



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:34 AM UTC

PDB ID : 8WEV / pdb_00008wev
Title : Crystal structure of Feruoyl-CoA Synthetase complexed with AMP from Amycolatopsis thermoflava
Authors : Seok, J.; Kim, K.-J.
Deposited on : 2023-09-18
Resolution : 2.29 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

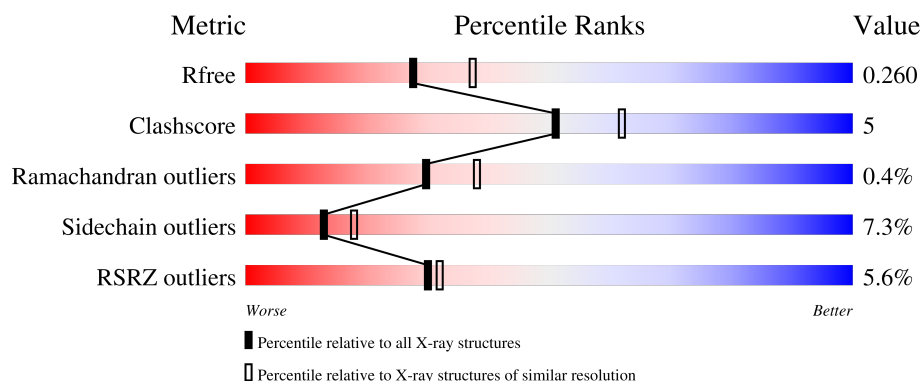
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	491	5% 84% 13% ..
1	B	491	6% 77% 17% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7342 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.

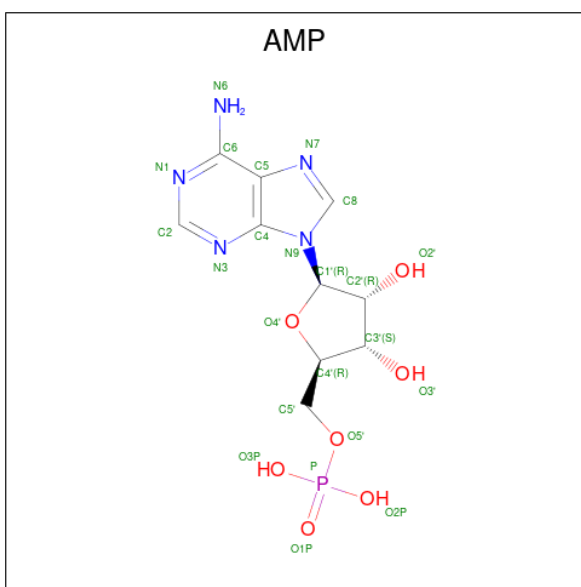
- Molecule 1 is a protein called Feruloyl-CoA Synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3632	2297	652	668	15			
1	B	476	Total	C	N	O	S	0	0	0
			3566	2256	638	657	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ARG	GLN	conflict	UNP A0A3N2H3K2
A	48	GLU	ALA	conflict	UNP A0A3N2H3K2
A	224	PRO	ALA	conflict	UNP A0A3N2H3K2
A	239	VAL	MET	conflict	UNP A0A3N2H3K2
A	256	ARG	HIS	conflict	UNP A0A3N2H3K2
A	258	THR	ALA	conflict	UNP A0A3N2H3K2
A	448	ALA	GLY	conflict	UNP A0A3N2H3K2
B	47	ARG	GLN	conflict	UNP A0A3N2H3K2
B	48	GLU	ALA	conflict	UNP A0A3N2H3K2
B	224	PRO	ALA	conflict	UNP A0A3N2H3K2
B	239	VAL	MET	conflict	UNP A0A3N2H3K2
B	256	ARG	HIS	conflict	UNP A0A3N2H3K2
B	258	THR	ALA	conflict	UNP A0A3N2H3K2
B	448	ALA	GLY	conflict	UNP A0A3N2H3K2

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	1	Total	Mg	0	0
			1	1		

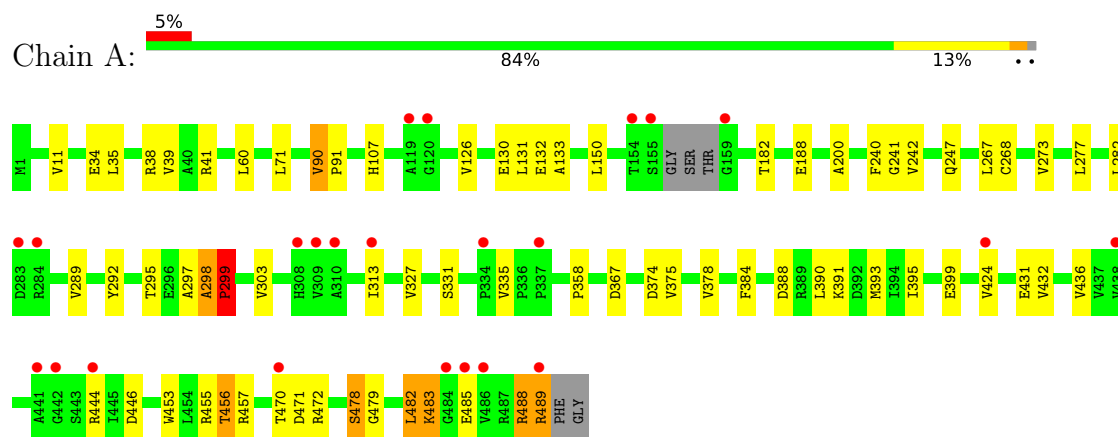
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	38	Total	O	0	0
			38	38		

