



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:39 AM UTC

PDB ID : 6HE2 / pdb_00006he2
Title : Crystal structure of an open conformation of 2-Hydroxyisobutyryl-CoA Ligase (HCL) in complex with 2-HIB-AMP and CoA
Authors : Zahn, M.; Rohwerder, T.; Strater, N.
Deposited on : 2018-08-20
Resolution : 2.30 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

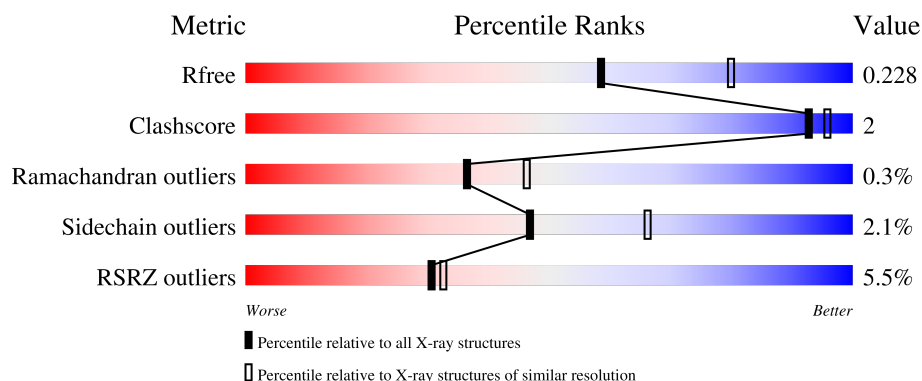
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	499	
1	B	499	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7501 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 2-hydroxyisobutyryl-CoA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3630	2292	651	663	24			
1	B	430	Total	C	N	O	S	0	0	0
			3380	2138	602	617	23			

There are 44 discrepancies between the modelled and reference sequences:

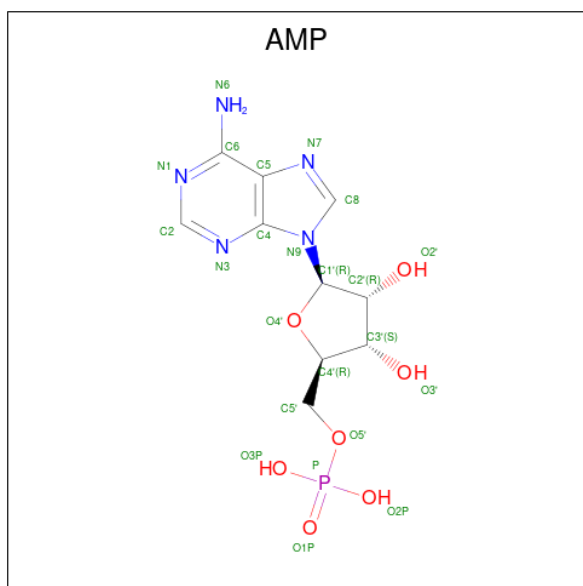
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP I3VE75
A	-9	ALA	-	expression tag	UNP I3VE75
A	-8	SER	-	expression tag	UNP I3VE75
A	-7	HIS	-	expression tag	UNP I3VE75
A	-6	HIS	-	expression tag	UNP I3VE75
A	-5	HIS	-	expression tag	UNP I3VE75
A	-4	HIS	-	expression tag	UNP I3VE75
A	-3	HIS	-	expression tag	UNP I3VE75
A	-2	HIS	-	expression tag	UNP I3VE75
A	-1	SER	-	expression tag	UNP I3VE75
A	0	GLY	-	expression tag	UNP I3VE75
A	478	GLY	-	expression tag	UNP I3VE75
A	479	SER	-	expression tag	UNP I3VE75
A	480	ALA	-	expression tag	UNP I3VE75
A	481	TRP	-	expression tag	UNP I3VE75
A	482	SER	-	expression tag	UNP I3VE75
A	483	HIS	-	expression tag	UNP I3VE75
A	484	PRO	-	expression tag	UNP I3VE75
A	485	GLN	-	expression tag	UNP I3VE75
A	486	PHE	-	expression tag	UNP I3VE75
A	487	GLU	-	expression tag	UNP I3VE75
A	488	LYS	-	expression tag	UNP I3VE75
B	-10	MET	-	initiating methionine	UNP I3VE75
B	-9	ALA	-	expression tag	UNP I3VE75
B	-8	SER	-	expression tag	UNP I3VE75

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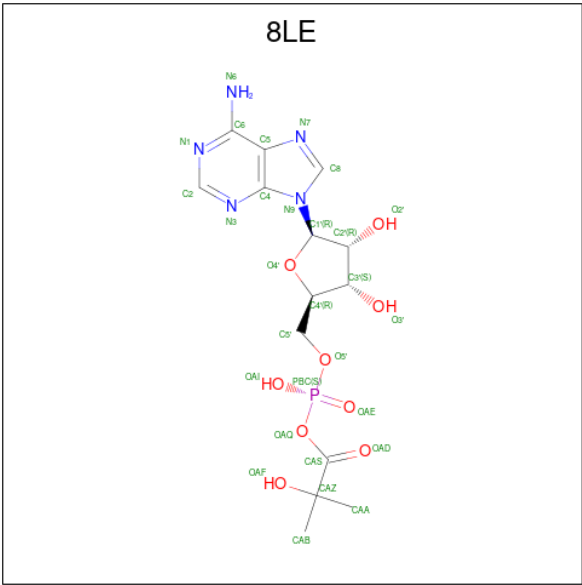
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP I3VE75
B	-6	HIS	-	expression tag	UNP I3VE75
B	-5	HIS	-	expression tag	UNP I3VE75
B	-4	HIS	-	expression tag	UNP I3VE75
B	-3	HIS	-	expression tag	UNP I3VE75
B	-2	HIS	-	expression tag	UNP I3VE75
B	-1	SER	-	expression tag	UNP I3VE75
B	0	GLY	-	expression tag	UNP I3VE75
B	478	GLY	-	expression tag	UNP I3VE75
B	479	SER	-	expression tag	UNP I3VE75
B	480	ALA	-	expression tag	UNP I3VE75
B	481	TRP	-	expression tag	UNP I3VE75
B	482	SER	-	expression tag	UNP I3VE75
B	483	HIS	-	expression tag	UNP I3VE75
B	484	PRO	-	expression tag	UNP I3VE75
B	485	GLN	-	expression tag	UNP I3VE75
B	486	PHE	-	expression tag	UNP I3VE75
B	487	GLU	-	expression tag	UNP I3VE75
B	488	LYS	-	expression tag	UNP I3VE75

