCP-O6A-P2A-O5A
4	A	503[B]	ACO	S1P-C2P-C3P-N4P
4	B	503[B]	ACO	C5B-O5B-P1A-O1A
4	B	503[B]	ACO	C5B-O5B-P1A-O2A
4	B	503[B]	ACO	C5B-O5B-P1A-O3A
4	B	503[B]	ACO	CCP-O6A-P2A-O4A
4	B	503[B]	ACO	CCP-O6A-P2A-O5A
8	B	505	EPE	C8-C7-N4-C3
4	A	503[B]	ACO	C3B-C4B-C5B-O5B
3	A	502[A]	COA	C3B-C4B-C5B-O5B
3	A	502[A]	COA	O4B-C4B-C5B-O5B
4	B	503[B]	ACO	S1P-C2P-C3P-N4P
7	B	501	NAI	C3D-C4D-C5D-O5D
7	B	501	NAI	O4D-C4D-C5D-O5D
4	A	503[B]	ACO	O-C-S1P-C2P
4	A	503[B]	ACO	C6P-C7P-N8P-C9P
7	B	501	NAI	C2B-C1B-N9A-C8A
7	B	501	NAI	PN-O3-PA-O1A
4	A	503[B]	ACO	CDP-CBP-CCP-O6A
7	B	501	NAI	C2D-C1D-N1N-C2N
4	A	503[B]	ACO	CAP-CBP-CCP-O6A
3	B	502[A]	COA	C5B-O5B-P1A-O1A
3	B	502[A]	COA	C5B-O5B-P1A-O2A
3	B	502[A]	COA	C5B-O5B-P1A-O3A
4	A	503[B]	ACO	CCP-O6A-P2A-O3A
4	B	503[B]	ACO	CCP-O6A-P2A-O3A
7	B	501	NAI	C2B-C1B-N9A-C4A
3	B	502[A]	COA	C3B-O3B-P3B-O9A
4	B	503[B]	ACO	C3B-O3B-P3B-O9A
7	B	501	NAI	C2D-C1D-N1N-C6N
2	A	501	NDP	O4D-C1D-N1N-C2N
7	B	501	NAI	O4D-C1D-N1N-C2N
4	B	503[B]	ACO	C6P-C7P-N8P-C9P
2	A	501	NDP	C2N-C3N-C7N-N7N
3	A	502[A]	COA	C3B-O3B-P3B-O7A
7	B	501	NAI	O4B-C1B-N9A-C8A
8	B	505	EPE	N4-C7-C8-O8
7	B	501	NAI	O4D-C1D-N1N-C6N
4	A	503[B]	ACO	CH3-C-S1P-C2P
3	A	502[A]	COA	C3B-O3B-P3B-O9A
3	B	502[A]	COA	C3B-O3B-P3B-O8A
4	A	503[B]	ACO	CEP-CBP-CCP-O6A

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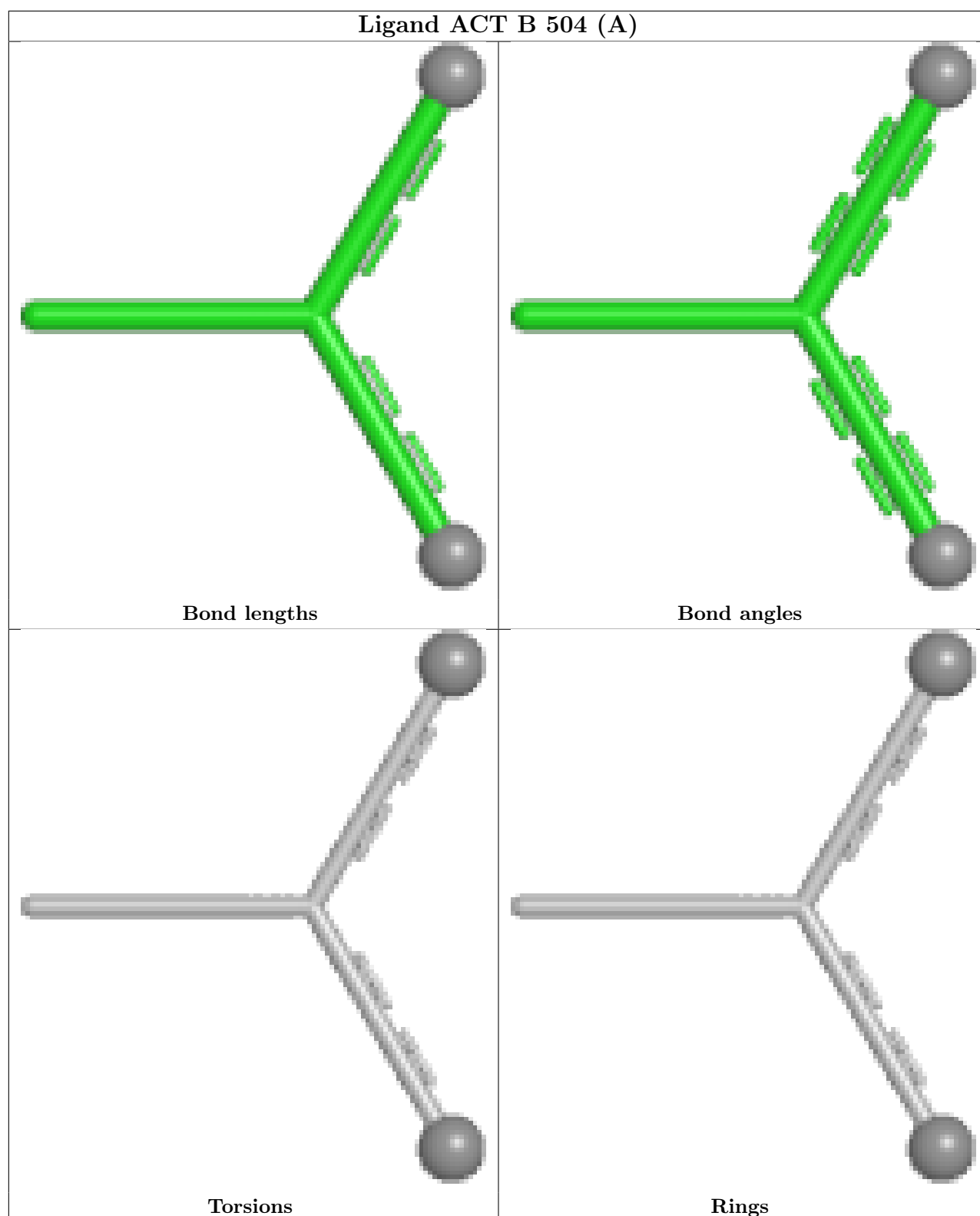
Mol	Chain	Res	Type	Atoms
2	A	501	NDP	PN-O3-PA-O2A
7	B	501	NAI	PN-O3-PA-O2A