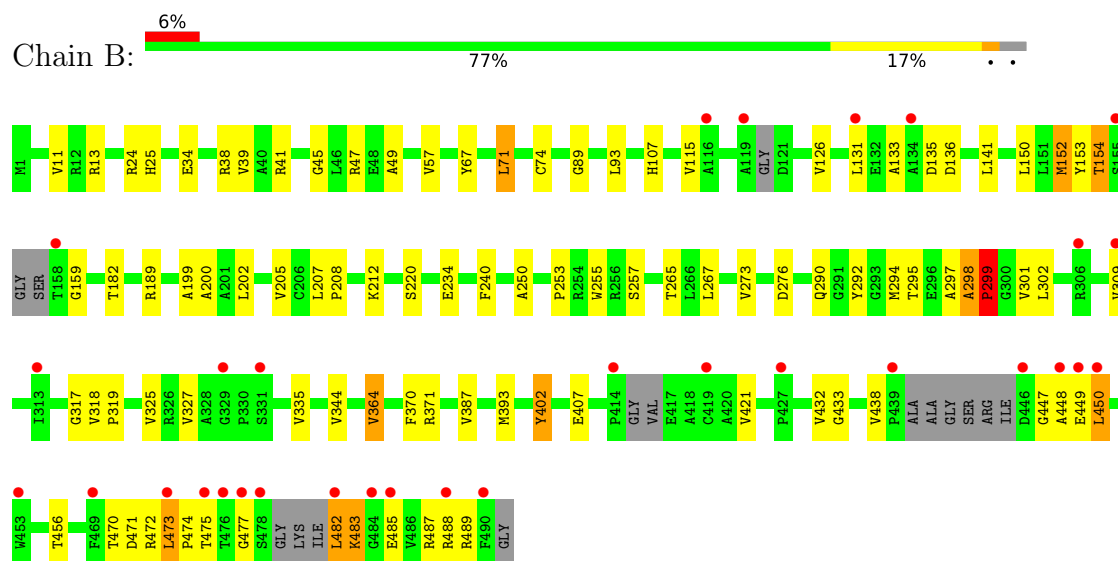
3 Residue-property plots

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: Feruloyl-CoA Synthetase



• Molecule 1: Feruloyl-CoA Synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.76Å 132.10Å 162.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.49 – 2.29 31.49 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.4 (31.49-2.29) 98.4 (31.49-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.261 0.203 , 0.260	Depositor DCC
R_{free} test set	2647 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.4	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	7342	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 2.95% 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: MG, AMP

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	1.07	1/3716 (0.0%)	1.41	9/5065 (0.2%)
1	B	1.05	0/3646	1.44	16/4966 (0.3%)
All	All	1.06	1/7362 (0.0%)	1.43	25/10031 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	VAL	N-CA	5.95	1.50	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	188	GLU	N-CA-CB	5.93	118.76	110.04
1	B	89	GLY	CA-C-N	5.83	124.99	120.33
1	B	89	GLY	C-N-CA	5.83	124.99	120.33
1	B	159	GLY	CA-C-O	-5.78	118.29	122.45
1	B	299	PRO	CA-C-N	5.78	125.47	119.92
1	B	299	PRO	C-N-CA	5.78	125.47	119.92
1	B	154	THR	CB-CA-C	-5.72	101.62	110.78
1	B	153	TYR	CB-CA-C	5.53	118.73	109.89
1	A	455	ARG	CA-C-N	5.43	127.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ARG	C-N-CA	5.43	127.56	120.28
1	B	402	TYR	CB-CA-C	5.41	115.31	110.44
1	B	387	VAL	N-CA-C	-5.38	106.56	111.67
1	A	446	ASP	CA-C-N	5.34	126.03	119.99
1	A	446	ASP	C-N-CA	5.34	126.03	119.99
1	A	34	GLU	CB-CG-CD	5.16	121.38	112.60
1	B	371	ARG	CA-C-N	5.15	127.70	120.28
1	B	371	ARG	C-N-CA	5.15	127.70	120.28
1	A	299	PRO	N-CA-CB	-5.11	96.98	102.60
1	A	295	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	364	VAL	CB-CA-C	5.06	115.39	110.63
1	B	317	GLY	CA-C-O	-5.05	117.25	122.25
1	A	367	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	202	LEU	CA-C-N	5.02	125.52	120.00
1	B	202	LEU	C-N-CA	5.02	125.52	120.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	450	LEU	Peptide