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



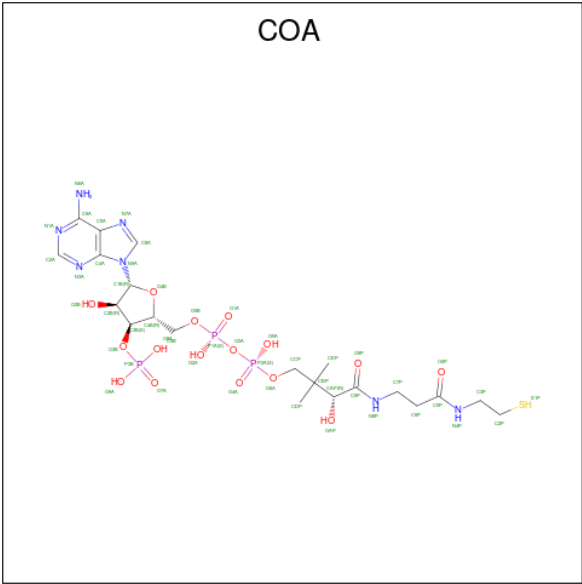
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	1
			23	10	5	7	1		

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] 2-methyl-2-oxidanyl-propanoate (CCD ID: 8LE) (formula: C₁₄H₂₀N₅O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			29	14	5	9	1		
3	B	1	Total	C	N	O	P	0	1
			29	14	5	9	1		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	11	0
4	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	17	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total 159	O 159	0	0
5	B	132	Total 132	O 132	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.85Å 101.85Å 109.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.30 39.72 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.72-2.30) 99.8 (39.72-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.184 , 0.222 0.186 , 0.228	Depositor DCC
R_{free} test set	1467 reflections (3.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.6	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	7501	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: AMP, COA, 8LE

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	0.86	0/3728	1.24	11/5056 (0.2%)
1	B	0.84	0/3474	1.29	15/4713 (0.3%)
All	All	0.85	0/7202	1.27	26/9769 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	GLY	CA-C-N	6.30	129.04	120.54
1	A	416	GLY	C-N-CA	6.30	129.04	120.54
1	B	241	GLU	N-CA-C	6.24	113.83	108.22
1	A	416	GLY	N-CA-C	6.13	119.54	111.70
1	B	234	LYS	N-CA-C	-5.98	104.13	112.45
1	A	101	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	11	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	416	GLY	CA-C-N	5.61	127.73	120.44
1	B	416	GLY	C-N-CA	5.61	127.73	120.44
1	A	97	PRO	N-CA-C	5.56	116.53	110.58
1	A	237	PHE	CA-CB-CG	5.55	119.35	113.80
1	B	129	GLY	CA-C-N	5.50	127.97	120.54
1	B	129	GLY	C-N-CA	5.50	127.97	120.54
1	B	276	VAL	N-CA-CB	5.45	118.53	111.67
1	A	289	TRP	CA-C-N	5.38	128.02	120.28
1	A	289	TRP	C-N-CA	5.38	128.02	120.28
1	A	5	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	109	GLU	CB-CG-CD	5.34	121.68	112.60
1	B	381	GLN	N-CA-C	-5.34	107.42	114.04
1	B	19	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	101	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	187	GLY	N-CA-C	5.17	120.98	114.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	TYR	N-CA-C	5.12	117.75	109.40
1	A	23	TRP	N-CA-C	-5.08	105.66	111.14
1	B	360	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	111	PHE	CA-CB-CG	5.04	118.84	113.80

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	3630	0	3507	8	0
1	B	3380	0	3254	13	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	48	0	32	0	0
4	B	48	0	32	0	0
5	A	159	0	0	0	0
5	B	132	0	0	0	0
All	All	7501	0	6849	21	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 2.

All (21) 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:199:LEU:HD22	1:A:204:PRO:HG3	1.82	0.61
1:B:199:LEU:HD22	1:B:204:PRO:HG3	1.88	0.56
1:B:211:PRO:HD2	1:B:241:GLU:HG3	1.89	0.54
1:B:428:SER:O	1:B:432:GLN:HB2	2.11	0.50
1:A:87:THR:HG22	1:A:90:ARG:HH12	1.77	0.49
1:A:366:ARG:HG3	1:A:399:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLU:HG3	1:B:24:PHE:CD1	2.51	0.46
1:A:114:HIS:HB3	1:A:163:LEU:O	2.16	0.46
1:A:271:SER:HA	1:A:273:PHE:N	2.31	0.45
1:B:271:SER:HA	1:B:273:PHE:N	2.31	0.45
1:A:286:MET:HE1	1:A:355:ILE:HD12	1.99	0.44
1:B:402:LEU:HD21	1:B:439:ALA:HA	2.00	0.44
1:B:286:MET:HE1	1:B:355:ILE:HD12	2.00	0.43
1:B:23:TRP:HB3	1:B:142:ARG:HG3	1.99	0.43
1:B:28:GLU:HB3	1:B:346:ARG:HG2	2.00	0.43
1:A:23:TRP:HB3	1:A:142:ARG:HG3	2.01	0.42
1:B:432:GLN:HE22	1:B:439:ALA:H	1.66	0.42
1:B:270:MET:HE2	1:B:316:TYR:HB3	2.00	0.42
1:A:12:GLU:OE2	1:A:134:ARG:HD3	2.21	0.41
1:B:205:ALA:HB1	1:B:234:LYS:HE2	2.02	0.41
1:B:311:ARG:HG2	1:B:336:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/499 (91%)	434 (96%)	19 (4%)	1 (0%)	43	55
1	B	424/499 (85%)	408 (96%)	14 (3%)	2 (0%)	24	31
All	All	878/998 (88%)	842 (96%)	33 (4%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ASP
1	B	162	SER
1	B	391	ILE