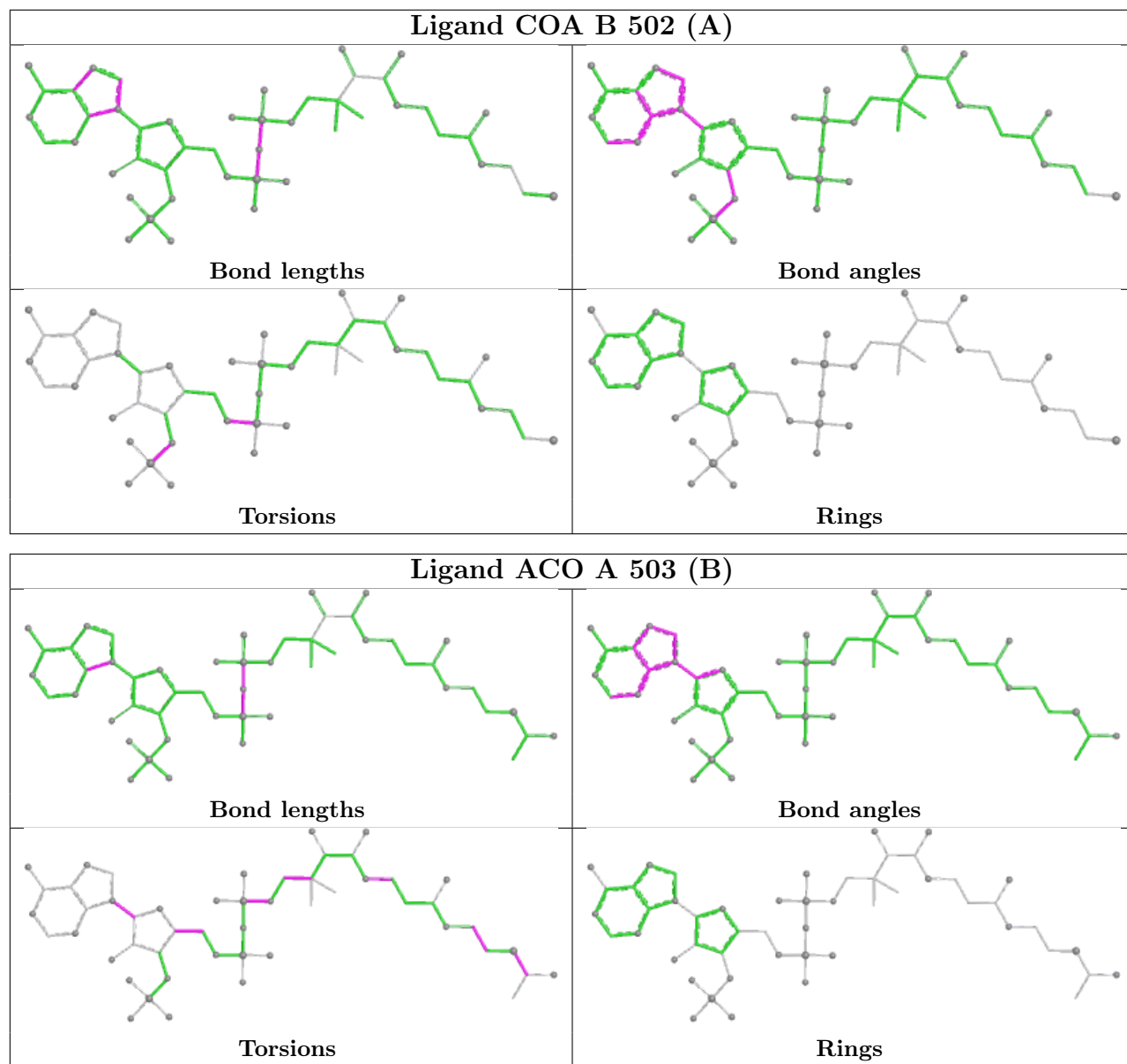
There are no ring outliers.