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	3632	0	3627	27	0
1	B	3566	0	3542	49	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	56	0	0	0	0
4	B	38	0	0	1	0
All	All	7342	0	7193	75	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 5.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MET:HE2	1:B:295:THR:HG23	1.63	0.80
1:B:154:THR:O	1:B:154:THR:OG1	2.03	0.73
1:B:71:LEU:C	1:B:71:LEU:HD23	2.16	0.71
1:B:327:VAL:HG23	1:B:335:VAL:HG22	1.73	0.69
1:B:24:ARG:HE	1:B:189:ARG:NH1	1.89	0.69
1:B:483:LYS:HB3	1:B:485:GLU:HG2	1.75	0.68
1:B:298:ALA:N	1:B:299:PRO:HA	2.10	0.66
1:A:453:TRP:O	1:A:456:THR:HB	1.97	0.65
1:A:298:ALA:N	1:A:299:PRO:HA	2.13	0.64
1:B:24:ARG:HE	1:B:189:ARG:HH12	1.45	0.63
1:B:126:VAL:HG11	1:B:131:LEU:HD22	1.84	0.60
1:A:60:LEU:O	1:A:107:HIS:HA	2.02	0.59
1:B:393:MET:HE2	1:B:402:TYR:CE1	2.38	0.58
1:B:150:LEU:C	1:B:150:LEU:HD12	2.29	0.58
1:B:71:LEU:C	1:B:71:LEU:CD2	2.79	0.55
1:B:473:LEU:HD23	1:B:482:LEU:HD11	1.88	0.55
1:B:475:THR:HG22	1:B:482:LEU:HG	1.90	0.54
1:B:205:VAL:HG21	1:B:240:PHE:HB2	1.89	0.54
1:A:483:LYS:C	1:A:485:GLU:H	2.16	0.54
1:B:71:LEU:HD23	1:B:71:LEU:O	2.08	0.54
1:A:485:GLU:HA	1:A:488:ARG:HG3	1.90	0.54
1:A:395:ILE:O	1:A:431:GLU:HB2	2.08	0.53
1:B:393:MET:HE2	1:B:402:TYR:HE1	1.72	0.53
1:A:297:ALA:C	1:A:299:PRO:HA	2.33	0.53
1:B:407:GLU:HG3	1:B:421:VAL:HG23	1.90	0.53
1:B:24:ARG:NE	1:B:189:ARG:HH12	2.05	0.53
1:B:297:ALA:C	1:B:299:PRO:HA	2.35	0.52
1:A:200:ALA:HB1	1:A:240:PHE:CZ	2.45	0.51
1:B:152:MET:HE1	1:B:199:ALA:H	1.76	0.51
1:B:34:GLU:O	1:B:38:ARG:HG3	2.10	0.50
1:A:242:VAL:HG21	1:A:478:SER:HB3	1.93	0.49
1:B:200:ALA:HB1	1:B:240:PHE:CZ	2.48	0.49
1:B:290:GLN:HE21	1:B:309:VAL:HG23	1.78	0.48
1:B:152:MET:HE2	1:B:295:THR:CG2	2.41	0.48
1:B:294:MET:HE3	1:B:301:VAL:HG21	1.95	0.48
1:A:327:VAL:HG23	1:A:335:VAL:HG22	1.96	0.48
1:B:438:VAL:HG12	1:B:470:THR:HG23	1.97	0.47
1:B:265:THR:HG22	1:B:267:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:N	1:A:91:PRO:CD	2.78	0.47
1:A:358:PRO:HG3	1:B:141:LEU:HD12	1.96	0.46
1:A:267:LEU:HD23	1:A:289:VAL:HB	1.97	0.46
1:A:38:ARG:NH2	1:A:132:GLU:OE2	2.48	0.46
1:B:250:ALA:HA	1:B:255:TRP:CD2	2.51	0.45
1:A:292:TYR:OH	1:A:374:ASP:OD2	2.27	0.45
1:B:57:VAL:HB	1:B:74:CYS:SG	2.57	0.45
1:A:241:GLY:O	1:A:268:CYS:HA	2.16	0.44
1:B:107:HIS:CG	1:B:115:VAL:HG21	2.53	0.44
1:B:49:ALA:HB2	1:B:131:LEU:HD11	2.00	0.44
1:B:152:MET:HE2	1:B:152:MET:HB3	1.90	0.44
1:A:436:VAL:HG21	1:A:489:ARG:HD3	1.99	0.44
1:B:189:ARG:NH2	1:B:234:GLU:O	2.45	0.44
1:B:273:VAL:HG22	1:B:290:GLN:OE1	2.18	0.44
1:A:375:VAL:HG22	1:A:390:LEU:HD13	2.00	0.43
1:B:25:HIS:HE1	1:B:220:SER:OG	2.02	0.43
1:B:67:TYR:CD1	1:B:67:TYR:C	2.97	0.43
1:A:393:MET:HE3	1:A:395:ILE:HD11	2.01	0.42
1:A:482:LEU:HD13	1:A:482:LEU:HA	1.90	0.42
1:B:273:VAL:HG22	1:B:290:GLN:CD	2.44	0.42
1:A:456:THR:HG22	1:A:457:ARG:HE	1.85	0.42
1:A:41:ARG:HD2	1:A:133:ALA:O	2.20	0.42
1:B:447:GLY:O	1:B:448:ALA:HB3	2.19	0.41
1:B:41:ARG:HG2	1:B:135:ASP:O	2.20	0.41
1:A:247:GLN:HG3	1:A:277:LEU:HD13	2.03	0.41
1:B:45:GLY:HA2	1:B:133:ALA:HB2	2.01	0.41
1:A:35:LEU:O	1:A:39:VAL:HG23	2.21	0.41
1:B:477:GLY:H	1:B:483:LYS:HZ1	1.68	0.41
1:A:90:VAL:HG22	1:A:91:PRO:HD3	2.03	0.41
1:A:378:VAL:HG22	1:A:384:PHE:CD2	2.56	0.41
1:B:207:LEU:N	1:B:208:PRO:CD	2.84	0.41
1:B:433:GLY:HA3	4:B:615:HOH:O	2.21	0.41
1:B:292:TYR:HB3	1:B:302:LEU:HB2	2.04	0.40
1:B:344:VAL:HA	1:B:370:PHE:O	2.20	0.40
1:B:205:VAL:C	1:B:208:PRO:HD2	2.45	0.40
1:B:318:VAL:HB	1:B:319:PRO:HD2	2.02	0.40
1:A:150:LEU:HD12	1:A:150:LEU:C	2.46	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	482/491 (98%)	464 (96%)	16 (3%)	2 (0%)	30	38
1	B	464/491 (94%)	436 (94%)	26 (6%)	2 (0%)	30	38
All	All	946/982 (96%)	900 (95%)	42 (4%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	ALA
1	B	298	ALA
1	B	474	PRO
1	A	479	GLY

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	371/374 (99%)	344 (93%)	27 (7%)	13	18
1	B	365/374 (98%)	338 (93%)	27 (7%)	13	17
All	All	736/748 (98%)	682 (93%)	54 (7%)	13	18