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	374/405 (92%)	364 (97%)	10 (3%)	39	58
1	B	346/405 (85%)	341 (99%)	5 (1%)	59	76
All	All	720/810 (89%)	705 (98%)	15 (2%)	47	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	311	ARG
1	A	393	ILE
1	A	399	MET
1	A	404	LEU
1	A	432	GLN
1	A	435	LEU
1	A	437	VAL
1	A	461	ASP
1	A	462	ASP
1	B	2	GLU
1	B	37	LYS
1	B	178	ARG
1	B	359	ILE
1	B	432	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	HIS
1	A	342	ASN
1	A	380	ASN
1	A	413	HIS
1	B	13	ASN
1	B	107	ASN
1	B	197	GLN

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	381	GLN
1	B	432	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 ⓘ

6 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	$\# Z > 2$
4	COA	A	503	-	47,50,50	0.44	0	69,75,75	0.54	0
3	8LE	B	502[A]	-	29,31,31	0.87	1 (3%)	43,48,48	1.84	10 (23%)
2	AMP	B	501[B]	-	25,25,25	0.16	0	37,38,38	0.38	0
2	AMP	A	501[B]	-	25,25,25	0.38	0	37,38,38	0.47	0
4	COA	B	503	-	47,50,50	0.41	0	69,75,75	0.46	0
3	8LE	A	502[A]	-	29,31,31	0.90	2 (6%)	43,48,48	1.79	7 (16%)

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
4	COA	A	503	-	-	13/48/64/64	0/3/3/3
3	8LE	B	502[A]	-	-	2/19/37/37	0/3/3/3
2	AMP	B	501[B]	-	-	4/10/26/26	0/3/3/3
2	AMP	A	501[B]	-	-	3/10/26/26	0/3/3/3
4	COA	B	503	-	-	8/48/64/64	0/3/3/3
3	8LE	A	502[A]	-	-	2/19/37/37	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	8LE	C5-N7	-2.17	1.35	1.39
3	B	502[A]	8LE	C5-N7	-2.14	1.35	1.39
3	A	502[A]	8LE	C8-N7	2.12	1.35	1.31

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[A]	8LE	C5-C4-N3	-5.33	119.37	126.72
3	B	502[A]	8LE	C5-C4-N3	-5.19	119.58	126.72
3	A	502[A]	8LE	N1-C2-N3	-5.12	120.83	128.58
3	B	502[A]	8LE	N1-C2-N3	-5.05	120.94	128.58
3	A	502[A]	8LE	C2-N3-C4	3.68	120.83	111.83
3	B	502[A]	8LE	C2-N3-C4	3.61	120.66	111.83
3	A	502[A]	8LE	N3-C4-N9	3.42	132.98	127.17
3	B	502[A]	8LE	N3-C4-N9	3.28	132.75	127.17
3	B	502[A]	8LE	N9-C8-N7	-3.27	109.29	113.94
3	A	502[A]	8LE	N9-C8-N7	-3.07	109.58	113.94
3	B	502[A]	8LE	C4-C5-N7	-3.02	107.12	110.58
3	B	502[A]	8LE	C5-N7-C8	2.82	107.88	103.45
3	A	502[A]	8LE	C4-C5-N7	-2.69	107.51	110.58
3	B	502[A]	8LE	OAI-PBC-OAQ	2.67	113.56	104.94
3	A	502[A]	8LE	C5-N7-C8	2.58	107.50	103.45
3	B	502[A]	8LE	C4-N9-C8	2.18	108.02	105.74
3	B	502[A]	8LE	C2'-C1'-N9	-2.16	107.94	113.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

