



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:26 PM UTC

PDB ID : 8JBI / pdb_00008jbi
Title : SteC 202-375 mutant- C276S
Authors : Zhang, M.; Dai, Y.; Li, B.
Deposited on : 2023-05-09
Resolution : 2.36 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

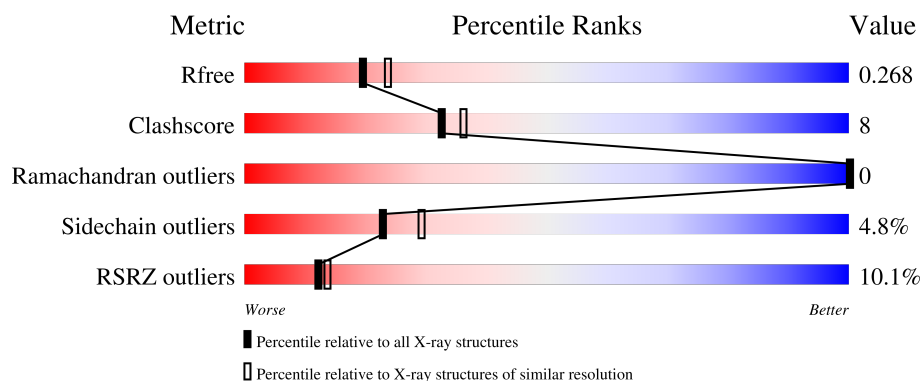
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	174	7% 72% 14% • 12%
1	B	174	10% 67% 16% • 14%
1	C	174	8% 78% 13% 10%
1	D	174	10% 71% 14% • 12%

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
3	MG	B	402	-	-	-	X
3	MG	D	402	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5158 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.

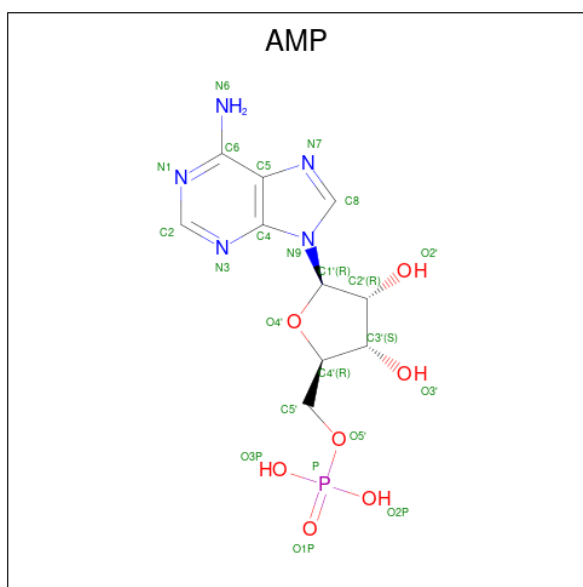
- Molecule 1 is a protein called Secreted effector kinase SteC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	153	Total	C	N	O	S	0	0	0
			1219	767	209	238	5			
1	A	153	Total	C	N	O	S	0	0	0
			1227	770	214	238	5			
1	B	149	Total	C	N	O	S	0	0	0
			1188	744	208	231	5			
1	C	157	Total	C	N	O	S	0	0	0
			1260	790	222	243	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	276	SER	CYS	engineered mutation	UNP D0ZIB5
A	276	SER	CYS	engineered mutation	UNP D0ZIB5
B	276	SER	CYS	engineered mutation	UNP D0ZIB5
C	276	SER	CYS	engineered mutation	UNP D0ZIB5

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	25	Total	O	0	0
			25	25		

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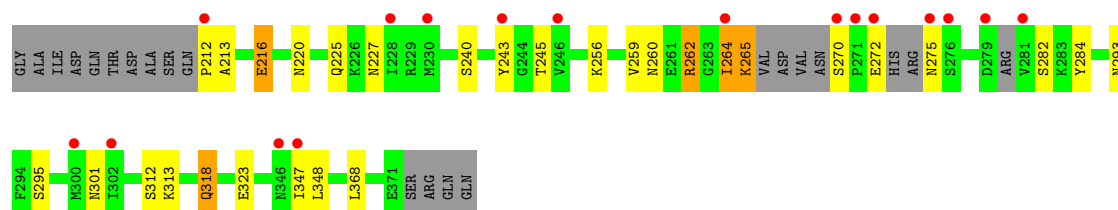
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total 54	O 54	0	0
4	B	29	Total 29	O 29	0	0
4	C	59	Total 59	O 59	0	0