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	71	LEU

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Mol	Chain	Res	Type
1	A	90	VAL
1	A	130	GLU
1	A	131	LEU
1	A	182	THR
1	A	273	VAL
1	A	282	LEU
1	A	299	PRO
1	A	303	VAL
1	A	313	ILE
1	A	331	SER
1	A	388	ASP
1	A	391	LYS
1	A	399	GLU
1	A	424	VAL
1	A	432	VAL
1	A	444	ARG
1	A	456	THR
1	A	470	THR
1	A	471	ASP
1	A	472	ARG
1	A	478	SER
1	A	482	LEU
1	A	483	LYS
1	A	488	ARG
1	A	489	ARG
1	B	11	VAL
1	B	13	ARG
1	B	39	VAL
1	B	47	ARG
1	B	71	LEU
1	B	93	LEU
1	B	152	MET
1	B	182	THR
1	B	212	LYS
1	B	253	PRO
1	B	257	SER
1	B	276	ASP
1	B	299	PRO
1	B	325	VAL
1	B	364	VAL
1	B	432	VAL
1	B	449	GLU

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Mol	Chain	Res	Type
1	B	450	LEU
1	B	456	THR
1	B	471	ASP
1	B	472	ARG
1	B	473	LEU
1	B	482	LEU
1	B	483	LYS
1	B	487	ARG
1	B	488	ARG
1	B	489	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	95	HIS
1	A	198	HIS
1	A	247	GLN
1	A	385	HIS
1	B	25	HIS
1	B	107	HIS
1	B	385	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
2	AMP	A	501	-	25,25,25	0.35	0	37,38,38	0.52	0
2	AMP	B	501	-	25,25,25	0.43	0	37,38,38	0.43	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	AMP	A	501	-	-	0/10/26/26	0/3/3/3
2	AMP	B	501	-	-	3/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

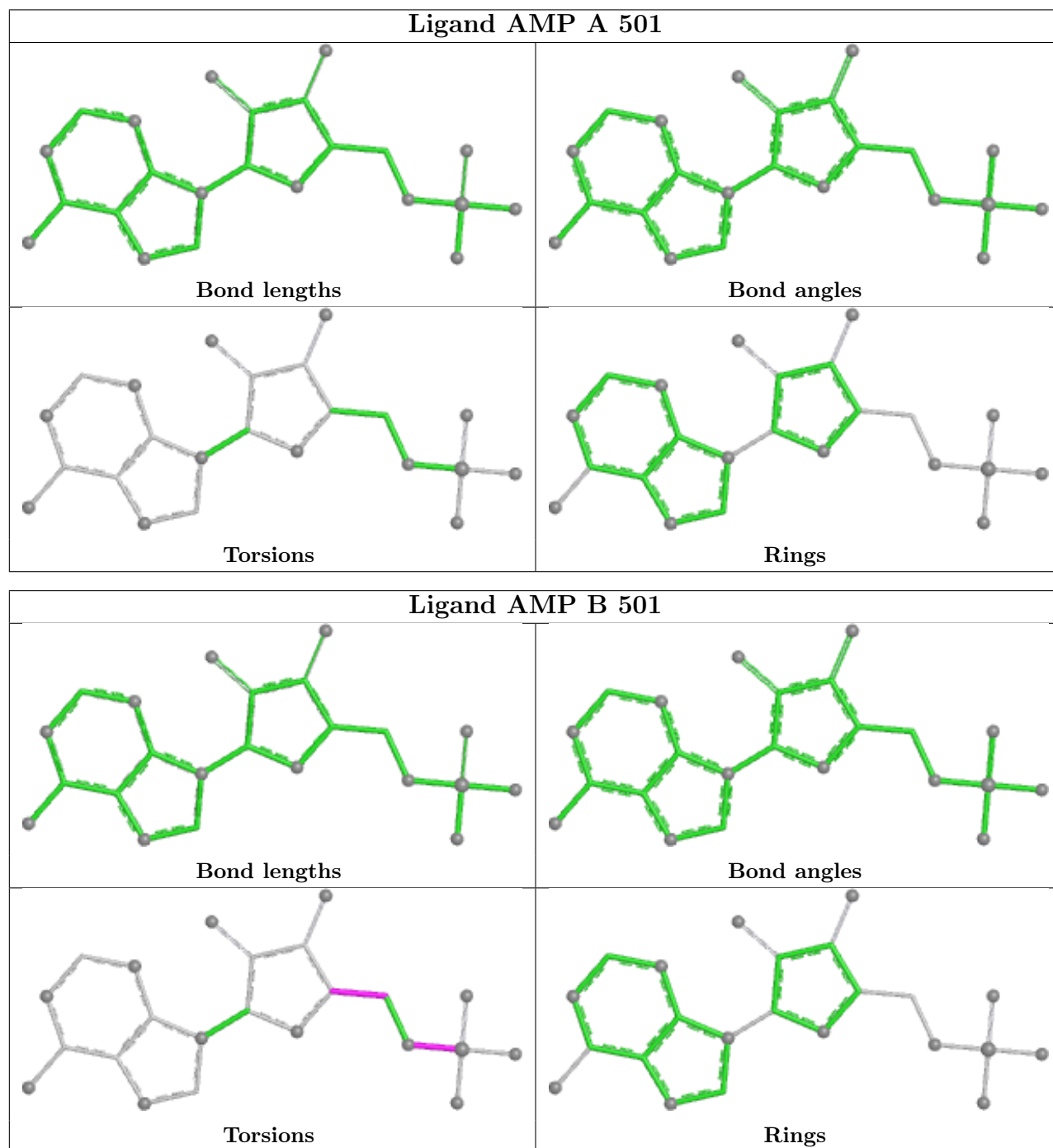
Mol	Chain	Res	Type	Atoms
2	B	501	AMP	C3'-C4'-C5'-O5'
2	B	501	AMP	O4'-C4'-C5'-O5'
2	B	501	AMP	C5'-O5'-P-O1P

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.