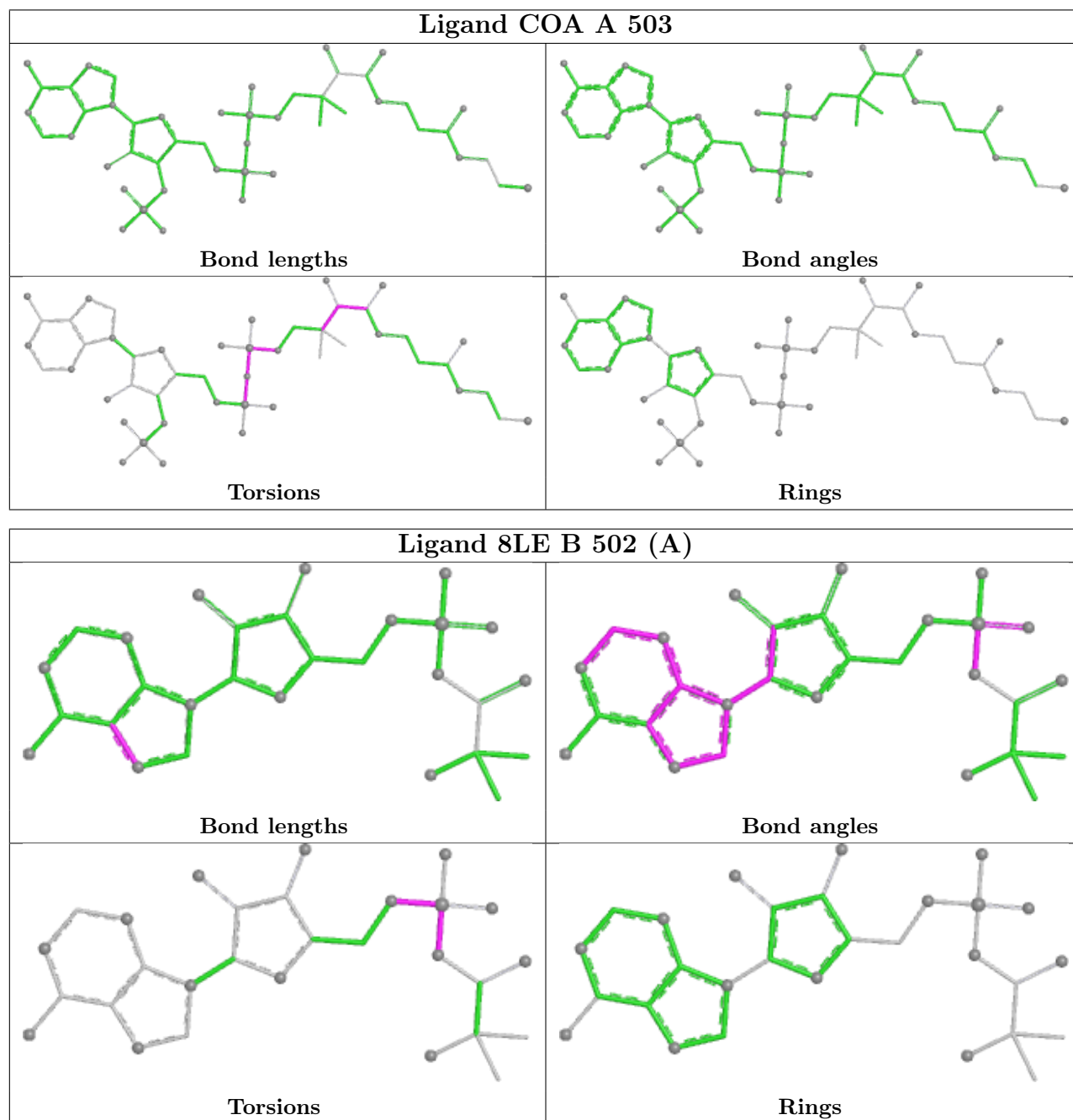
Mol	Chain	Res	Type	Atoms
2	B	501[B]	AMP	C5'-O5'-P-O1P
2	B	501[B]	AMP	C5'-O5'-P-O3P
2	B	501[B]	AMP	C3'-C4'-C5'-O5'
4	A	503	COA	P2A-O3A-P1A-O5B
4	A	503	COA	OAP-CAP-CBP-CCP
4	A	503	COA	C9P-CAP-CBP-CCP
4	A	503	COA	OAP-CAP-CBP-CDP
4	A	503	COA	C9P-CAP-CBP-CDP
4	A	503	COA	OAP-CAP-CBP-CEP
4	A	503	COA	O9P-C9P-CAP-CBP
4	B	503	COA	C5B-O5B-P1A-O1A
4	B	503	COA	C5B-O5B-P1A-O3A
2	A	501[B]	AMP	C3'-C4'-C5'-O5'
2	A	501[B]	AMP	O4'-C4'-C5'-O5'
2	B	501[B]	AMP	O4'-C4'-C5'-O5'
4	A	503	COA	N8P-C9P-CAP-CBP
4	A	503	COA	P1A-O3A-P2A-O6A
4	A	503	COA	C9P-CAP-CBP-CEP
3	A	502[A]	8LE	C5'-O5'-PBC-OAE
3	B	502[A]	8LE	C5'-O5'-PBC-OAE
4	A	503	COA	CCP-O6A-P2A-O4A
4	B	503	COA	C5B-O5B-P1A-O2A
4	B	503	COA	CCP-O6A-P2A-O4A
4	B	503	COA	P1A-O3A-P2A-O5A
4	B	503	COA	C3B-O3B-P3B-O9A
4	A	503	COA	N8P-C9P-CAP-OAP
3	A	502[A]	8LE	CAS-OAQ-PBC-OAE
3	B	502[A]	8LE	CAS-OAQ-PBC-OAE
2	A	501[B]	AMP	C5'-O5'-P-O3P
4	B	503	COA	P1A-O3A-P2A-O4A
4	B	503	COA	N8P-C9P-CAP-OAP
4	A	503	COA	P1A-O3A-P2A-O5A

There are no ring outliers.

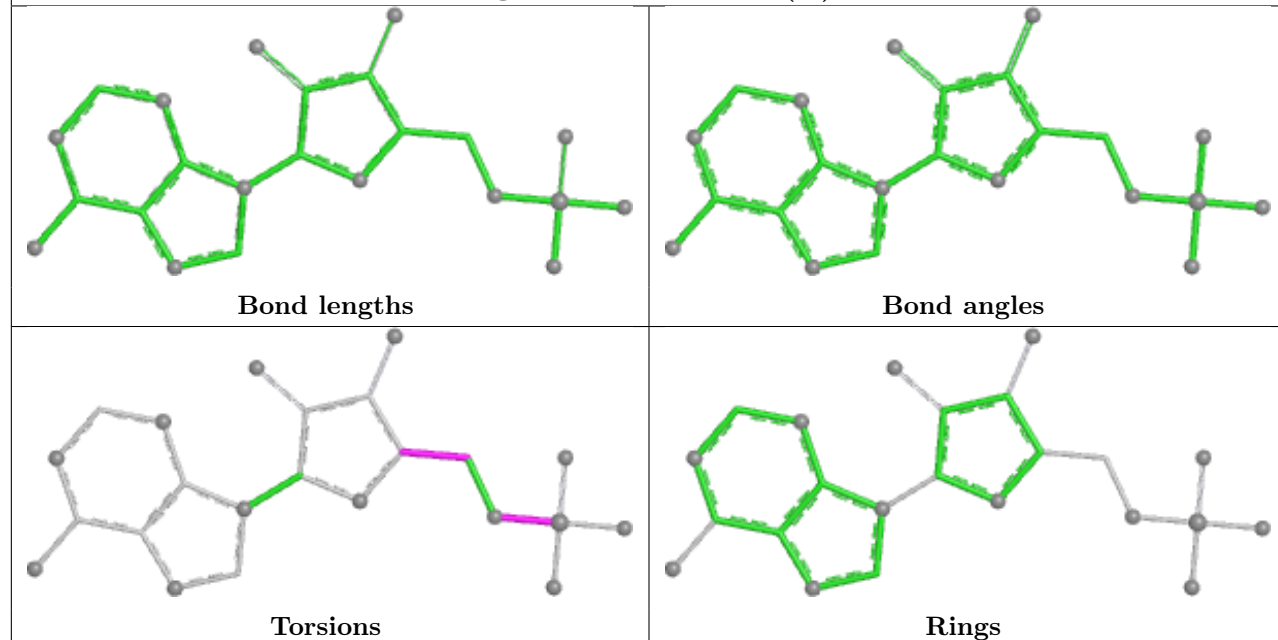
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