3 Residue-property plots [i](#)

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

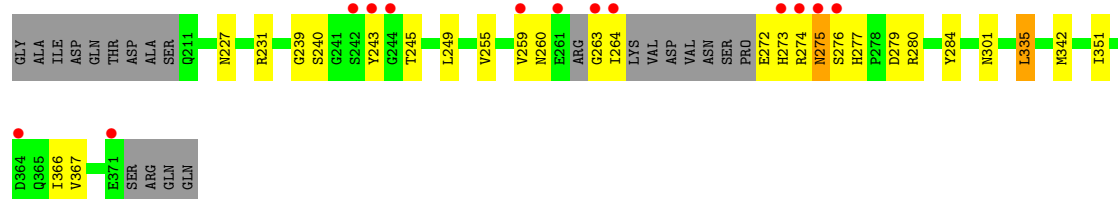
• Molecule 1: Secreted effector kinase SteC

Chain D: 



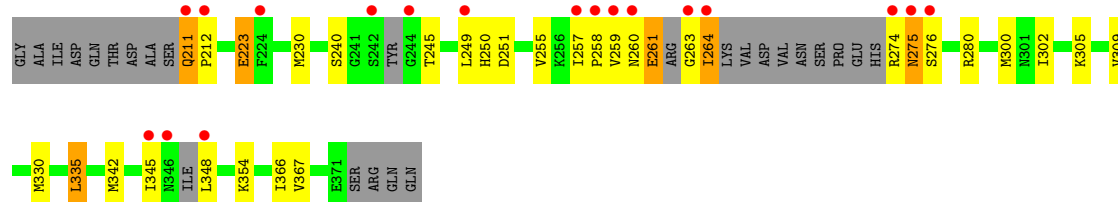
• Molecule 1: Secreted effector kinase SteC

Chain A: 



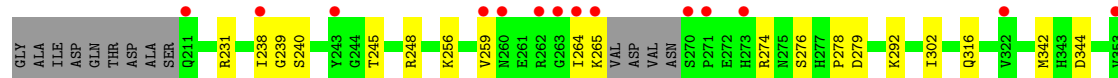
• Molecule 1: Secreted effector kinase SteC

Chain B: 



• Molecule 1: Secreted effector kinase SteC

Chain C: 



D364	D374
Q365	SER
I366	ARG
V367	GLN
	GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.00Å 92.88Å 88.84Å 90.00° 107.82° 90.00°	Depositor
Resolution (Å)	40.40 – 2.36 40.40 – 2.36	Depositor EDS
% Data completeness (in resolution range)	96.9 (40.40-2.36) 96.8 (40.40-2.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.195 , 0.242 0.227 , 0.268	Depositor DCC
R_{free} test set	1666 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5158	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, MG

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	0.53	0/1245	0.88	1/1673 (0.1%)
1	B	0.53	0/1202	0.88	0/1611
1	C	0.54	0/1280	0.85	0/1721
1	D	0.56	0/1236	0.96	2/1659 (0.1%)
All	All	0.54	0/4963	0.89	3/6664 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	323	GLU	N-CA-C	-5.88	104.95	111.36
1	A	275	ASN	N-CA-C	-5.59	104.37	110.91
1	D	284	TYR	CB-CA-C	5.32	120.37	109.67

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	1227	0	1201	27	0
1	B	1188	0	1166	21	0
1	C	1260	0	1240	16	0
1	D	1219	0	1198	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	23	0	12	2	0
2	B	23	0	12	0	0
2	C	23	0	12	3	0
2	D	23	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	54	0	0	1	0
4	B	29	0	0	1	0
4	C	59	0	0	3	0
4	D	25	0	0	0	0
All	All	5158	0	4853	78	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 8.