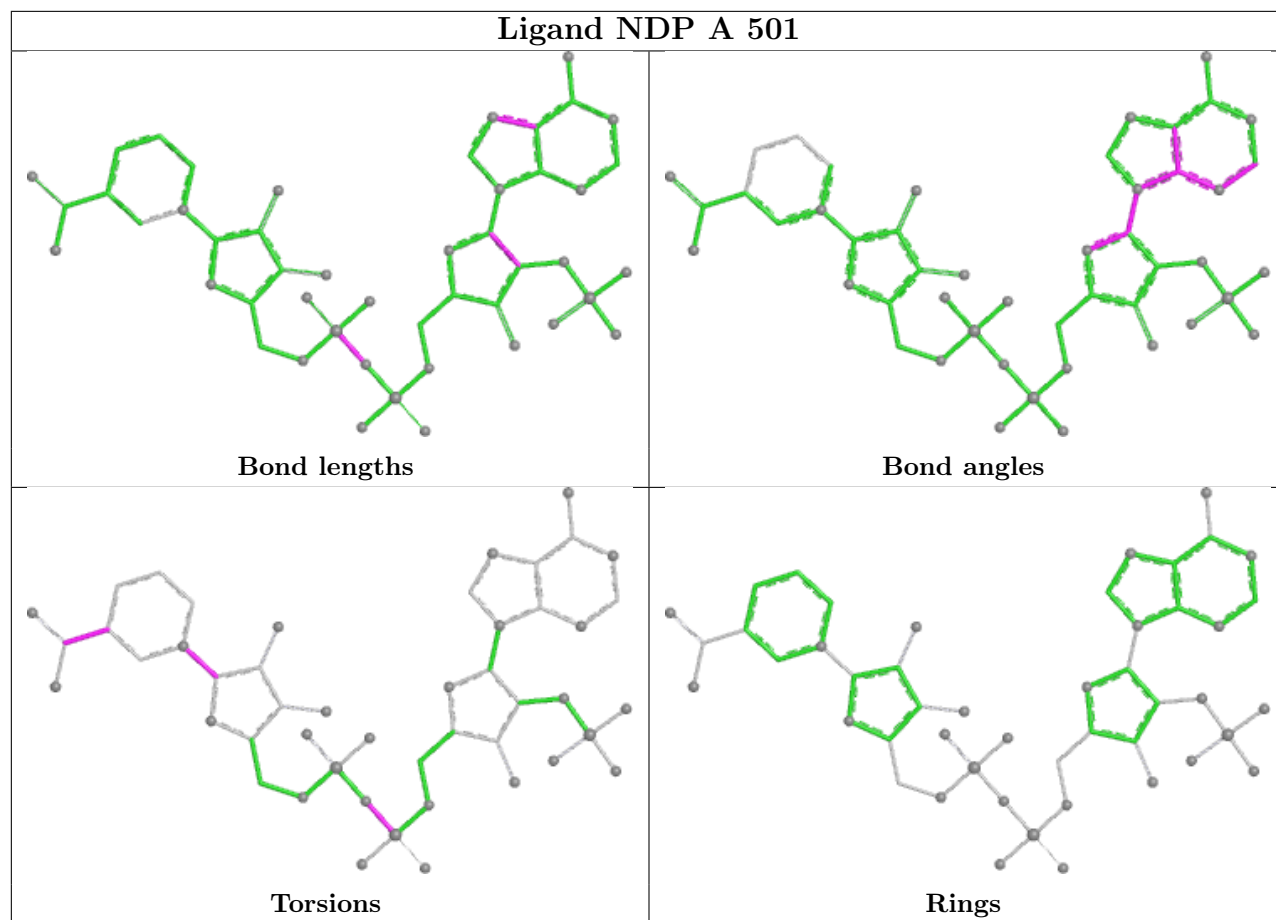
7 monomers are involved in 12 short contacts:

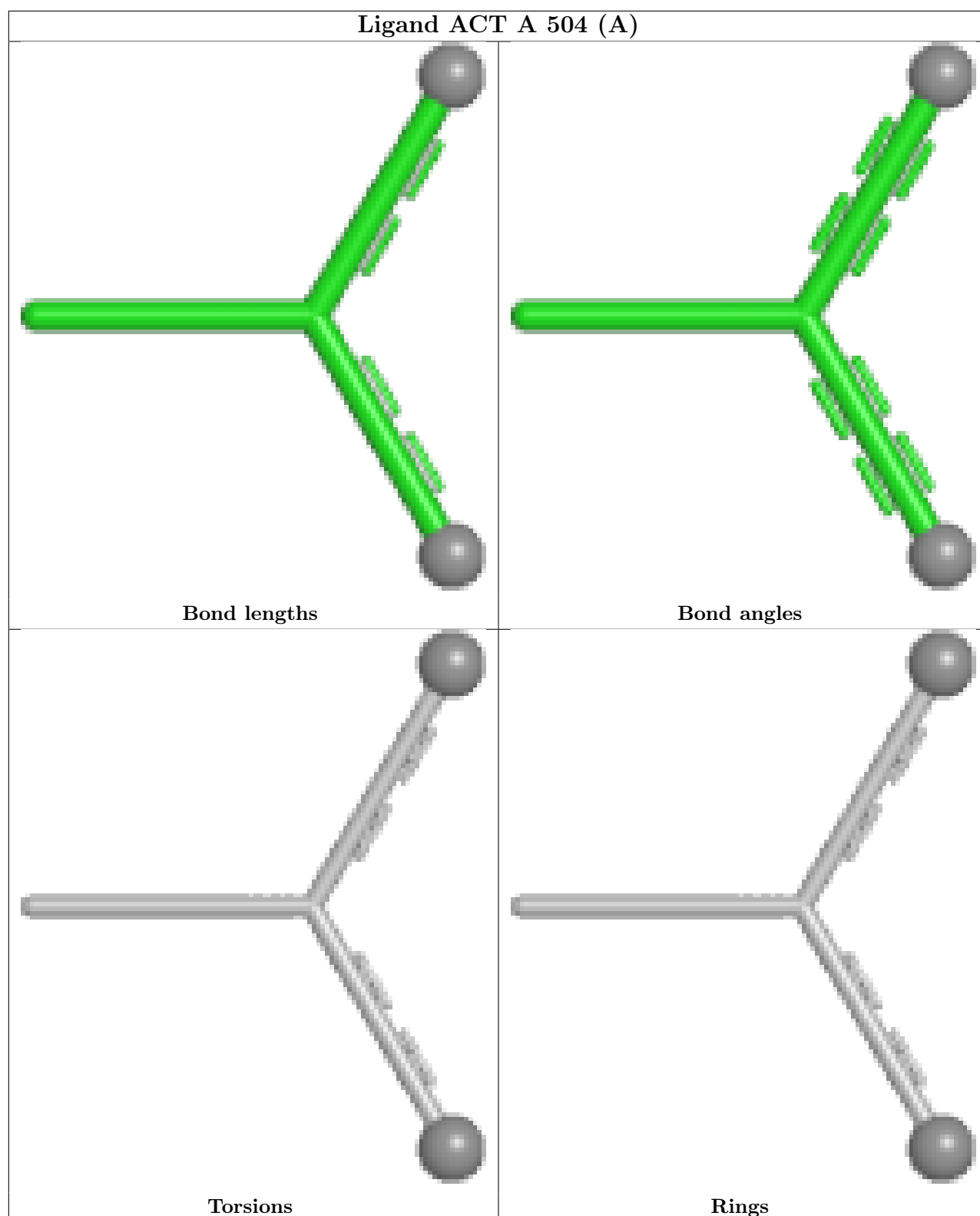
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[A]	COA	1	0
4	A	503[B]	ACO	2	0
7	B	501	NAI	3	0
8	B	505	EPE	2	0
4	B	503[B]	ACO	1	0
6	A	505	SO4	1	0
3	A	502[A]	COA	2	0