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	486/491 (98%)	0.13	23 (4%) 36 38	29, 48, 89, 127	0
1	B	476/491 (96%)	0.46	31 (6%) 25 27	35, 56, 98, 130	0
All	All	962/982 (97%)	0.29	54 (5%) 30 32	29, 52, 94, 130	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	PHE	5.5
1	B	450	LEU	5.5
1	B	313	ILE	4.7
1	B	484	GLY	4.4
1	A	284	ARG	4.2
1	A	154	THR	4.2
1	A	310	ALA	3.7
1	A	334	PRO	3.6
1	B	448	ALA	3.5
1	B	482	LEU	3.4
1	B	473	LEU	3.4
1	A	309	VAL	3.3
1	B	488	ARG	3.3
1	B	427	PRO	3.2
1	B	119	ALA	3.1
1	B	158	THR	3.0
1	A	484	GLY	3.0
1	A	441	ALA	3.0
1	B	155	SER	2.9
1	A	313	ILE	2.8
1	B	306	ARG	2.8
1	B	476	THR	2.8
1	A	424	VAL	2.7
1	B	331	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	470	THR	2.7
1	B	414	PRO	2.6
1	B	131	LEU	2.6
1	B	477	GLY	2.6
1	A	489	ARG	2.5
1	A	120	GLY	2.5
1	B	449	GLU	2.5
1	A	442	GLY	2.5
1	A	485	GLU	2.5
1	A	438	VAL	2.4
1	B	116	ALA	2.4
1	B	453	TRP	2.3
1	B	475	THR	2.3
1	B	478	SER	2.3
1	B	309	VAL	2.3
1	A	444	ARG	2.2
1	B	439	PRO	2.2
1	B	134	ALA	2.2
1	B	485	GLU	2.1
1	A	155	SER	2.1
1	A	337	PRO	2.1
1	A	119	ALA	2.1
1	A	486	VAL	2.1
1	A	159	GLY	2.1
1	B	419	CYS	2.0
1	A	308	HIS	2.0
1	A	283	ASP	2.0
1	B	446	ASP	2.0
1	B	329	GLY	2.0
1	B	469	PHE	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](#)

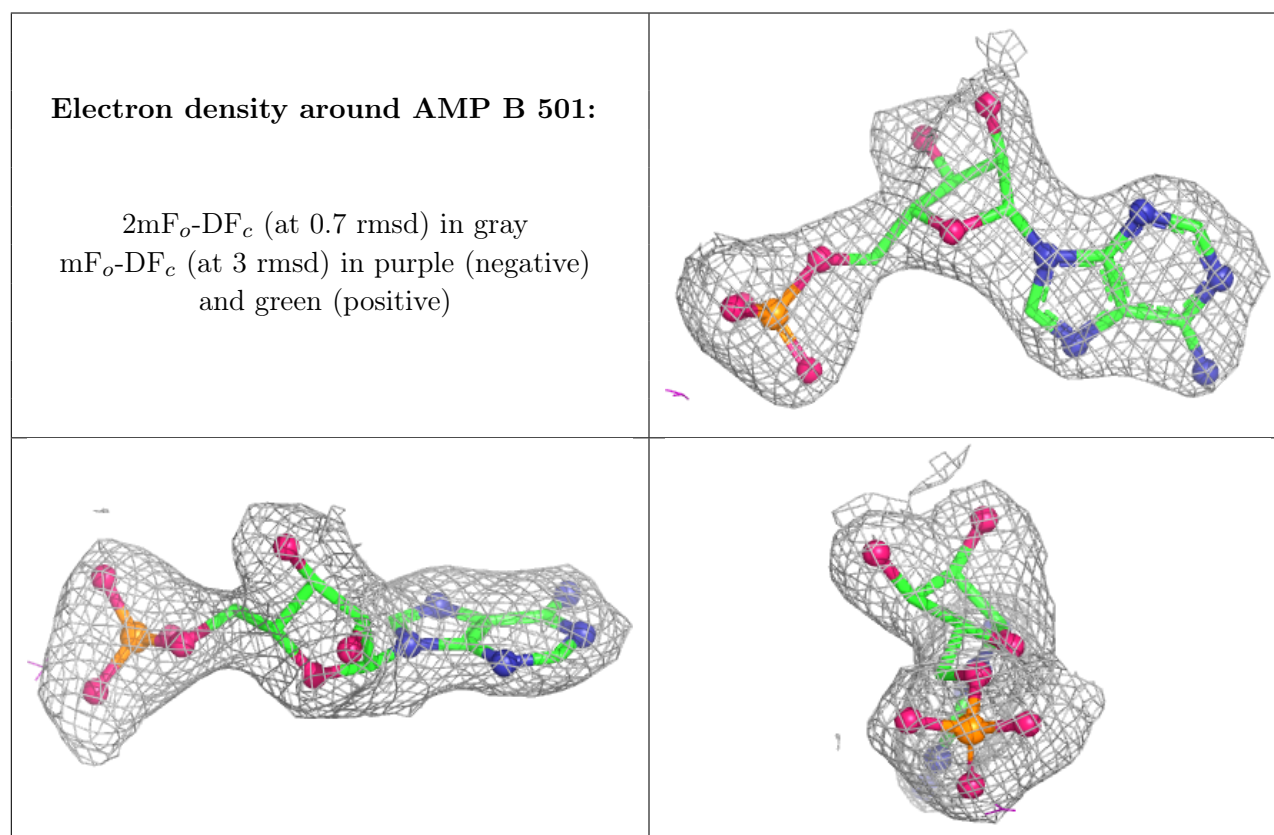
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