All (78) 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:D:347:ILE:HG21	1:A:284:TYR:CD2	1.92	1.04
1:D:348:LEU:H	1:A:275:ASN:HD21	1.05	1.02
1:C:239:GLY:HA3	2:C:401:AMP:H5'2	1.41	0.99
1:D:213:ALA:HB3	1:D:216:GLU:HG3	1.56	0.85
1:C:238:ILE:HD11	1:C:248:ARG:HB2	1.63	0.80
1:D:348:LEU:H	1:A:275:ASN:ND2	1.84	0.74
1:B:230:MET:HE3	1:B:259:VAL:HG11	1.71	0.72
1:B:230:MET:HE2	1:B:302:ILE:HG21	1.74	0.68
1:C:364:ASP:OD1	1:C:365:GLN:NE2	2.28	0.67
1:A:277:HIS:NE2	1:A:279:ASP:HB2	2.09	0.67
1:D:347:ILE:HG21	1:A:284:TYR:CE2	2.30	0.65
1:D:227:ASN:HA	1:D:301:ASN:HD21	1.63	0.63
1:C:259:VAL:HA	1:C:265:LYS:HB3	1.81	0.63
1:B:255:VAL:HG11	1:B:300:MET:HE1	1.81	0.63
1:D:347:ILE:CG2	1:A:284:TYR:CD2	2.77	0.62
1:A:240:SER:HB3	1:A:245:THR:HG23	1.82	0.62
1:A:260:ASN:H	1:A:263:GLY:HA3	1.63	0.61
1:D:227:ASN:HA	1:D:301:ASN:ND2	2.15	0.61
1:D:348:LEU:N	1:A:275:ASN:HD21	1.88	0.60
1:C:231:ARG:NH1	4:C:502:HOH:O	2.24	0.58
1:C:276:SER:O	1:C:278:PRO:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:OD1	1:A:301:ASN:ND2	2.36	0.58
1:B:240:SER:HA	1:B:245:THR:HG22	1.89	0.55
1:A:263:GLY:O	1:A:264:ILE:C	2.49	0.55
1:C:240:SER:HB3	1:C:245:THR:HG23	1.89	0.54
1:B:345:ILE:HG13	1:C:274:ARG:HA	1.88	0.54
1:A:231:ARG:HB3	1:A:231:ARG:NH1	2.22	0.54
1:D:240:SER:HB3	1:D:245:THR:HG23	1.89	0.54
1:D:347:ILE:HG22	1:D:368:LEU:HB2	1.90	0.54
1:D:243:TYR:HD1	1:D:256:LYS:HE3	1.75	0.52
1:D:260:ASN:OD1	1:D:262:ARG:HG2	2.10	0.51
1:D:293:ASN:O	1:D:313:LYS:HE3	2.11	0.51
1:A:280:ARG:HD2	4:A:539:HOH:O	2.11	0.51
1:C:239:GLY:HA3	2:C:401:AMP:C5'	2.29	0.51
1:A:260:ASN:N	1:A:263:GLY:HA3	2.26	0.50
1:B:211:GLN:N	1:B:212:PRO:HD3	2.27	0.49
1:A:259:VAL:HA	1:A:263:GLY:O	2.13	0.49
1:A:335:LEU:HD23	1:A:342:MET:HB2	1.95	0.49
1:A:260:ASN:OD1	1:A:263:GLY:HA2	2.14	0.48
1:A:273:HIS:CE1	1:A:276:SER:HA	2.49	0.48
1:C:292:LYS:HE3	1:C:292:LYS:HB2	1.46	0.48
1:B:366:ILE:HG21	1:C:342:MET:HE3	1.96	0.47
1:D:264:ILE:HD13	1:D:265:LYS:H	1.78	0.47
1:B:274:ARG:HD2	1:B:276:SER:H	1.80	0.47