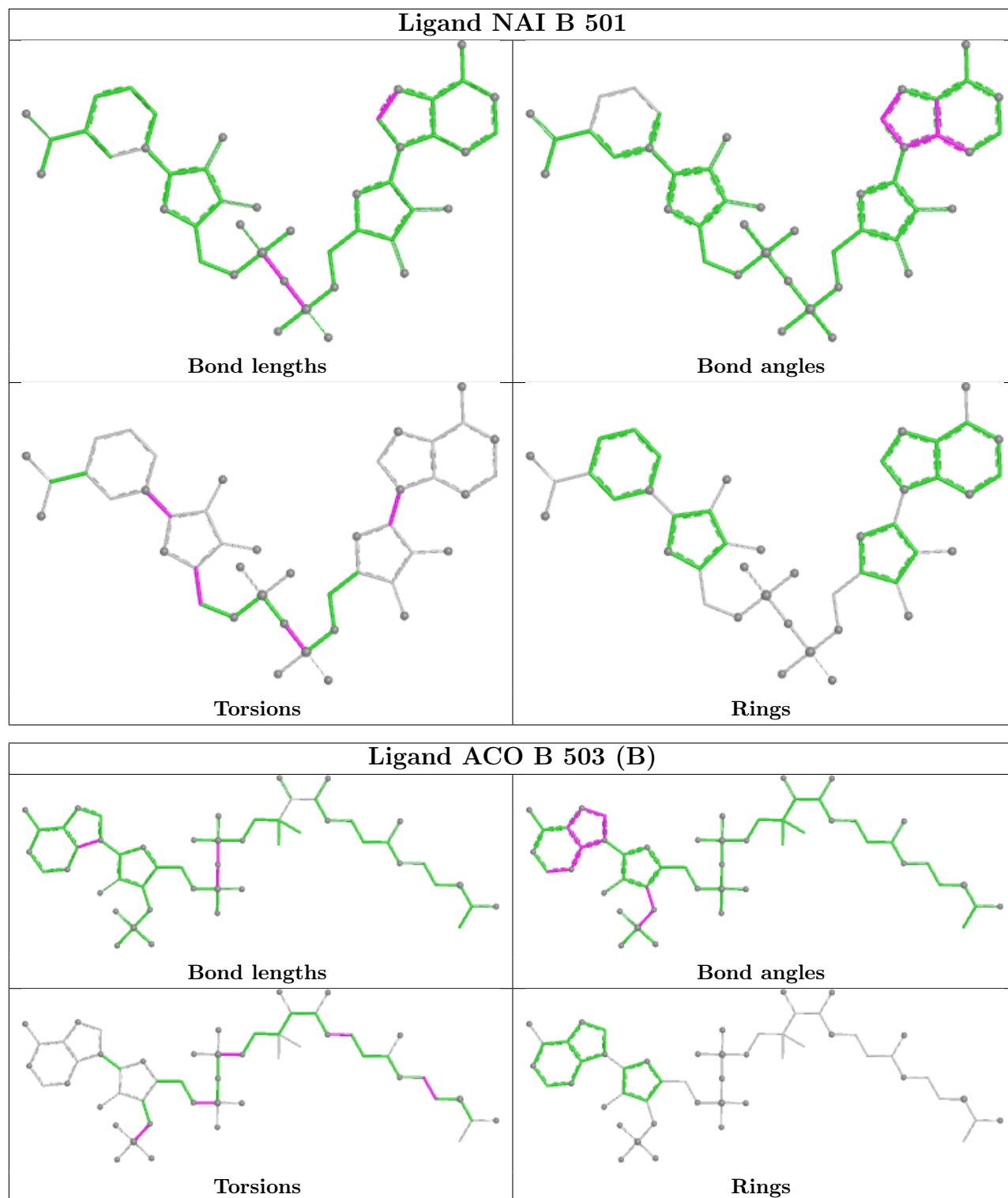
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