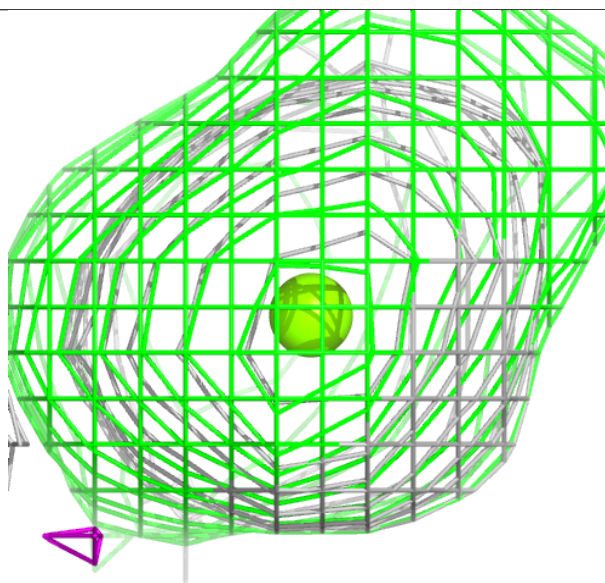
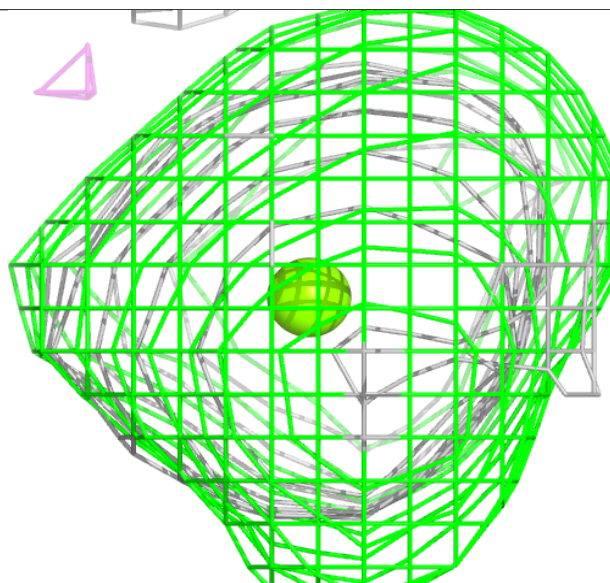
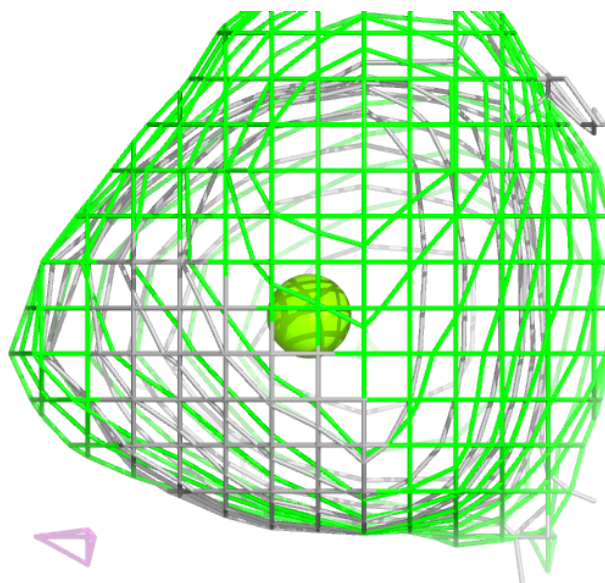
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AMP	B	501	23/23	0.94	0.07	50,62,66,67	0
3	MG	A	502	1/1	0.94	0.38	36,36,36,36	0
3	MG	A	504	1/1	0.94	0.31	60,60,60,60	0
3	MG	A	503	1/1	0.95	0.35	44,44,44,44	0
2	AMP	A	501	23/23	0.96	0.06	43,48,52,55	0
3	MG	B	502	1/1	0.98	0.40	38,38,38,38	0

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.



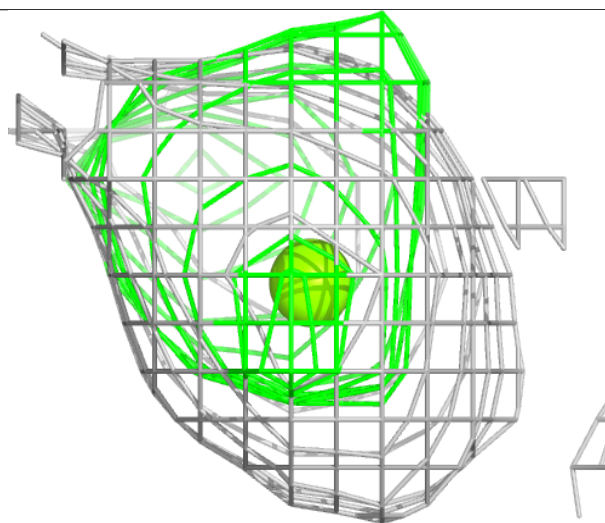
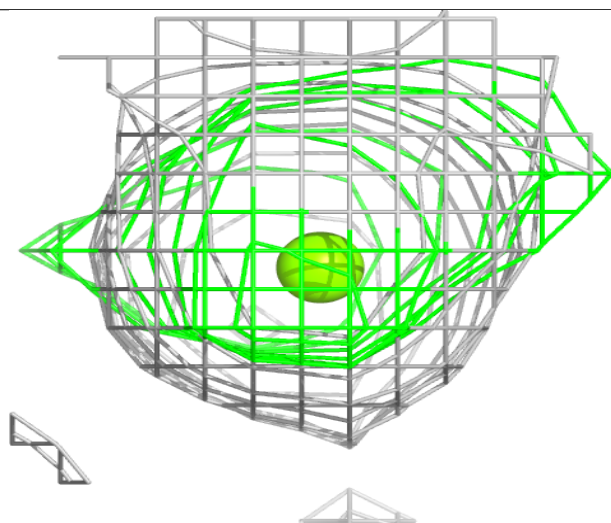
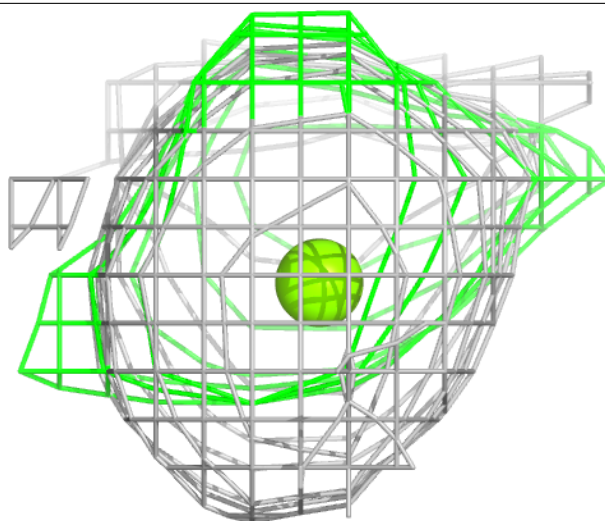
Electron density around MG A 502:

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



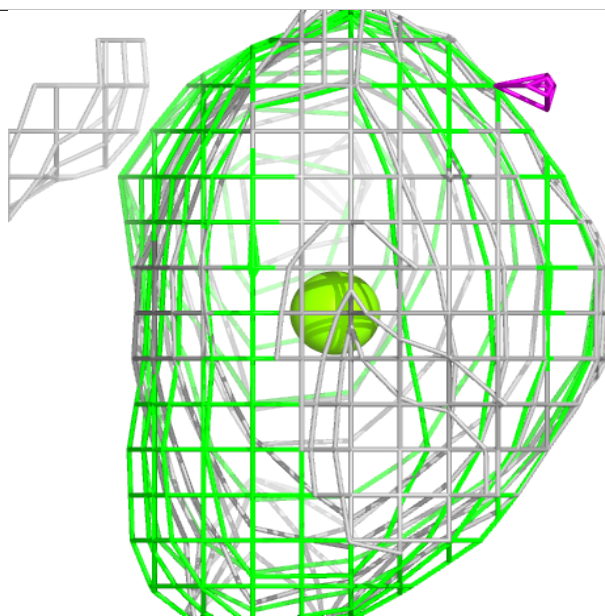
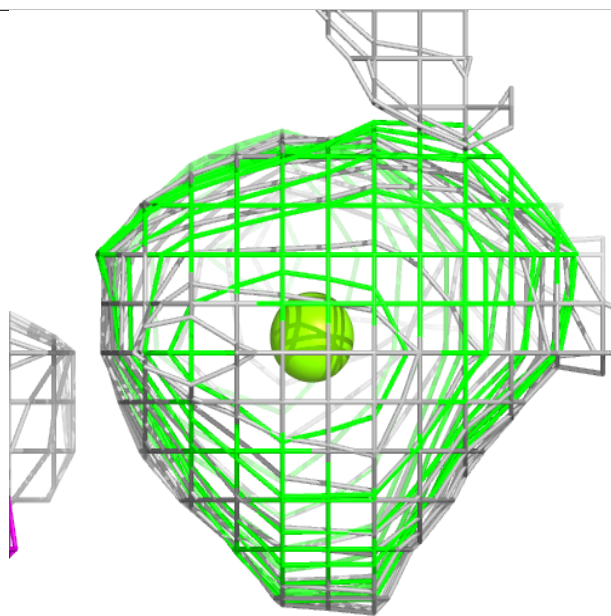
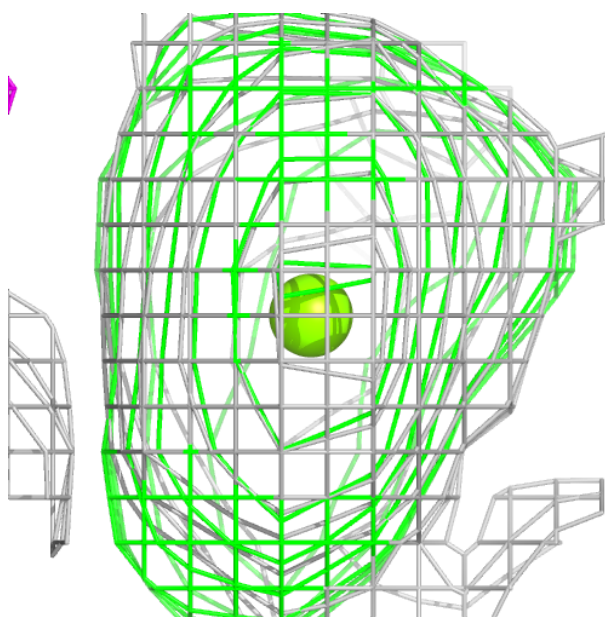
Electron density around MG A 504:

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



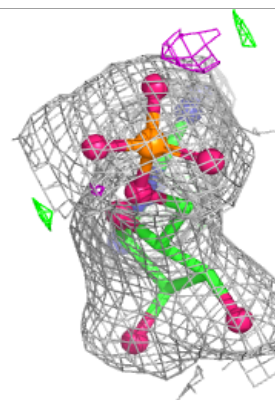
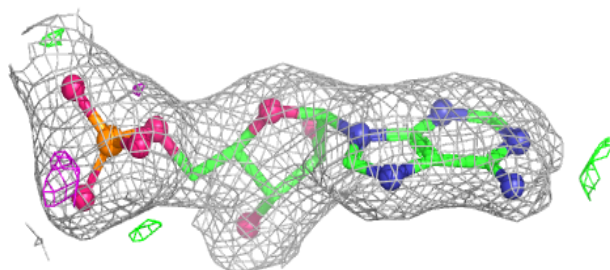
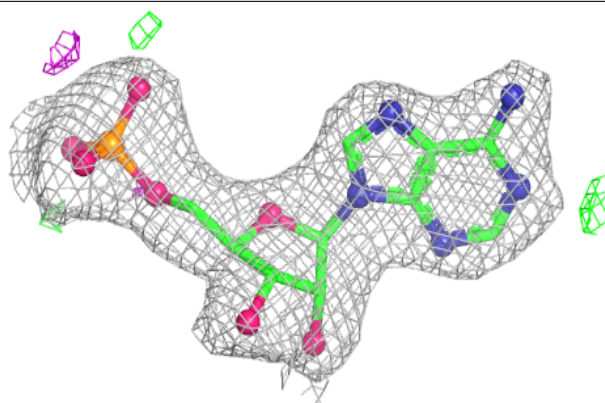
Electron density around MG A 503:

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



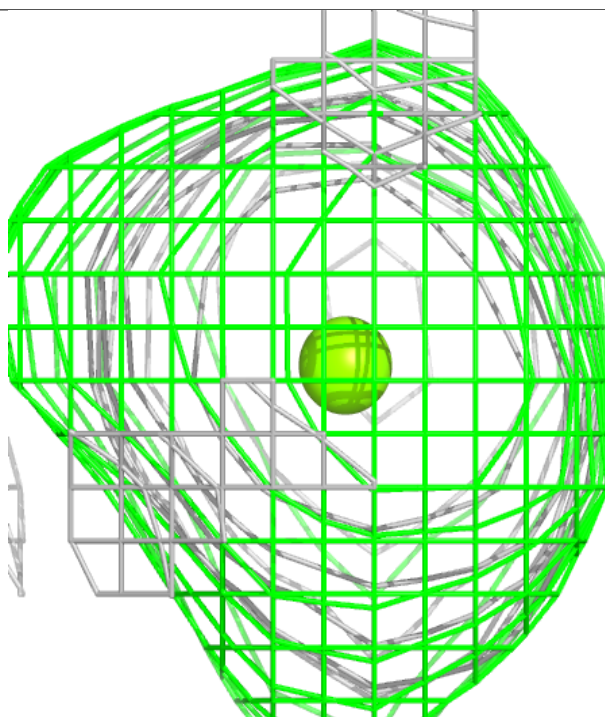
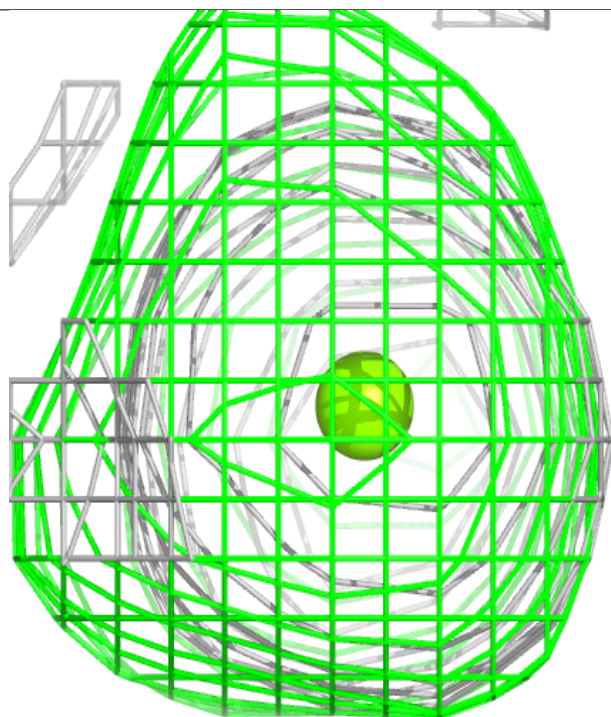
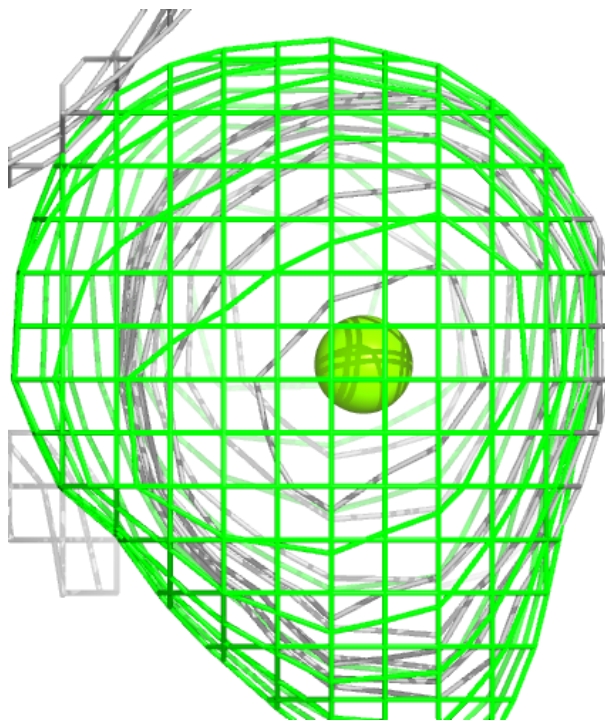
Electron density around AMP A 501:

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



Electron density around MG B 502:

$2mF_o-DF_c$ (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.