



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:06 AM UTC

PDB ID : 4RVN / pdb_00004rvn
Title : Crystal structure of a Putative Acyl-CoA ligase (BT_0428) from Bacteroides
thetaiotaomicron VPI-5482 at 2.20 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2014-11-26
Resolution : 2.20 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

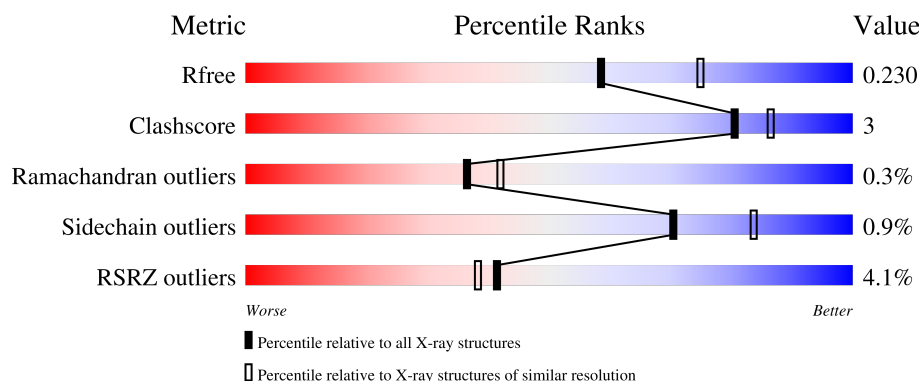
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

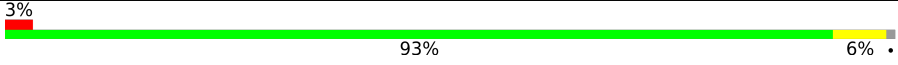
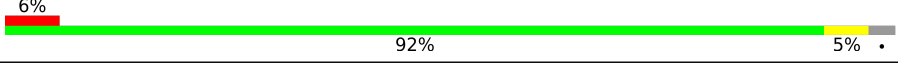
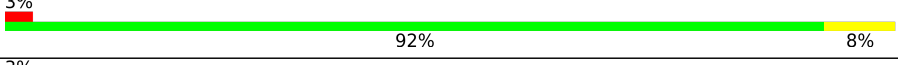
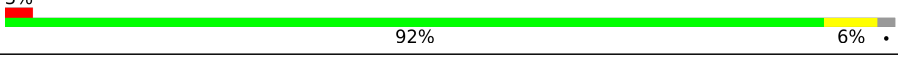
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	436	
1	B	436	
1	C	436	
1	D	436	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	UNL	A	507	-	-	X	-
6	UNL	B	503	-	-	X	-
6	UNL	C	507	-	-	X	-
6	UNL	D	503	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14520 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 Phenylacetate-coenzyme A ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	Se	0	6	0
			3445	2173	593	658	6	15			
1	B	424	Total	C	N	O	S	Se	0	8	0
			3356	2115	581	639	6	15			
1	C	434	Total	C	N	O	S	Se	0	3	0
			3427	2162	597	647	6	15			
1	D	426	Total	C	N	O	S	Se	0	6	0
			3362	2124	577	640	6	15			

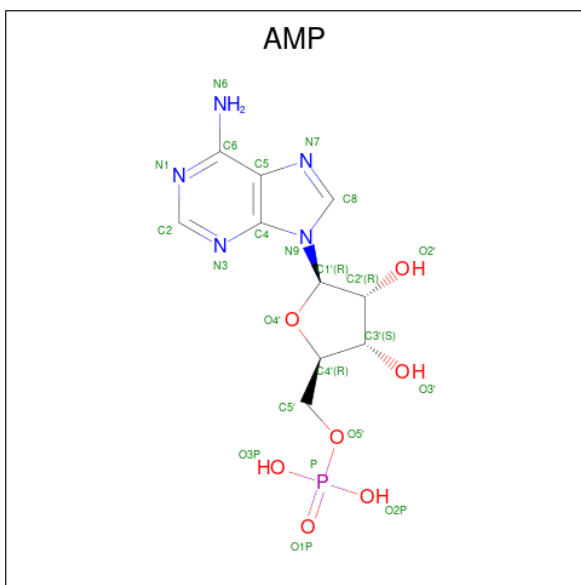
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8AAN6
B	0	GLY	-	expression tag	UNP Q8AAN6
C	0	GLY	-	expression tag	UNP Q8AAN6
D	0	GLY	-	expression tag	UNP Q8AAN6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

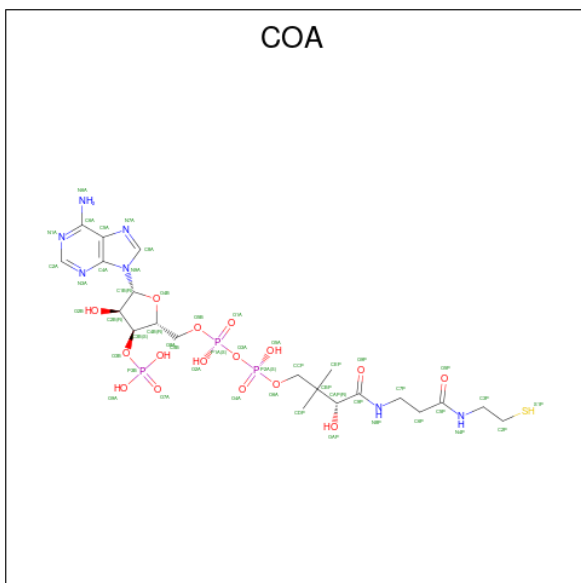
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 23	C 10	N 5	O 7	P 1	0	1
3	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	D	1	Total 23	C 10	N 5	O 7	P 1	0	0

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: $\text{C}_{21}\text{H}_{36}\text{N}_7\text{O}_{16}\text{P}_3\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