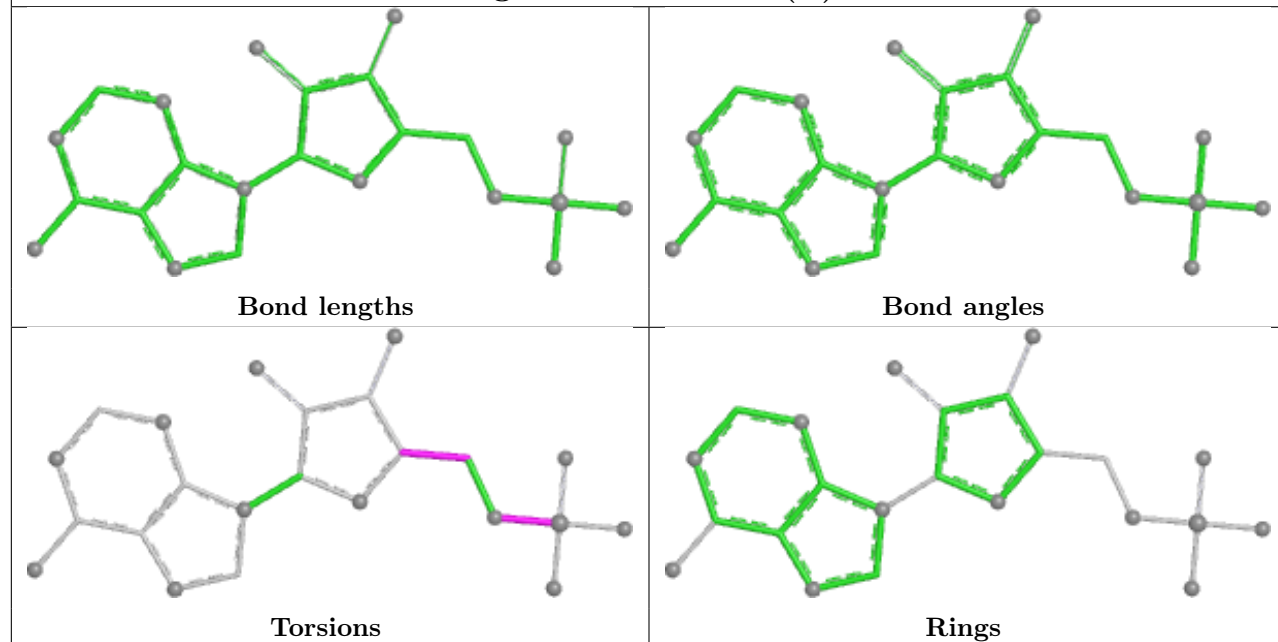
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