1:B:230:MET:CE	1:B:259:VAL:HG21	2.45	0.46
1:A:239:GLY:HA3	2:A:401:AMP:O5'	2.16	0.46
1:A:231:ARG:HH12	1:C:302:ILE:HG22	1.80	0.46
1:B:223:GLU:CD	1:B:223:GLU:H	2.24	0.46
1:B:260:ASN:O	1:B:261:GLU:C	2.59	0.46
1:D:347:ILE:HD11	1:A:280:ARG:CZ	2.45	0.46
2:C:401:AMP:O3P	2:C:401:AMP:H3'	2.15	0.46
1:A:243:TYR:OH	2:A:401:AMP:P	2.74	0.46
1:C:292:LYS:HG3	4:C:529:HOH:O	2.15	0.46
1:A:275:ASN:N	1:A:275:ASN:HD22	2.13	0.45
1:A:277:HIS:CD2	1:A:279:ASP:HB2	2.51	0.45
1:D:260:ASN:ND2	1:D:264:ILE:HG22	2.31	0.45
1:B:348:LEU:CD2	1:B:367:VAL:HG22	2.47	0.45
4:B:501:HOH:O	1:C:256:LYS:HD3	2.16	0.45
1:B:354:LYS:HG3	1:C:316:GLN:O	2.16	0.44
1:B:263:GLY:C	1:B:264:ILE:HG13	2.41	0.43
1:B:230:MET:HE3	1:B:259:VAL:HG21	2.00	0.43
1:B:300:MET:HE3	1:B:309:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ASN:HA	1:D:301:ASN:CG	2.44	0.43
1:A:231:ARG:HB3	1:A:231:ARG:HH11	1.84	0.42
1:D:227:ASN:CA	1:D:301:ASN:HD21	2.32	0.42
1:B:250:HIS:ND1	1:B:251:ASP:N	2.66	0.42
1:B:257:ILE:HA	1:B:258:PRO:HD3	1.86	0.42
1:B:275:ASN:O	1:B:280:ARG:HD3	2.19	0.42
1:B:275:ASN:OD1	1:B:275:ASN:N	2.53	0.42
1:B:335:LEU:HD23	1:B:342:MET:HB2	2.02	0.41
1:D:245:THR:OG1	1:D:259:VAL:O	2.32	0.41
1:D:243:TYR:CD1	1:D:256:LYS:HE3	2.53	0.41
1:A:351:ILE:HD11	1:A:366:ILE:HD13	2.02	0.41
1:D:282:SER:HA	1:D:295:SER:OG	2.21	0.41
1:D:318:GLN:H	1:D:318:GLN:HG2	1.73	0.41
1:A:249:LEU:HD12	1:A:255:VAL:HG21	2.03	0.41
1:D:220:ASN:O	1:D:225:GLN:NE2	2.54	0.40
1:C:344:ASP:OD1	4:C:501:HOH:O	2.22	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	147/174 (84%)	143 (97%)	4 (3%)	0	100	100
1	B	139/174 (80%)	135 (97%)	4 (3%)	0	100	100
1	C	153/174 (88%)	146 (95%)	7 (5%)	0	100	100
1	D	145/174 (83%)	139 (96%)	6 (4%)	0	100	100
All	All	584/696 (84%)	563 (96%)	21 (4%)	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	136/154 (88%)	132 (97%)	4 (3%)	37	49
1	B	132/154 (86%)	123 (93%)	9 (7%)	14	16
1	C	140/154 (91%)	137 (98%)	3 (2%)	47	61
1	D	136/154 (88%)	126 (93%)	10 (7%)	13	14
All	All	544/616 (88%)	518 (95%)	26 (5%)	23	29