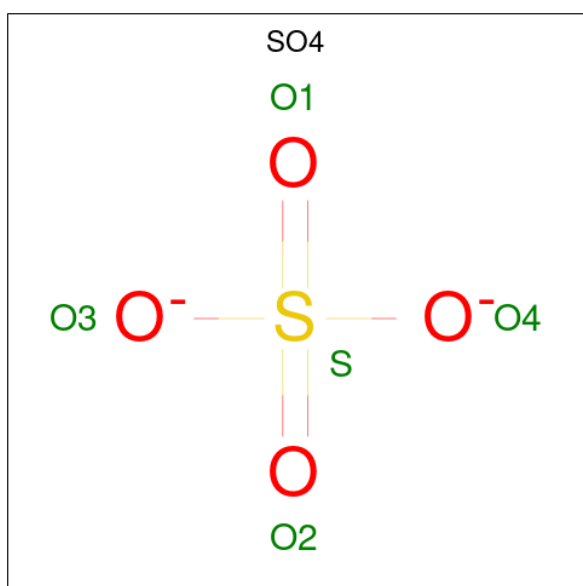
- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	K	0	0
			3	3		
5	C	3	Total	K	0	0
			3	3		

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

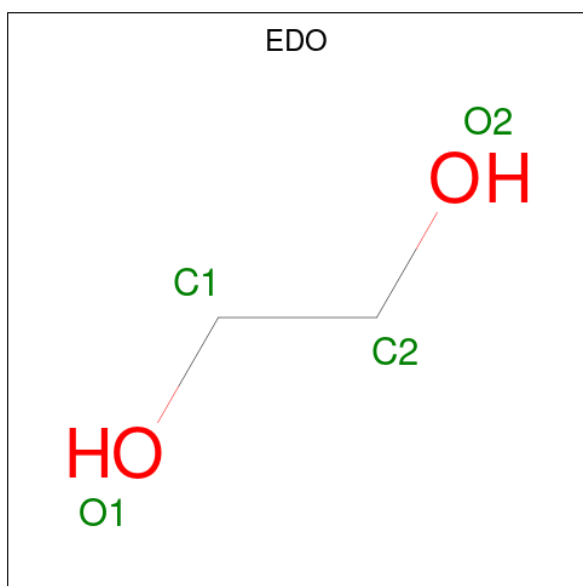
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			10	10		
6	B	1	Total	O	0	0
			9	9		
6	C	1	Total	O	0	0
			6	6		
6	D	1	Total	O	0	0
			7	7		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0

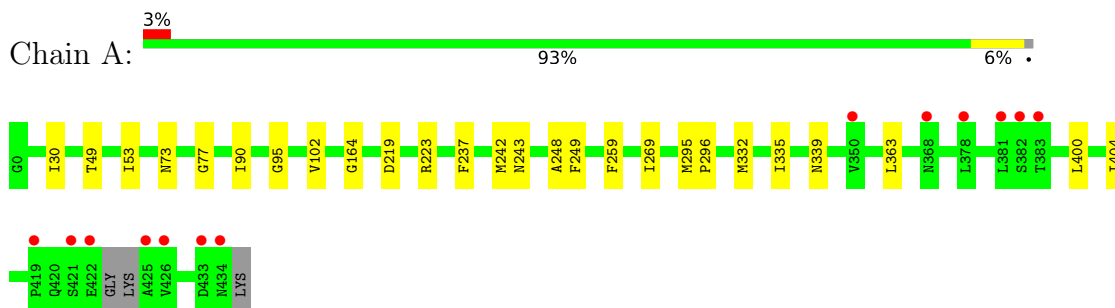
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	213	Total O 214 214	0	1
9	B	142	Total O 143 143	0	1
9	C	134	Total O 135 135	0	1
9	D	173	Total O 173 173	0	1

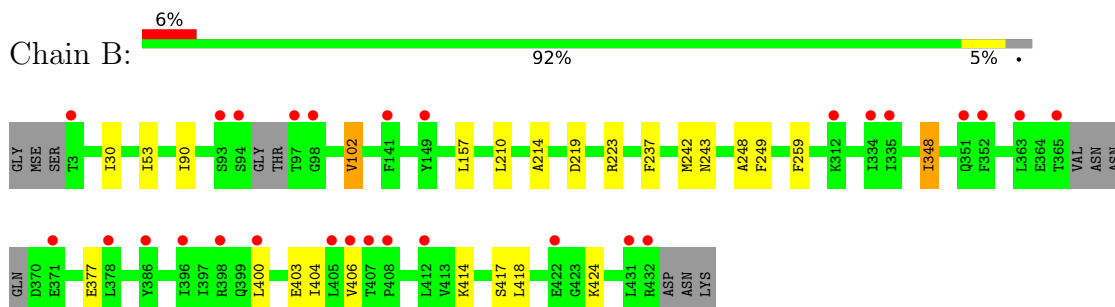
3 Residue-property plots [i](#)

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.

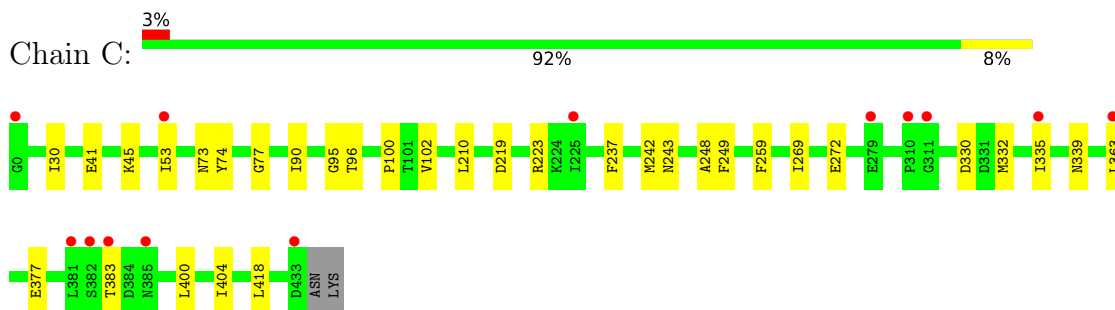
- Molecule 1: Phenylacetate-coenzyme A ligase



- Molecule 1: Phenylacetate-coenzyme A ligase

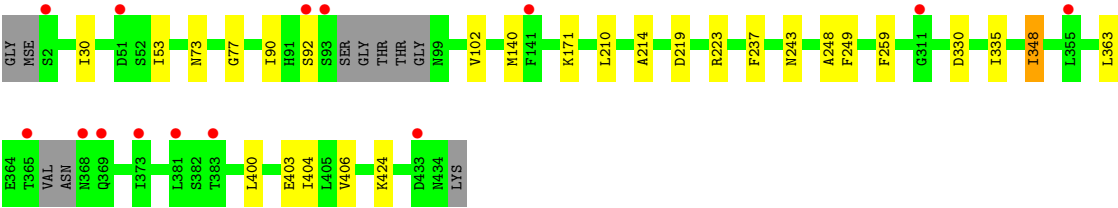


- Molecule 1: Phenylacetate-coenzyme A ligase



- Molecule 1: Phenylacetate-coenzyme A ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	127.78Å 211.30Å 71.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.20 47.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.78-2.20) 99.9 (47.78-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.20Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.192 , 0.219 0.204 , 0.230	Depositor DCC
R_{free} test set	4990 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14520	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: AMP, ZN, UNL, SO4, K, EDO, COA