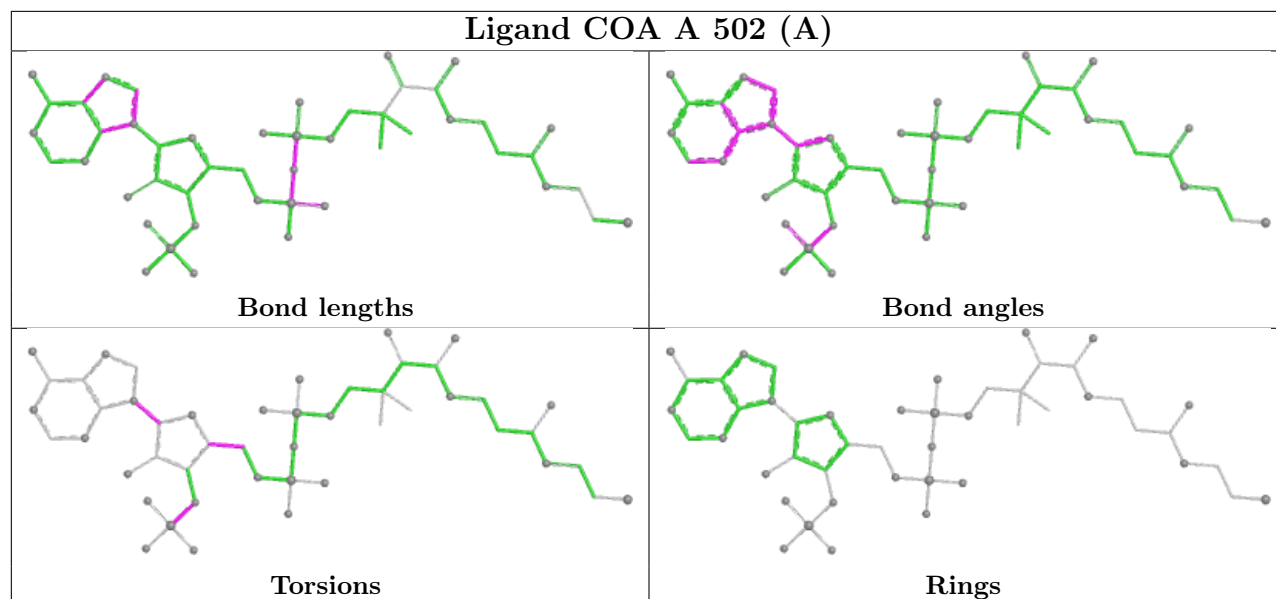












5.7 Other polymers [i](#)

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	339/352 (96%)	0.06	15 (4%) 39 38	12, 26, 46, 91	4 (1%)
1	B	340/352 (96%)	0.22	20 (5%) 28 27	10, 27, 57, 100	3 (0%)
All	All	679/704 (96%)	0.14	35 (5%) 33 31	10, 27, 53, 100	7 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	ALA	8.7
1	B	147	CYS	6.2
1	A	253	ARG	5.7
1	B	254	ASP	5.2
1	B	28	ALA	4.3
1	A	231	GLU	3.9
1	A	11	ALA	3.7
1	B	257	GLY	3.4
1	A	254	ASP	3.1
1	B	102	SER	3.1
1	B	27	SER	3.1
1	B	12	SER	2.9
1	B	89	LEU	2.9
1	A	260	ILE	2.8
1	B	30	ALA	2.8
1	B	162	TRP	2.8
1	B	88	SER	2.7
1	B	24	GLU	2.7
1	A	28	ALA	2.7
1	B	17	VAL	2.6
1	A	91[A]	ARG	2.6
1	B	29	GLY	2.6
1	A	30	ALA	2.6
1	B	253	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	18	ASP	2.6
1	A	29	GLY	2.5
1	A	102	SER	2.4
1	A	177	TRP	2.3
1	B	258	GLN	2.3
1	A	21	ASP	2.3
1	B	145	ASP	2.3
1	A	27	SER	2.3
1	A	237	HIS	2.2
1	B	25	ILE	2.2
1	A	293	TRP	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](#)

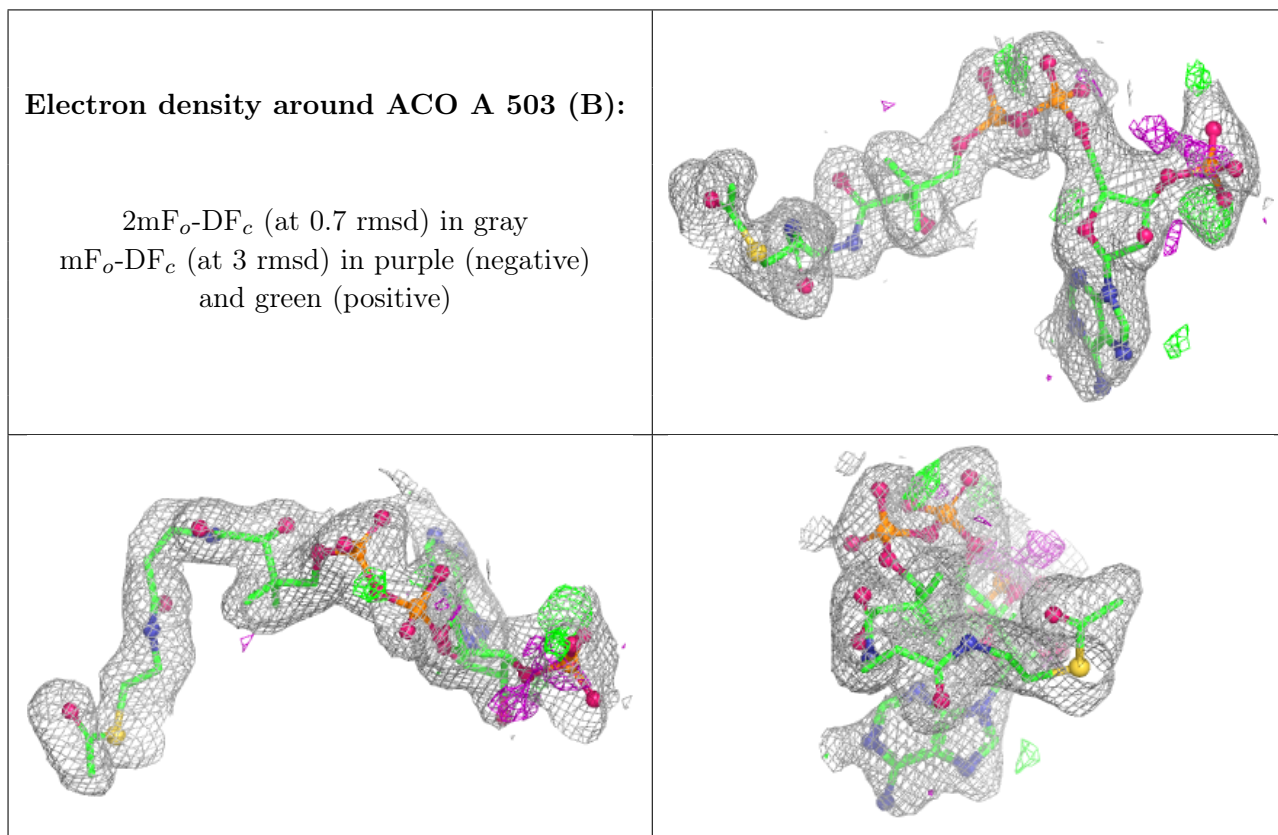
There are no oligosaccharides in this entry.