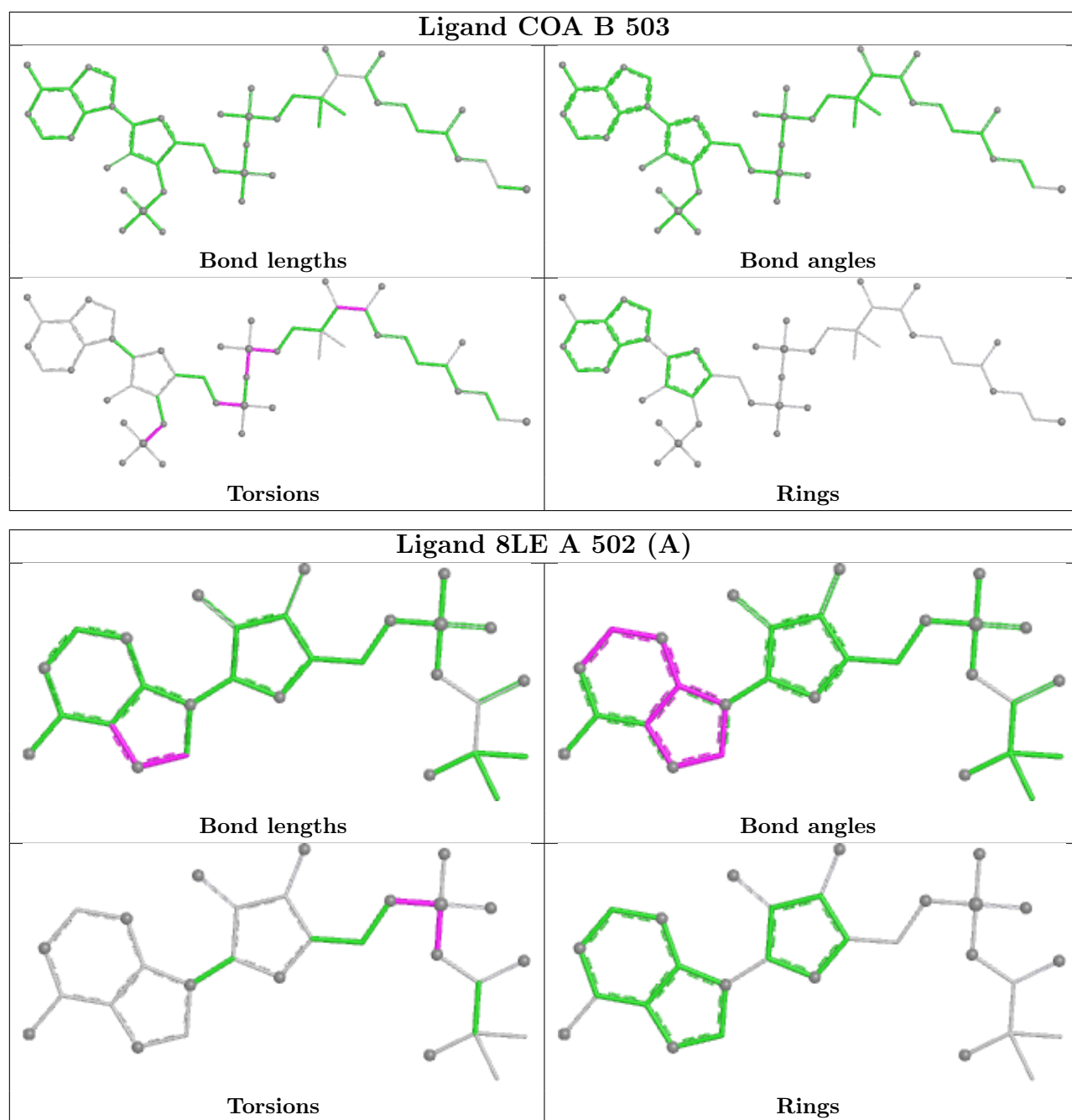


Ligand AMP B 501 (B)



Ligand AMP A 501 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/499 (92%)	-0.26	10 (2%) 62 64	25, 37, 63, 114	0
1	B	430/499 (86%)	0.09	39 (9%) 15 16	25, 39, 86, 106	0
All	All	890/998 (89%)	-0.10	49 (5%) 30 32	25, 38, 81, 114	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	ALA	7.2
1	B	402	LEU	5.9
1	B	392	VAL	5.9
1	B	406	VAL	5.3
1	B	439	ALA	4.9
1	B	391	ILE	4.9
1	B	419	ALA	4.7
1	B	415	ALA	4.6
1	B	405	ARG	4.5
1	B	412	VAL	4.5
1	B	423	PHE	4.5
1	B	403	LEU	4.4
1	B	408	PRO	3.9
1	B	417	ALA	3.9
1	B	404	LEU	3.8
1	A	-3	HIS	3.8
1	B	420	LEU	3.6
1	A	454	PHE	3.6
1	B	117	SER	3.6
1	B	411	SER	3.5
1	B	382	MET	3.5
1	A	462	ASP	3.5
1	B	418	ALA	3.5
1	B	409	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	425	THR	3.3
1	B	383	SER	3.3
1	A	395	ARG	3.1
1	A	461	ASP	3.0
1	B	426	GLU	3.0
1	A	-4	HIS	2.9
1	A	399	MET	2.9
1	B	422	THR	2.8
1	B	413	HIS	2.7
1	B	410	GLU	2.6
1	B	365	ILE	2.6
1	B	-2	HIS	2.6
1	B	429	HIS	2.5
1	B	407	GLU	2.5
1	A	122	ARG	2.5
1	B	121	GLY	2.5
1	B	387	GLY	2.4
1	A	-2	HIS	2.4
1	B	438	ARG	2.4
1	B	414	ALA	2.3
1	B	366	ARG	2.3
1	A	437	VAL	2.2
1	B	384	GLY	2.2
1	B	424	ARG	2.1
1	B	430	ARG	2.1

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

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

6.3 Carbohydrates ⓘ

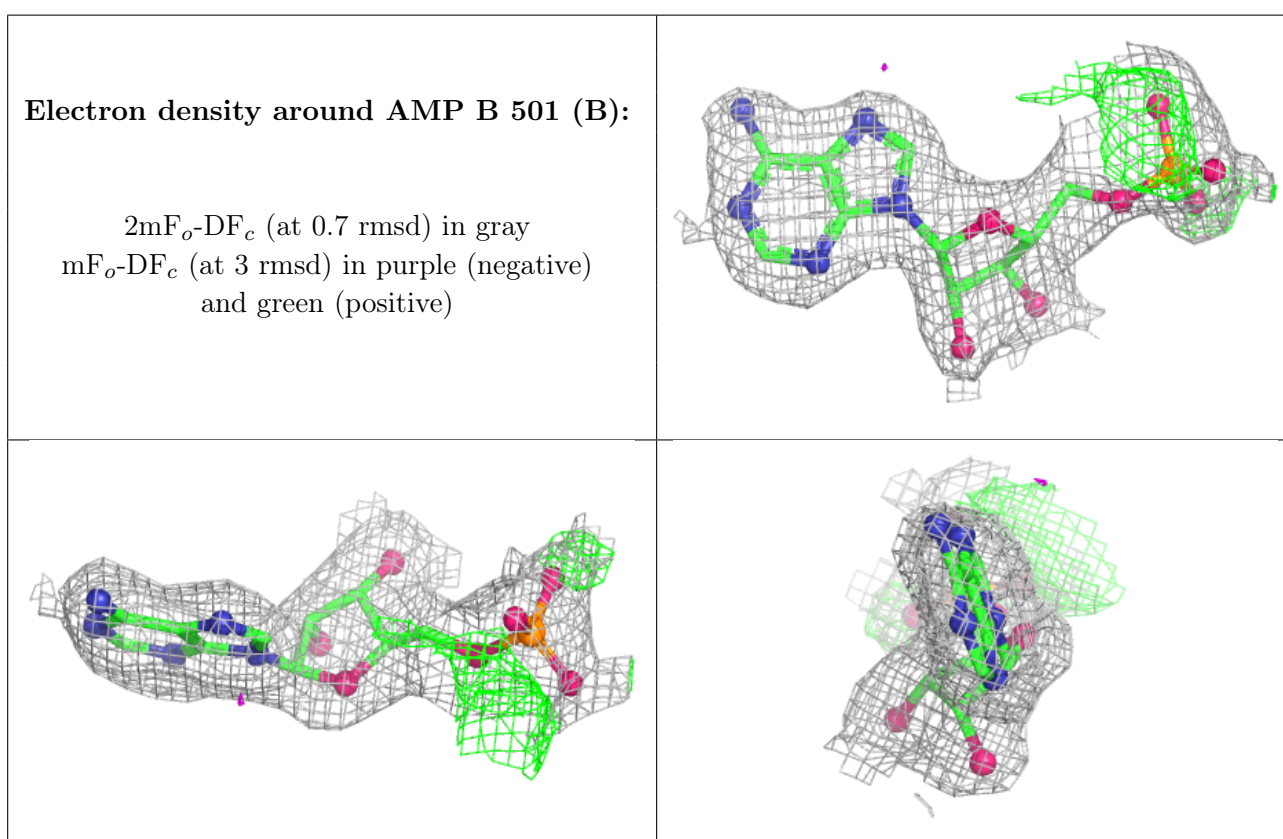
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