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	0.78	0/3506	1.18	4/4709 (0.1%)
1	B	0.77	1/3423 (0.0%)	1.18	3/4601 (0.1%)
1	C	0.78	0/3480	1.20	5/4675 (0.1%)
1	D	0.78	1/3423 (0.0%)	1.20	2/4602 (0.0%)
All	All	0.78	2/13832 (0.0%)	1.19	14/18587 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	ILE	CG1-CD1	-6.12	1.27	1.51
1	D	348	ILE	CG1-CD1	-6.08	1.28	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	GLY	N-CA-C	6.91	120.77	111.72
1	A	95	GLY	N-CA-C	6.70	120.50	111.72
1	A	249	PHE	CA-CB-CG	6.02	119.82	113.80
1	C	249	PHE	CA-CB-CG	5.98	119.78	113.80
1	B	249	PHE	CA-CB-CG	5.90	119.70	113.80
1	D	249	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	242	MSE	CA-C-N	5.33	131.71	121.54
1	B	242	MSE	C-N-CA	5.33	131.71	121.54
1	C	330	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	330	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	242	MSE	CA-C-N	5.04	131.16	121.54
1	C	242	MSE	C-N-CA	5.04	131.16	121.54
1	A	242	MSE	CA-C-N	5.02	131.12	121.54
1	A	242	MSE	C-N-CA	5.02	131.12	121.54

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	3445	0	3434	14	0
1	B	3356	0	3309	13	0
1	C	3427	0	3417	13	0
1	D	3362	0	3307	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	0	1	0
3	B	23	0	12	2	0
3	C	23	0	12	3	0
3	D	23	0	12	2	0
4	A	31	0	11	1	0
4	C	31	0	11	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	10	0	0	7	0
6	B	9	0	0	3	0
6	C	6	0	0	5	0
6	D	7	0	0	5	0
7	A	10	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	A	20	0	30	2	0
8	B	4	0	6	0	0
8	C	12	0	18	0	0
8	D	8	0	12	0	0
9	A	214	0	0	1	0
9	B	143	0	0	0	0
9	C	135	0	0	0	0
9	D	173	0	0	0	0
All	All	14520	0	13591	72	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 (72) 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)
3:D:502:AMP:O1P	6:D:503:UNL:O2	1.65	1.13
6:D:503:UNL:O2	6:D:503:UNL:O1	1.96	0.84
6:D:503:UNL:O2	6:D:503:UNL:O3	1.98	0.81
3:D:502:AMP:P	6:D:503:UNL:O2	2.39	0.80
3:B:502:AMP:O2P	6:B:503:UNL:O3	1.99	0.80
3:A:502[A]:AMP:O3P	6:A:507:UNL:O4	2.06	0.73
6:C:507:UNL:O5	6:C:507:UNL:O6	2.10	0.70
1:B:214:ALA:HB1	1:B:424:LYS:HE2	1.74	0.69
3:C:502:AMP:P	6:C:507:UNL:O1	2.51	0.68
3:C:502:AMP:O2P	6:C:507:UNL:O1	2.12	0.67
3:C:502:AMP:O3P	6:C:507:UNL:O1	2.14	0.65
1:A:30:ILE:HD13	1:A:53:ILE:HG13	1.80	0.64
1:D:30:ILE:HD13	1:D:53:ILE:HG13	1.80	0.63
6:A:507:UNL:O4	6:A:507:UNL:O2	2.17	0.63
1:B:30:ILE:HD13	1:B:53:ILE:HG13	1.81	0.62
1:C:30:ILE:HD13	1:C:53:ILE:HG13	1.81	0.62
6:C:507:UNL:O1	6:C:507:UNL:O2	2.18	0.62
1:D:90:ILE:HG23	1:D:102:VAL:HG13	1.83	0.60
6:A:507:UNL:O4	6:A:507:UNL:O5	2.21	0.59
6:A:507:UNL:O5	6:A:507:UNL:O6	2.21	0.58
1:D:348:ILE:HD12	1:D:400:LEU:HD23	1.87	0.57
1:B:348:ILE:HD12	1:B:400:LEU:HD23	1.87	0.57
1:D:214:ALA:HB1	1:D:424:LYS:HE2	1.89	0.54
6:B:503:UNL:O3	6:B:503:UNL:O2	2.27	0.52
1:D:335:ILE:HD13	1:D:363:LEU:HD22	1.92	0.52
1:C:335:ILE:HD13	1:C:363:LEU:HD22	1.92	0.51
1:A:335:ILE:HD13	1:A:363:LEU:HD22	1.94	0.50
1:C:237:PHE:HB3	1:C:248:ALA:HB3	1.95	0.49
1:C:41:GLU:HG3	1:C:45:LYS:HE2	1.96	0.48
1:A:296:PRO:HD2	9:A:606:HOH:O	2.13	0.48
1:B:237:PHE:HB3	1:B:248:ALA:HB3	1.96	0.48
1:D:237:PHE:HB3	1:D:248:ALA:HB3	1.95	0.47
1:D:30:ILE:CD1	1:D:53:ILE:HG13	2.44	0.47
1:A:295:MSE:HE1	8:A:512:EDO:H22	1.97	0.46
1:C:96:THR:HA	1:D:171:LYS:HD2	1.98	0.46
1:A:30:ILE:CD1	1:A:53:ILE:HG13	2.46	0.45
1:A:332:MSE:SE	1:A:339:ASN:HB3	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:HA	8:A:510:EDO:H21	1.98	0.45
1:A:90:ILE:HG23	1:A:102:VAL:HG13	1.98	0.45
1:B:90:ILE:HG23	1:B:102:VAL:HG13	1.99	0.44
6:A:507:UNL:O6	6:A:507:UNL:O7	2.35	0.44
1:A:237:PHE:HB3	1:A:248:ALA:HB3	1.99	0.44
6:D:503:UNL:O1	6:D:503:UNL:O5	2.36	0.44
1:B:30:ILE:CD1	1:B:53:ILE:HG13	2.46	0.44
1:B:414:LYS:HB3	1:B:417:SER:OG	2.17	0.44
1:D:92:SER:HB3	1:D:140:MSE:HE3	2.00	0.43
1:C:400:LEU:O	1:C:404:ILE:HG12	2.18	0.43
1:C:219:ASP:O	1:C:223:ARG:HG2	2.19	0.43
1:B:400:LEU:O	1:B:404:ILE:HG12	2.19	0.43
1:D:348:ILE:HD11	1:D:403:GLU:HG2	2.01	0.43
1:A:400:LEU:O	1:A:404:ILE:HG12	2.18	0.43
1:C:74:TYR:CE1	1:C:100:PRO:HD2	2.53	0.43
1:D:348:ILE:HD11	1:D:403:GLU:CB	2.49	0.43
1:C:30:ILE:CD1	1:C:53:ILE:HG13	2.47	0.43
1:A:90:ILE:HD11	1:B:157:LEU:HD21	2.01	0.43
1:C:73:ASN:HB3	1:C:77:GLY:HA3	2.00	0.42
1:D:219:ASP:O	1:D:223:ARG:HG2	2.19	0.42
1:D:400:LEU:O	1:D:404:ILE:HG12	2.19	0.42
1:A:219:ASP:O	1:A:223:ARG:HG2	2.19	0.42
1:B:377:GLU:HG3	1:B:418:LEU:HD12	2.01	0.42
1:B:348:ILE:HD11	1:B:403:GLU:HG2	2.00	0.42
1:A:73:ASN:HB3	1:A:77:GLY:HA3	2.01	0.42
1:B:219:ASP:O	1:B:223:ARG:HG2	2.19	0.42
1:B:348:ILE:HD11	1:B:403:GLU:CB	2.49	0.42
1:A:164:GLY:HA2	4:A:503:COA:H1B	2.01	0.42
1:C:332:MSE:SE	1:C:339:ASN:HB3	2.70	0.41
1:C:90:ILE:HG23	1:C:102:VAL:HG13	2.02	0.41
1:D:73:ASN:HB3	1:D:77:GLY:HA3	2.01	0.41
3:B:502:AMP:O2P	6:B:503:UNL:O2	2.38	0.41
1:C:377:GLU:HG3	1:C:418:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