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.

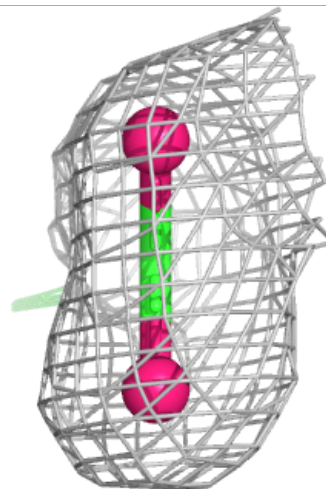
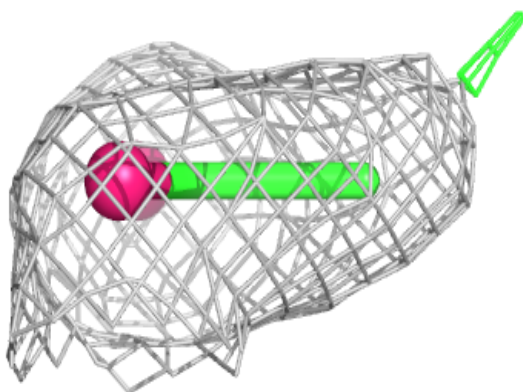
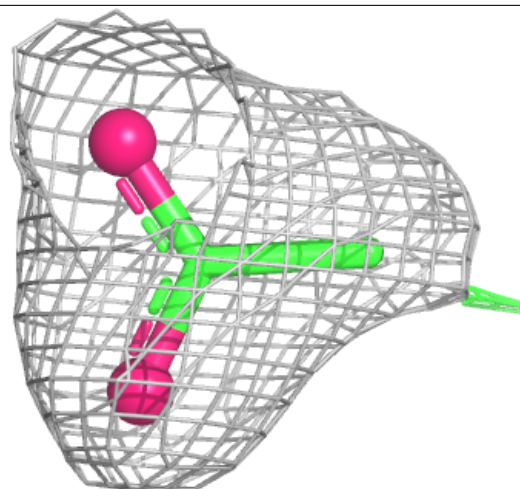
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	505	5/5	0.79	0.18	68,69,71,75	0
8	EPE	B	505	15/15	0.86	0.23	31,41,62,65	15
4	ACO	A	503[B]	51/51	0.90	0.13	19,27,59,63	51
5	ACT	B	504[A]	4/4	0.91	0.10	18,21,21,23	4
5	ACT	A	504[A]	4/4	0.92	0.09	19,19,19,22	4
6	SO4	B	506	5/5	0.92	0.10	44,52,65,68	0
7	NAI	B	501	44/44	0.92	0.12	22,32,40,45	44
2	NDP	A	501	48/48	0.92	0.12	18,28,59,62	48
4	ACO	B	503[B]	51/51	0.93	0.12	17,27,70,71	51
3	COA	A	502[A]	48/48	0.94	0.12	20,28,60,63	48
3	COA	B	502[A]	48/48	0.94	0.11	19,29,69,71	48

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.



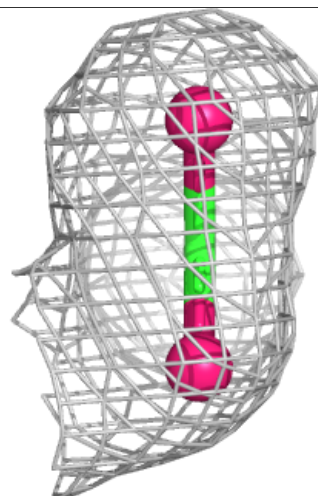
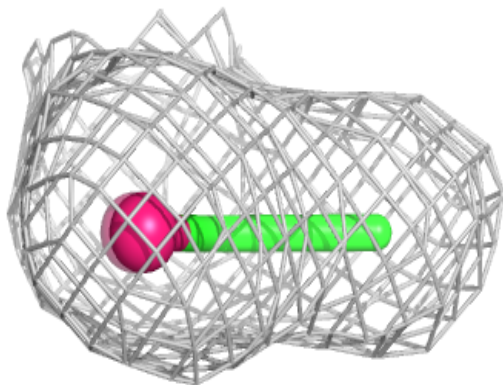
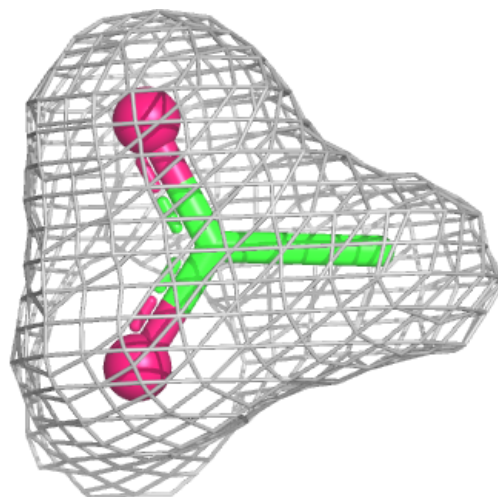
Electron density around ACT B 504 (A):