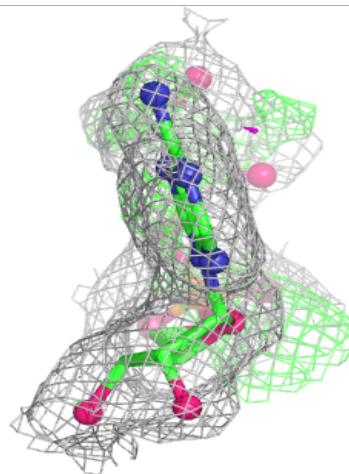
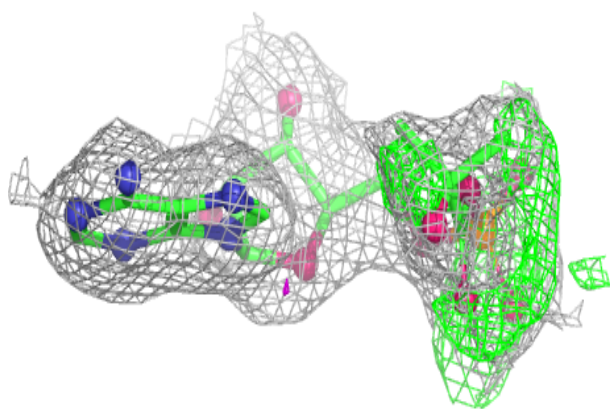
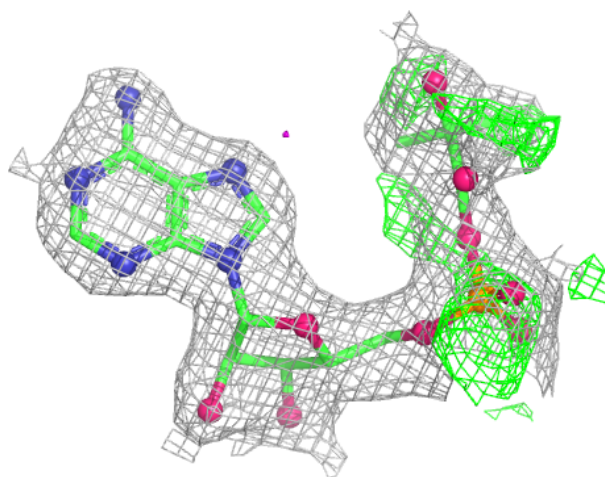
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	B	501[B]	23/23	0.86	0.11	25,38,40,41	23
3	8LE	B	502[A]	29/29	0.86	0.14	23,38,40,41	29
3	8LE	A	502[A]	29/29	0.89	0.10	23,31,39,44	29
4	COA	A	503	48/48	0.91	0.11	38,76,95,95	11
4	COA	B	503	48/48	0.93	0.09	42,74,98,98	17
2	AMP	A	501[B]	23/23	0.95	0.08	13,30,32,32	23

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.



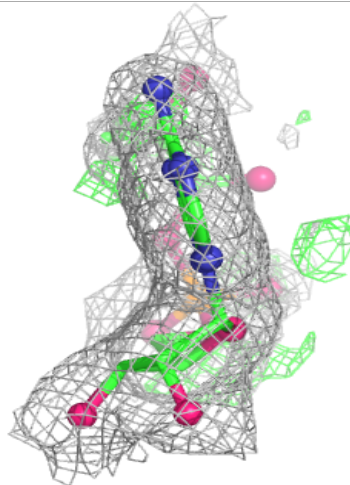
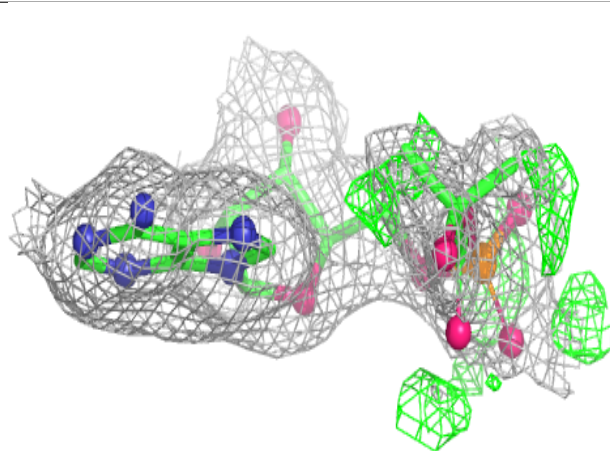
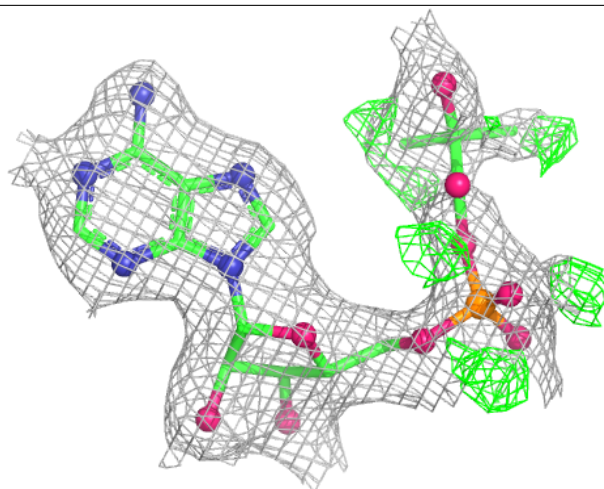
Electron density around 8LE B 502 (A):