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	435/436 (100%)	418 (96%)	16 (4%)	1 (0%)	43	51
1	B	426/436 (98%)	411 (96%)	14 (3%)	1 (0%)	43	51
1	C	435/436 (100%)	414 (95%)	19 (4%)	2 (0%)	24	27
1	D	426/436 (98%)	408 (96%)	17 (4%)	1 (0%)	43	51
All	All	1722/1744 (99%)	1651 (96%)	66 (4%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	B	243	ASN
1	C	243	ASN
1	D	243	ASN
1	C	383	THR

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	377/370 (102%)	375 (100%)	2 (0%)	81	90
1	B	363/370 (98%)	359 (99%)	4 (1%)	65	79
1	C	371/370 (100%)	367 (99%)	4 (1%)	65	79
1	D	361/370 (98%)	358 (99%)	3 (1%)	73	85
All	All	1472/1480 (100%)	1459 (99%)	13 (1%)	70	84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	PHE
1	A	269	ILE
1	B	102	VAL
1	B	210	LEU
1	B	259	PHE
1	B	406	VAL
1	C	210	LEU
1	C	259	PHE
1	C	269	ILE
1	C	272	GLU
1	D	210	LEU
1	D	259	PHE
1	D	406	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	24	GLN
1	A	35	ASN
1	A	252	GLN
1	A	351	GLN
1	A	369	GLN
1	B	24	GLN
1	B	35	ASN
1	B	252	GLN
1	C	24	GLN
1	C	35	ASN
1	C	252	GLN
1	C	351	GLN
1	D	19	GLN
1	D	24	GLN
1	D	196	GLN
1	D	252	GLN
1	D	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 10 are monoatomic and 4 are unknown - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	COA	A	503	-	32,33,50	0.84	1 (3%)	50,52,75	1.23	7 (14%)
7	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.13	0
8	EDO	A	510	-	3,3,3	0.53	0	2,2,2	0.22	0
8	EDO	C	510	-	3,3,3	0.53	0	2,2,2	0.32	0
8	EDO	A	512	-	3,3,3	0.40	0	2,2,2	0.38	0
7	SO4	A	508	-	4,4,4	0.27	0	6,6,6	0.18	0
8	EDO	D	506	-	3,3,3	0.51	0	2,2,2	0.37	0
3	AMP	D	502	-	25,25,25	0.13	0	37,38,38	0.33	0
3	AMP	C	502	5	25,25,25	0.17	0	37,38,38	0.37	0
4	COA	C	503	-	32,33,50	0.82	3 (9%)	50,52,75	1.16	7 (14%)
8	EDO	D	505	-	3,3,3	0.53	0	2,2,2	0.31	0
7	SO4	C	508	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	B	504	-	4,4,4	0.27	0	6,6,6	0.14	0
8	EDO	C	509	-	3,3,3	0.49	0	2,2,2	0.40	0
8	EDO	B	505	-	3,3,3	0.49	0	2,2,2	0.39	0
3	AMP	B	502	-	25,25,25	0.18	0	37,38,38	0.38	0
7	SO4	A	509	-	4,4,4	0.26	0	6,6,6	0.06	0
8	EDO	A	513	-	3,3,3	0.60	0	2,2,2	0.25	0
8	EDO	C	511	-	3,3,3	0.55	0	2,2,2	0.30	0
8	EDO	A	514	-	3,3,3	0.50	0	2,2,2	0.39	0
8	EDO	A	511	-	3,3,3	0.50	0	2,2,2	0.39	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
8	EDO	B	505	-	-	0/1/1/1	-
3	AMP	B	502	-	-	1/10/26/26	0/3/3/3
4	COA	A	503	-	-	4/21/37/64	0/3/3/3
4	COA	C	503	-	-	4/21/37/64	0/3/3/3
8	EDO	D	505	-	-	0/1/1/1	-
8	EDO	D	506	-	-	0/1/1/1	-
8	EDO	A	513	-	-	0/1/1/1	-
8	EDO	C	511	-	-	0/1/1/1	-
3	AMP	D	502	-	-	0/10/26/26	0/3/3/3
8	EDO	A	510	-	-	0/1/1/1	-
8	EDO	A	511	-	-	0/1/1/1	-
8	EDO	A	512	-	-	0/1/1/1	-
8	EDO	C	510	-	-	0/1/1/1	-
8	EDO	A	514	-	-	0/1/1/1	-
8	EDO	C	509	-	-	0/1/1/1	-
3	AMP	C	502	5	-	0/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	COA	P1A-O3A	3.73	1.63	1.59
4	C	503	COA	P1A-O3A	2.93	1.62	1.59
4	C	503	COA	P3B-O3B	2.34	1.63	1.59
4	C	503	COA	P2A-O6A	2.20	1.63	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	COA	O6A-P2A-O3A	4.29	119.02	104.64
4	C	503	COA	O6A-P2A-O3A	3.77	117.27	104.64
4	A	503	COA	O3A-P1A-O1A	-3.12	101.31	110.70
4	C	503	COA	O3A-P1A-O1A	-3.12	101.33	110.70
4	A	503	COA	O5A-P2A-O4A	3.03	122.64	110.83
4	C	503	COA	O5A-P2A-O4A	2.76	121.60	110.83
4	A	503	COA	O6A-P2A-O5A	-2.61	98.03	107.80
4	C	503	COA	O6A-P2A-O5A	-2.56	98.22	107.80
4	A	503	COA	O3A-P2A-O4A	-2.43	98.28	111.04
4	C	503	COA	O2A-P1A-O1A	2.41	123.65	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	COA	O2A-P1A-O1A	2.36	123.41	112.44
4	C	503	COA	O3A-P2A-O4A	-2.23	99.30	111.04
4	C	503	COA	O3B-P3B-O7A	2.22	117.25	109.33
4	A	503	COA	O3B-P3B-O7A	2.16	117.03	109.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