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	212	PRO
1	D	216	GLU
1	D	262	ARG
1	D	264	ILE
1	D	265	LYS
1	D	270	SER
1	D	272	GLU
1	D	275	ASN
1	D	312	SER
1	D	318	GLN
1	A	272	GLU
1	A	274	ARG
1	A	335	LEU
1	A	367	VAL
1	B	211	GLN
1	B	223	GLU
1	B	249	LEU
1	B	261	GLU
1	B	264	ILE
1	B	275	ASN
1	B	305	LYS
1	B	330	MET
1	B	335	LEU
1	C	264	ILE

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Mol	Chain	Res	Type
1	C	279	ASP
1	C	367	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	236	ASN
1	A	260	ASN
1	A	273	HIS
1	A	275	ASN
1	A	301	ASN
1	A	343	HIS
1	B	303	ASN
1	C	343	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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	D	401	3	25,25,25	0.36	0	37,38,38	0.44	0
2	AMP	B	401	-	25,25,25	0.37	0	37,38,38	0.42	0
2	AMP	A	401	3	25,25,25	0.40	0	37,38,38	0.53	0
2	AMP	C	401	3	25,25,25	0.43	0	37,38,38	0.67	1 (2%)

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	D	401	3	-	6/10/26/26	0/3/3/3
2	AMP	B	401	-	-	2/10/26/26	0/3/3/3
2	AMP	A	401	3	-	6/10/26/26	0/3/3/3
2	AMP	C	401	3	-	6/10/26/26	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	AMP	O3P-P-O5'	-2.35	100.54	106.67

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	AMP	C5'-O5'-P-O2P
2	D	401	AMP	C5'-O5'-P-O3P
2	A	401	AMP	C5'-O5'-P-O3P
2	C	401	AMP	C5'-O5'-P-O1P
2	C	401	AMP	C5'-O5'-P-O2P
2	C	401	AMP	C5'-O5'-P-O3P
2	C	401	AMP	O4'-C4'-C5'-O5'
2	A	401	AMP	O4'-C4'-C5'-O5'
2	C	401	AMP	C3'-C4'-C5'-O5'
2	A	401	AMP	C3'-C4'-C5'-O5'
2	B	401	AMP	O4'-C4'-C5'-O5'
2	D	401	AMP	C5'-O5'-P-O1P
2	A	401	AMP	C5'-O5'-P-O1P
2	C	401	AMP	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	A	401	AMP	C5'-O5'-P-O2P
2	D	401	AMP	O4'-C4'-C5'-O5'
2	B	401	AMP	C3'-C4'-C5'-O5'
2	A	401	AMP	C4'-C5'-O5'-P
2	D	401	AMP	C4'-C5'-O5'-P
2	D	401	AMP	C3'-C4'-C5'-O5'

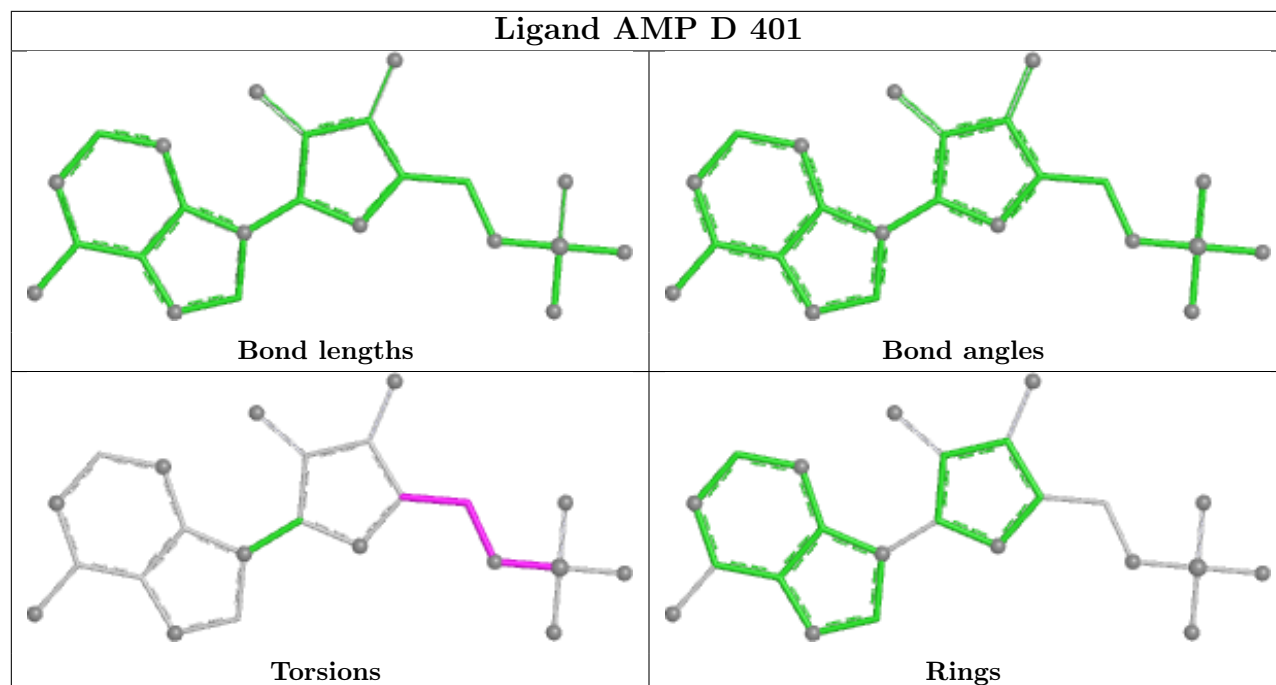
There are no ring outliers.