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



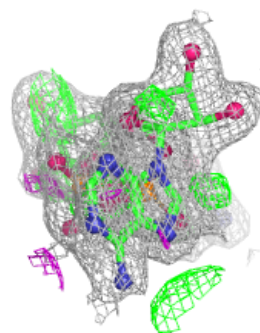
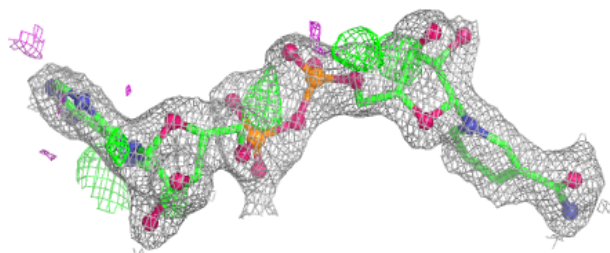
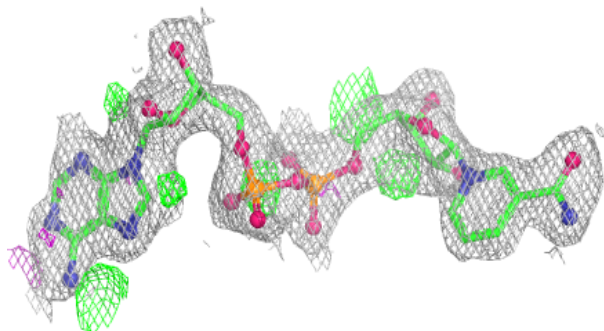
Electron density around ACT A 504 (A):

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

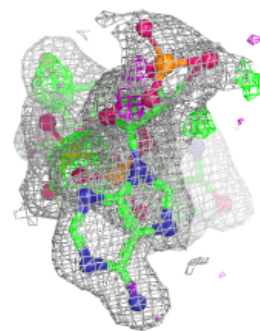
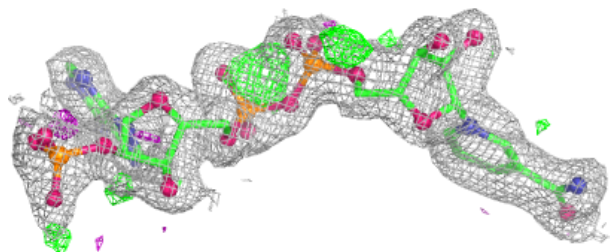
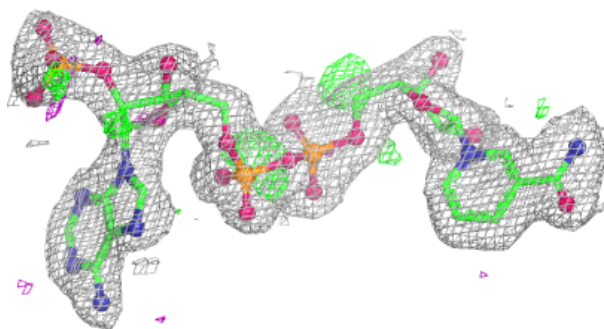


Electron density around NAI B 501:

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

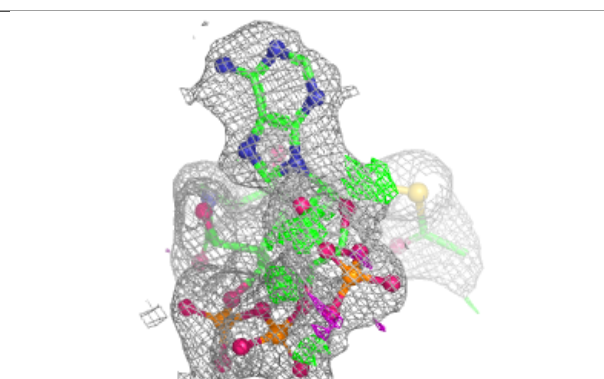
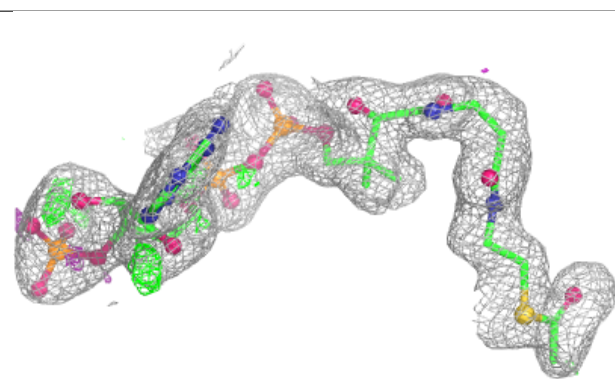
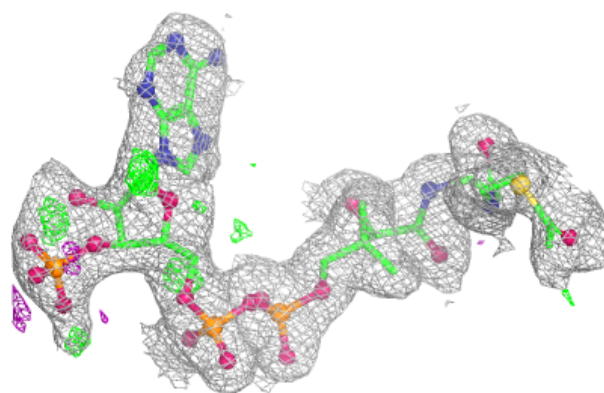
**Electron density around NDP A 501:**