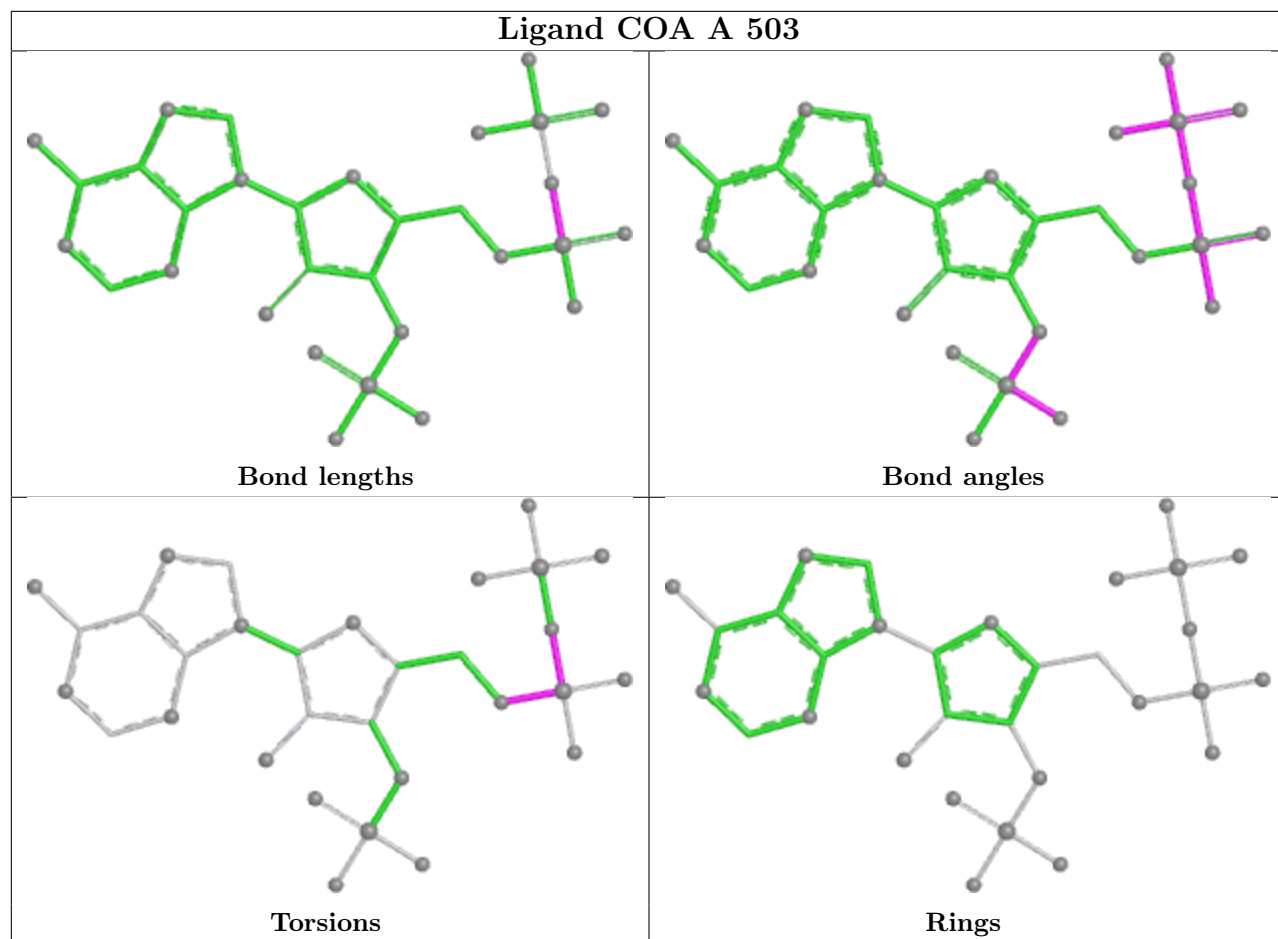
Mol	Chain	Res	Type	Atoms
4	A	503	COA	C5B-O5B-P1A-O1A
4	A	503	COA	C5B-O5B-P1A-O2A
4	A	503	COA	C5B-O5B-P1A-O3A
4	C	503	COA	C5B-O5B-P1A-O1A
4	C	503	COA	C5B-O5B-P1A-O2A
4	C	503	COA	C5B-O5B-P1A-O3A
3	B	502	AMP	C5'-O5'-P-O3P
4	A	503	COA	P2A-O3A-P1A-O2A
4	C	503	COA	P2A-O3A-P1A-O2A