2 monomers are involved in 5 short contacts:

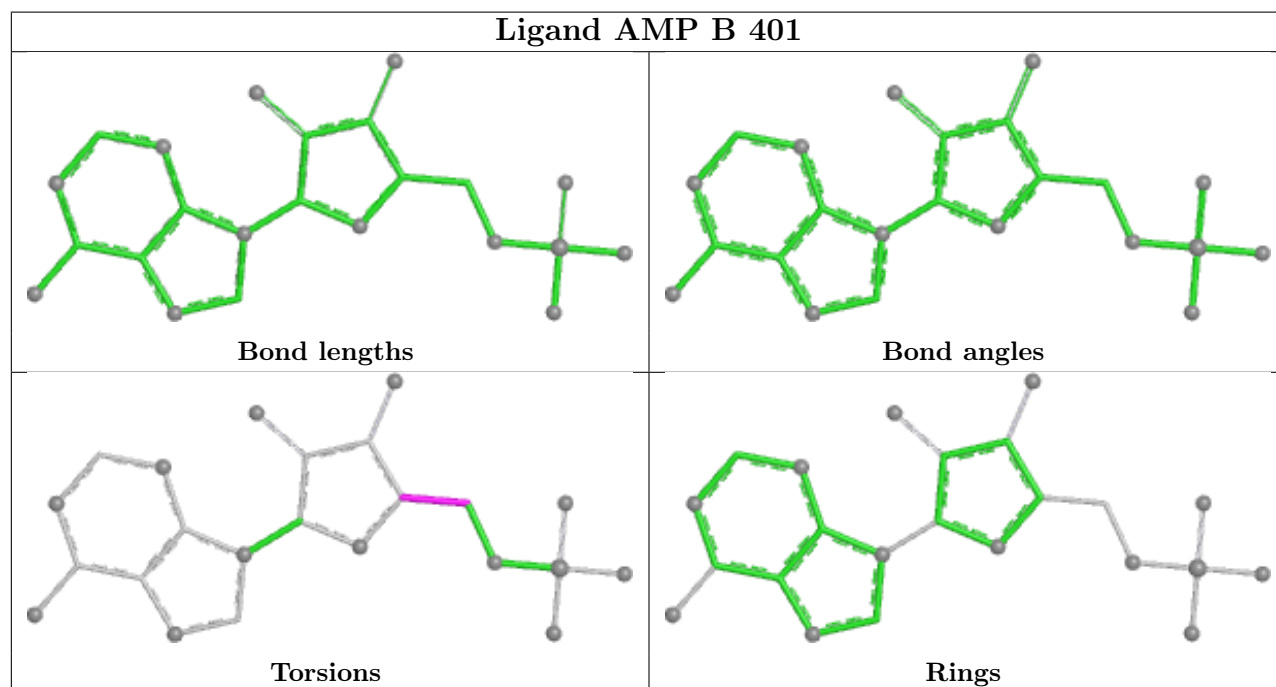
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AMP	2	0
2	C	401	AMP	3	0