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



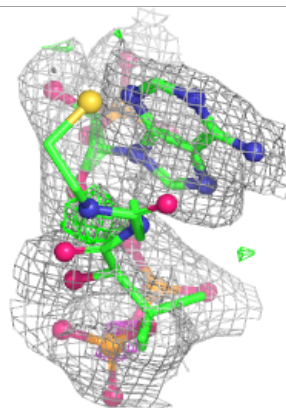
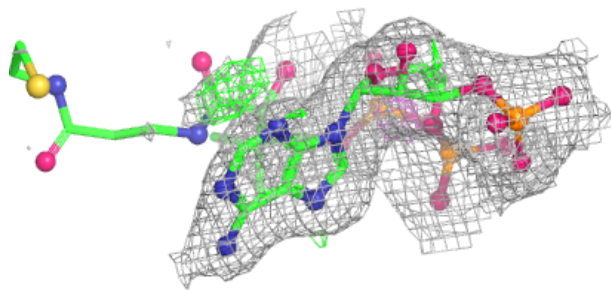
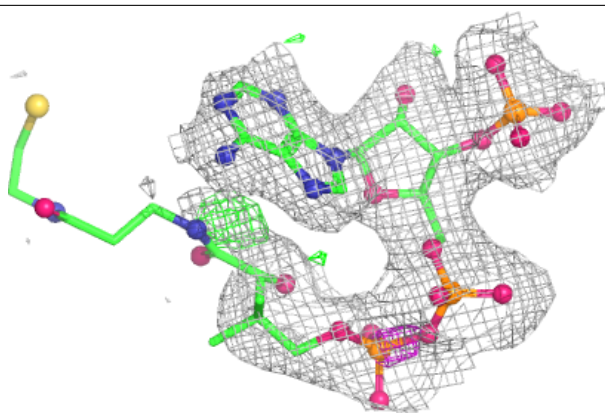
Electron density around 8LE A 502 (A):

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

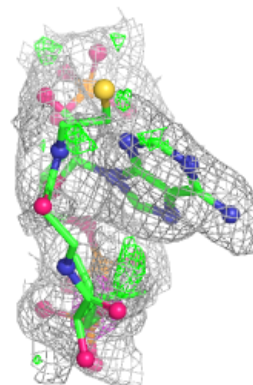
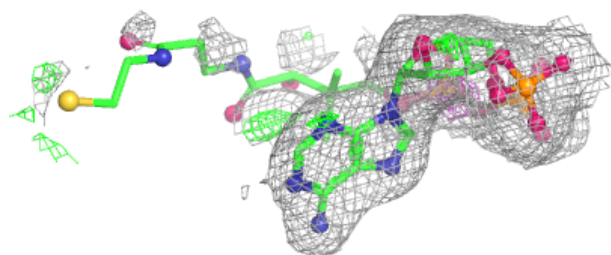
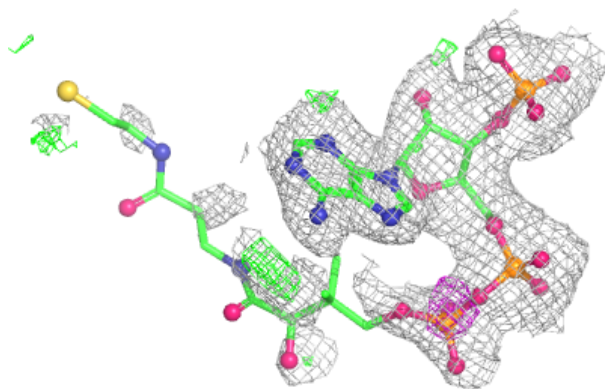


Electron density around COA A 503:

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

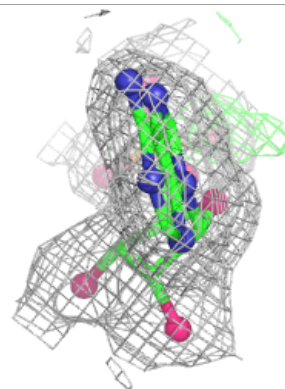
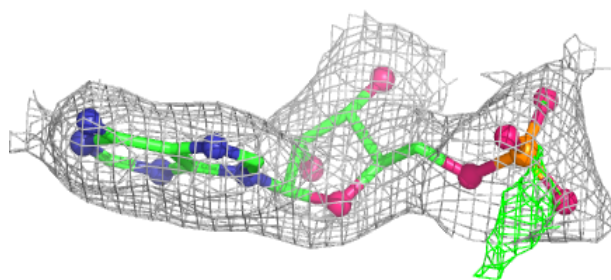
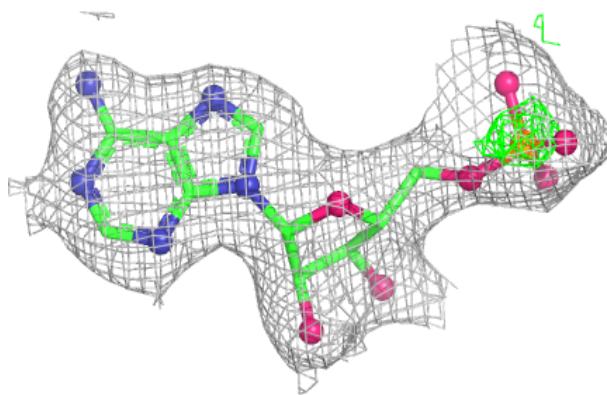
**Electron density around COA B 503:**

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



Electron density around AMP A 501 (B):

$2mF_o-DF_c$ (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.