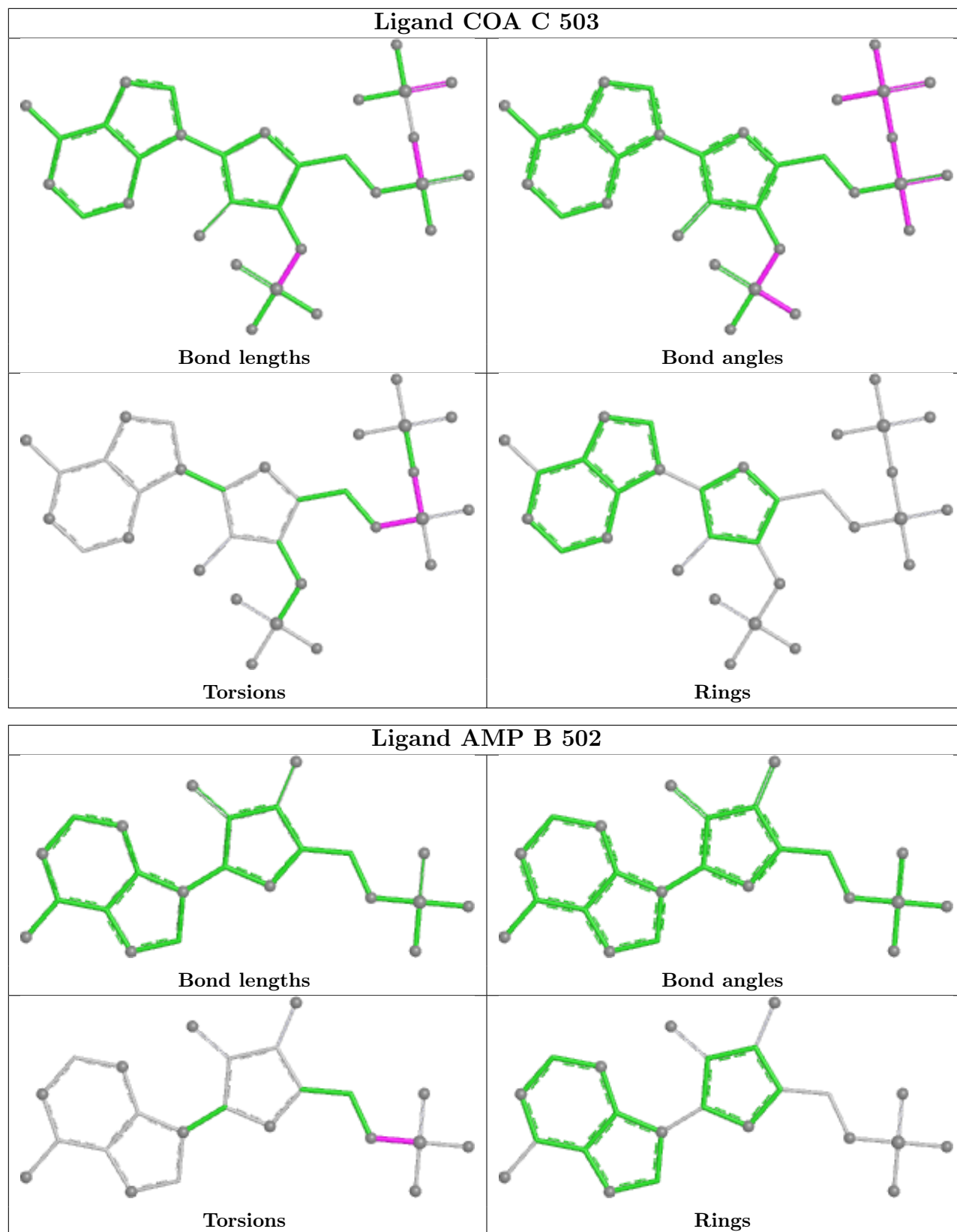
There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	COA	1	0
8	A	510	EDO	1	0
8	A	512	EDO	1	0
3	D	502	AMP	2	0
3	C	502	AMP	3	0
3	B	502	AMP	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	418/436 (95%)	0.16	13 (3%)	51	48	28, 47, 83, 133	5 (1%)
1	B	410/436 (94%)	0.38	28 (6%)	23	20	32, 57, 106, 133	7 (1%)
1	C	419/436 (96%)	0.32	13 (3%)	51	48	28, 58, 95, 114	3 (0%)
1	D	412/436 (94%)	0.27	14 (3%)	48	45	30, 50, 92, 119	5 (1%)
All	All	1659/1744 (95%)	0.28	68 (4%)	41	38	28, 53, 97, 133	20 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	433	ASP	5.8
1	A	422	GLU	4.9
1	A	426	VAL	4.1
1	D	368	ASN	4.0
1	D	433	ASP	3.9
1	B	94	SER	3.9
1	D	369	GLN	3.7
1	B	365	THR	3.6
1	D	383	THR	3.6
1	A	421	SER	3.6
1	A	434	ASN	3.5
1	A	425	ALA	3.5
1	D	93	SER	3.5
1	D	365	THR	3.4
1	C	382	SER	3.3
1	A	368	ASN	3.3
1	D	2	SER	3.3
1	C	381	LEU	3.2
1	B	312	LYS	3.1
1	B	406	VAL	3.0
1	A	419	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	383	THR	2.9
1	B	97	THR	2.9
1	C	383	THR	2.9
1	B	378	LEU	2.8
1	C	385	ASN	2.8
1	B	93	SER	2.8
1	B	400	LEU	2.6
1	C	311	GLY	2.6
1	D	92	SER	2.6
1	B	431	LEU	2.5
1	C	0	GLY	2.5
1	C	53	ILE	2.5
1	B	371	GLU	2.5
1	D	355	LEU	2.5
1	A	382	SER	2.4
1	C	225	ILE	2.4
1	B	363	LEU	2.4
1	B	412	LEU	2.4
1	C	363	LEU	2.4
1	B	407	THR	2.4
1	A	350	VAL	2.4
1	B	149	TYR	2.4
1	B	396	ILE	2.4
1	D	141	PHE	2.4
1	B	422	GLU	2.4
1	A	433	ASP	2.3
1	D	311	GLY	2.3
1	B	335	ILE	2.3
1	C	279	GLU	2.3
1	B	386	TYR	2.3
1	B	398[A]	ARG	2.3
1	B	351[A]	GLN	2.3
1	B	334	ILE	2.3
1	C	310	PRO	2.2
1	B	98	GLY	2.2
1	D	373	ILE	2.2
1	B	3	THR	2.2
1	B	405	LEU	2.2
1	B	141	PHE	2.2
1	A	378	LEU	2.2
1	D	381	LEU	2.1
1	D	51	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	2.1
1	B	352	PHE	2.1
1	B	408	PRO	2.0
1	B	432	ARG	2.0
1	C	335	ILE	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
8	EDO	B	505	4/4	0.67	0.22	78,78,78,79	0
8	EDO	C	511	4/4	0.72	0.19	51,52,53,54	0
7	SO4	C	508	5/5	0.74	0.09	114,114,114,114	0
8	EDO	A	514	4/4	0.74	0.17	74,74,74,75	0
8	EDO	D	505	4/4	0.74	0.18	76,77,78,78	0
7	SO4	A	509	5/5	0.77	0.10	127,127,127,127	0
8	EDO	D	506	4/4	0.78	0.17	55,56,57,58	0
6	UNL	D	503	7/-	0.79	0.17	32,43,56,62	0
8	EDO	C	509	4/4	0.80	0.17	69,69,70,70	0
7	SO4	B	504	5/5	0.81	0.11	103,103,103,104	0
4	COA	A	503	31/48	0.81	0.13	82,90,109,110	0
8	EDO	A	511	4/4	0.81	0.16	73,73,74,75	0
8	EDO	C	510	4/4	0.82	0.17	68,68,69,69	0
6	UNL	C	507	6/-	0.85	0.14	34,42,56,71	0
8	EDO	A	510	4/4	0.85	0.14	54,55,55,55	0
8	EDO	A	512	4/4	0.86	0.19	60,60,61,61	0
6	UNL	A	507	10/-	0.87	0.13	26,36,54,56	0
4	COA	C	503	31/48	0.87	0.12	71,76,90,90	0