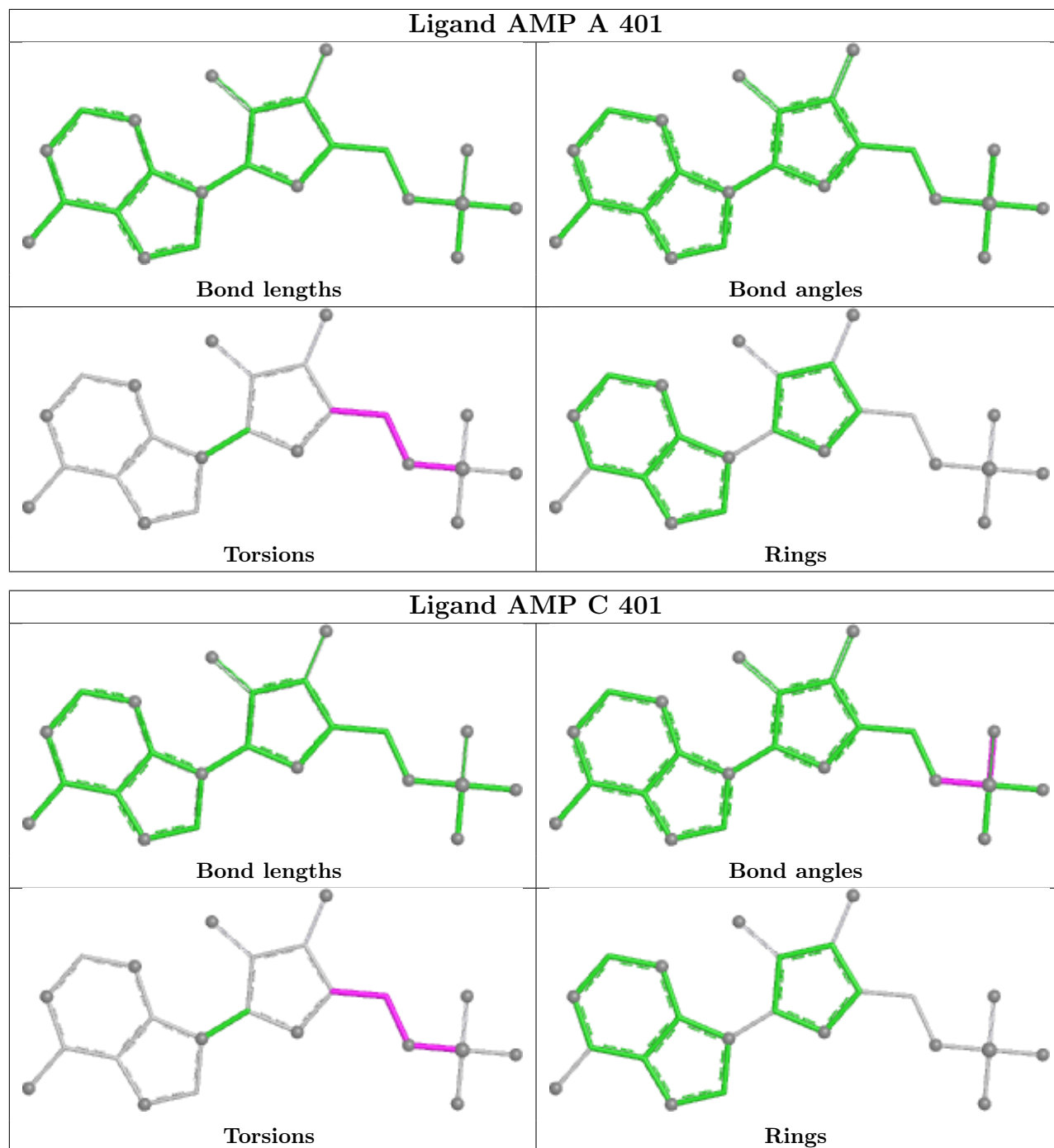
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand AMP D 401