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

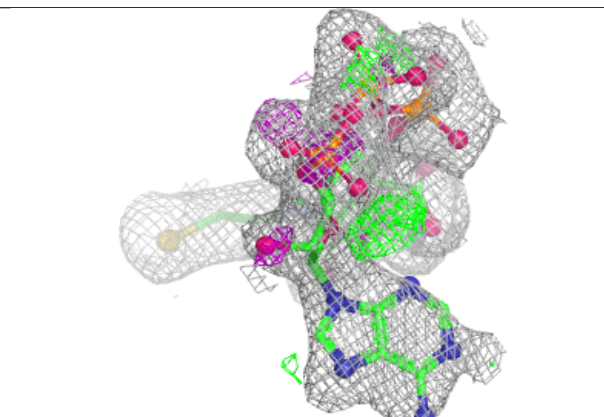
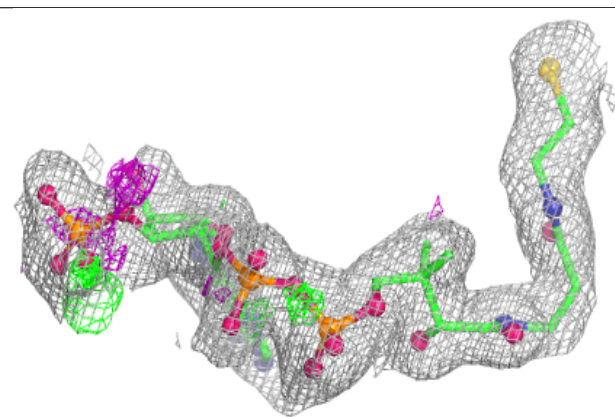
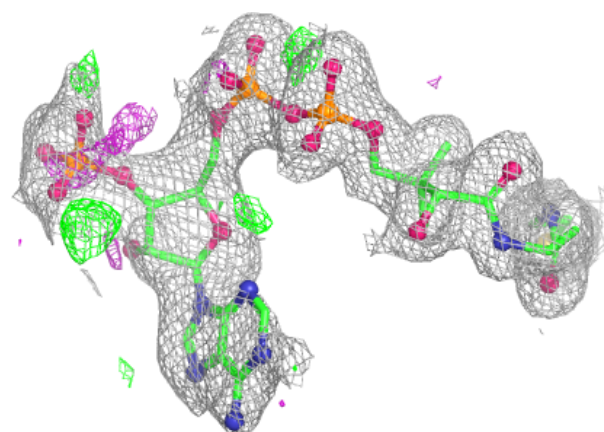


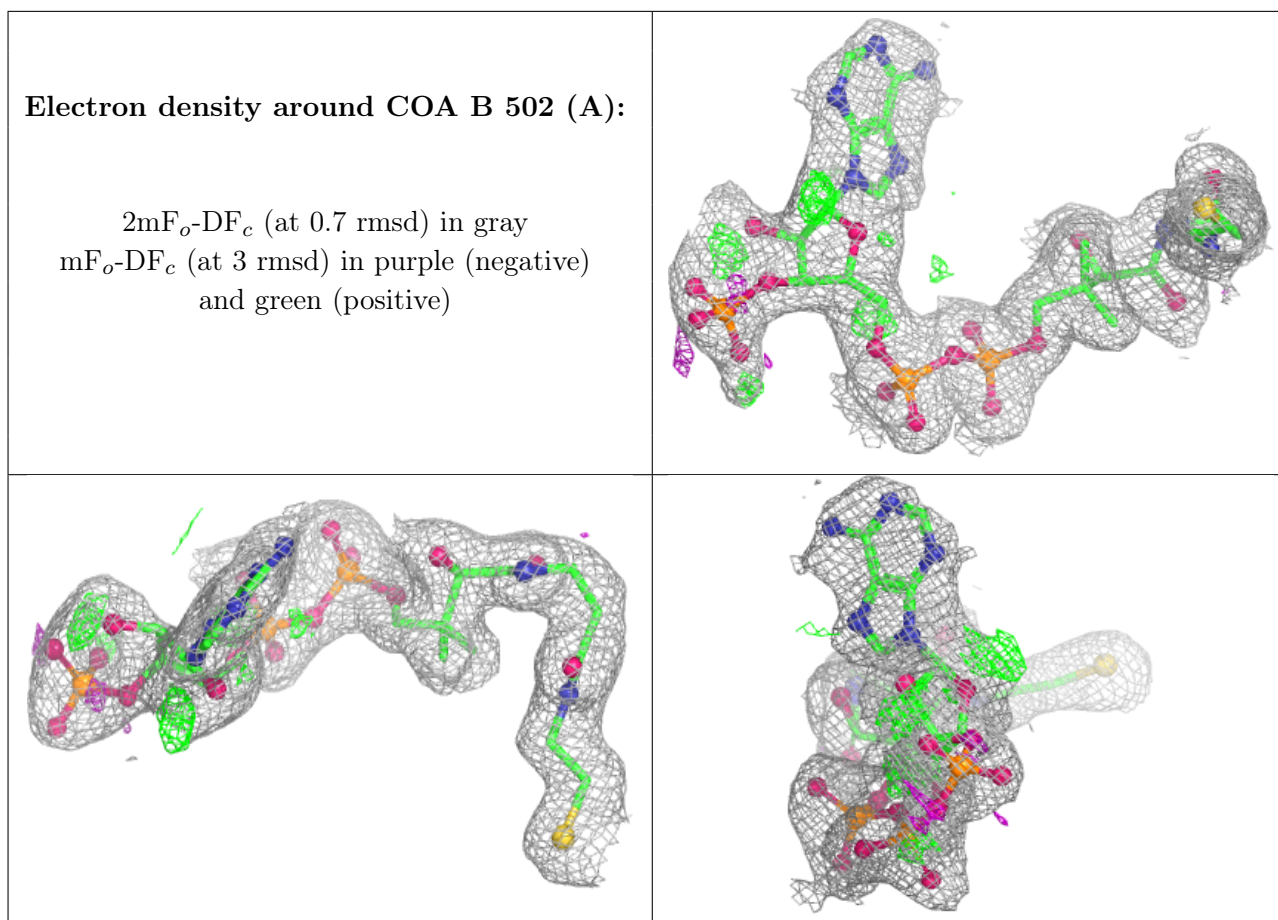
Electron density around ACO B 503 (B):

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

**Electron density around COA A 502 (A):**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.