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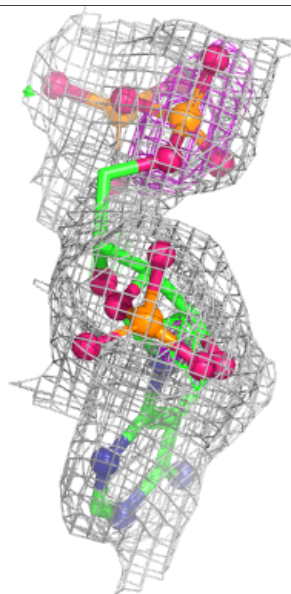
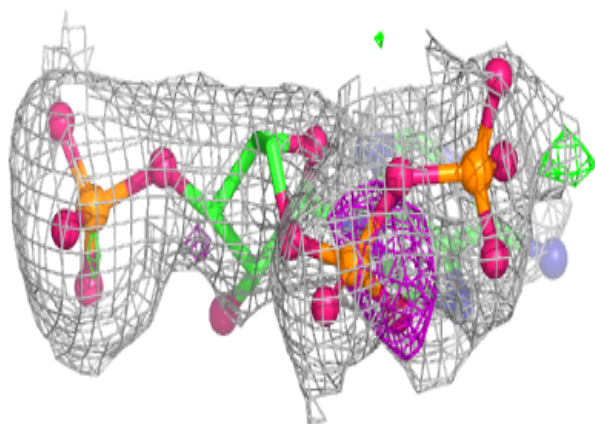
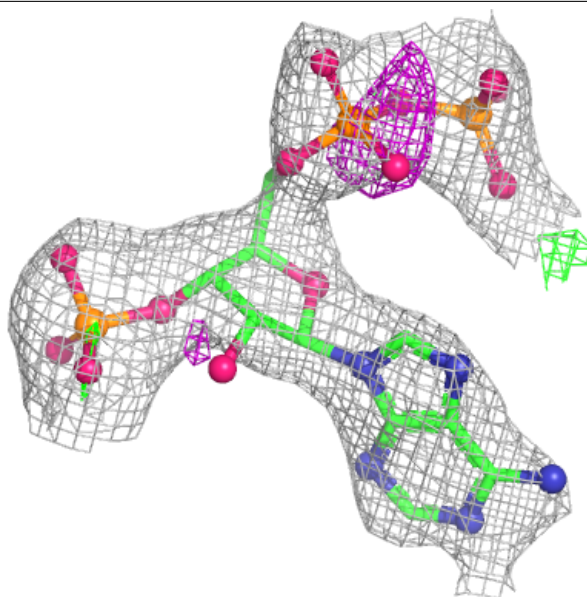
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	UNL	B	503	9/-	0.89	0.12	40,42,59,60	0
7	SO4	D	504	5/5	0.89	0.09	86,86,87,87	0
3	AMP	B	502	23/23	0.92	0.08	45,48,49,50	0
8	EDO	A	513	4/4	0.93	0.10	38,39,39,40	0
3	AMP	D	502	23/23	0.94	0.07	35,39,52,55	0
7	SO4	A	508	5/5	0.95	0.06	51,51,53,54	0
3	AMP	C	502	23/23	0.95	0.07	39,42,43,45	0
2	ZN	B	501	1/1	0.96	0.07	47,47,47,47	0
5	K	A	505	1/1	0.96	0.07	43,43,43,43	0
2	ZN	C	501	1/1	0.97	0.05	57,57,57,57	0
3	AMP	A	502[A]	23/23	0.97	0.06	29,32,34,36	0
5	K	C	505	1/1	0.97	0.06	37,37,37,37	0
5	K	C	506	1/1	0.97	0.07	38,38,38,38	0
2	ZN	D	501	1/1	0.98	0.04	48,48,48,48	0
5	K	C	504	1/1	0.98	0.09	44,44,44,44	0
5	K	A	504	1/1	0.98	0.07	38,38,38,38	0
5	K	A	506	1/1	0.99	0.07	30,30,30,30	0
2	ZN	A	501	1/1	0.99	0.03	43,43,43,43	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.

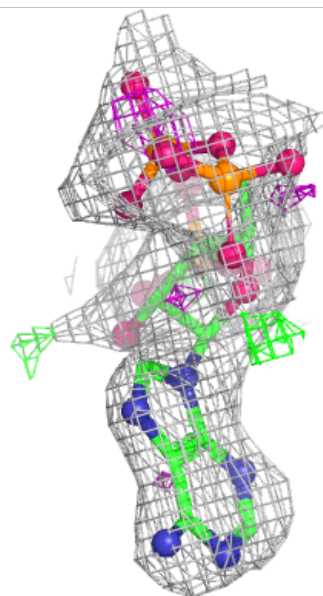
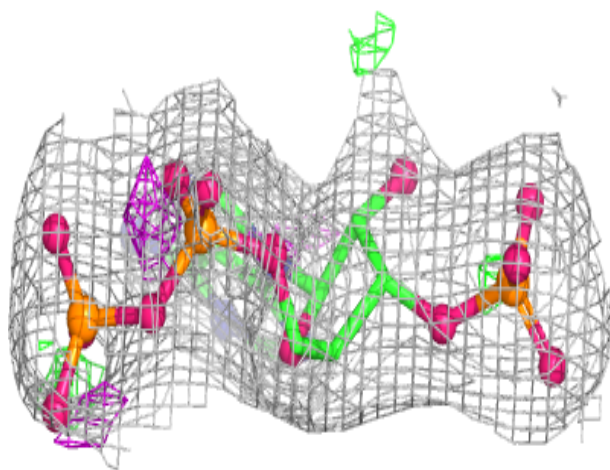
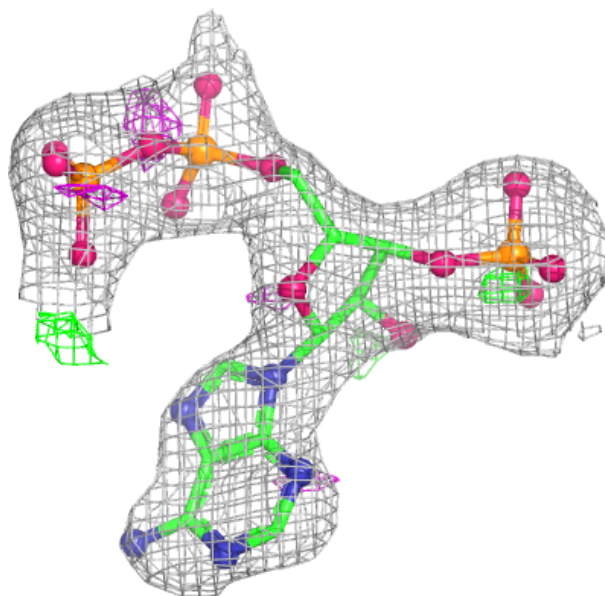
Electron density around COA A 503:

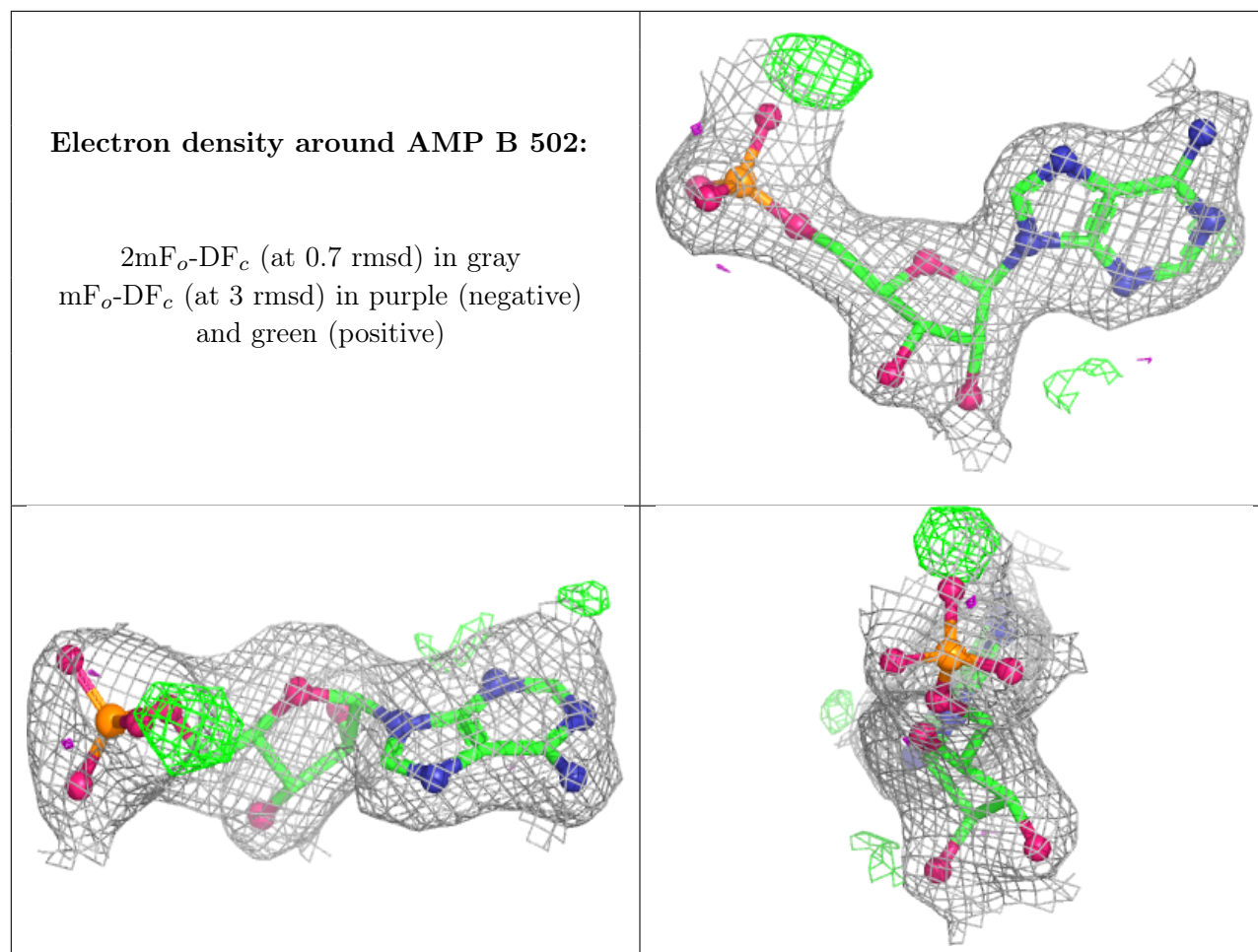
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA C 503:

$2mF_o-DF_c$ (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.