Ligand AMP B 401





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	153/174 (87%)	0.71	13 (8%) 16 18	30, 60, 102, 114	0
1	B	149/174 (85%)	0.87	18 (12%) 8 10	30, 70, 109, 142	0
1	C	157/174 (90%)	0.56	14 (8%) 15 17	42, 59, 94, 114	0
1	D	153/174 (87%)	0.94	17 (11%) 10 12	30, 76, 122, 130	0
All	All	612/696 (87%)	0.77	62 (10%) 12 14	30, 64, 112, 142	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	347	ILE	6.6
1	B	259	VAL	6.1
1	A	263	GLY	5.5
1	B	264	ILE	4.8
1	A	275	ASN	4.5
1	B	263	GLY	4.4
1	B	258	PRO	4.3
1	A	273	HIS	4.3
1	B	257	ILE	4.0
1	B	211	GLN	3.9
1	C	211	GLN	3.8
1	A	274	ARG	3.8
1	C	264	ILE	3.7
1	D	281	VAL	3.6
1	A	259	VAL	3.6
1	A	264	ILE	3.5
1	D	275	ASN	3.5
1	A	244	GLY	3.5
1	C	271	PRO	3.5
1	C	243	TYR	3.4
1	D	270	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	348	LEU	3.2
1	A	243	TYR	3.1
1	D	276	SER	3.1
1	D	212	PRO	3.1
1	D	302	ILE	3.1
1	C	265	LYS	3.0
1	A	276	SER	3.0
1	B	346	ASN	2.9
1	C	353	VAL	2.9
1	B	275	ASN	2.9
1	B	212	PRO	2.8
1	D	228	ILE	2.8
1	C	270	SER	2.8
1	B	244	GLY	2.8
1	B	276	SER	2.8
1	B	260	ASN	2.7
1	C	238	ILE	2.6
1	B	345	ILE	2.6
1	C	263	GLY	2.6
1	D	230	MET	2.6
1	C	322	VAL	2.5
1	A	261	GLU	2.4
1	B	274	ARG	2.4
1	B	242	SER	2.4
1	D	271	PRO	2.4
1	C	273	HIS	2.3
1	D	279	ASP	2.3
1	D	346	ASN	2.3
1	C	260	ASN	2.2
1	D	264	ILE	2.2
1	D	300	MET	2.1
1	A	364	ASP	2.1
1	D	272	GLU	2.1
1	A	371	GLU	2.1
1	D	246	VAL	2.1
1	A	242	SER	2.1
1	B	249	LEU	2.1
1	C	262	ARG	2.1
1	D	243	TYR	2.0
1	C	259	VAL	2.0
1	B	224	PHE	2.0

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 ⓘ

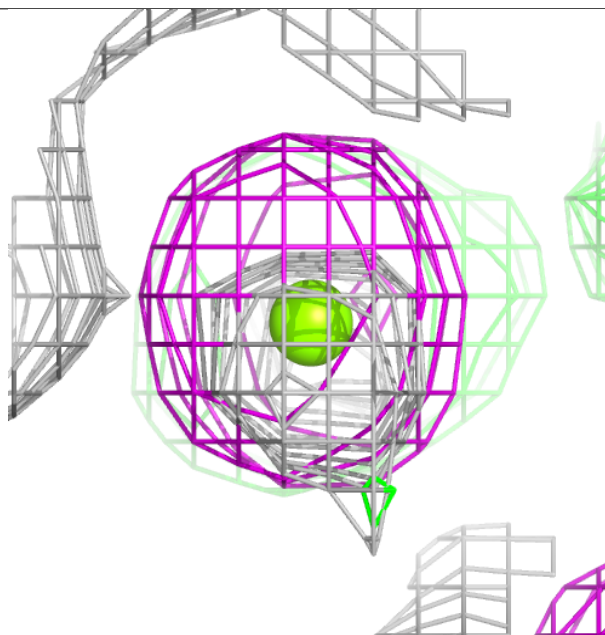
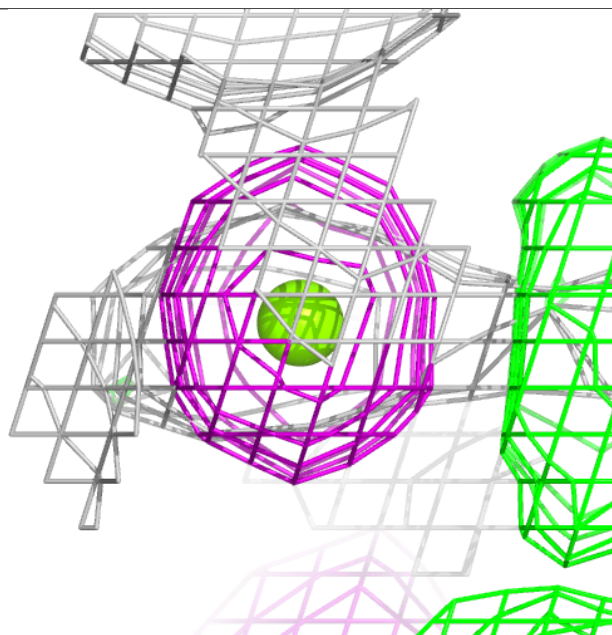
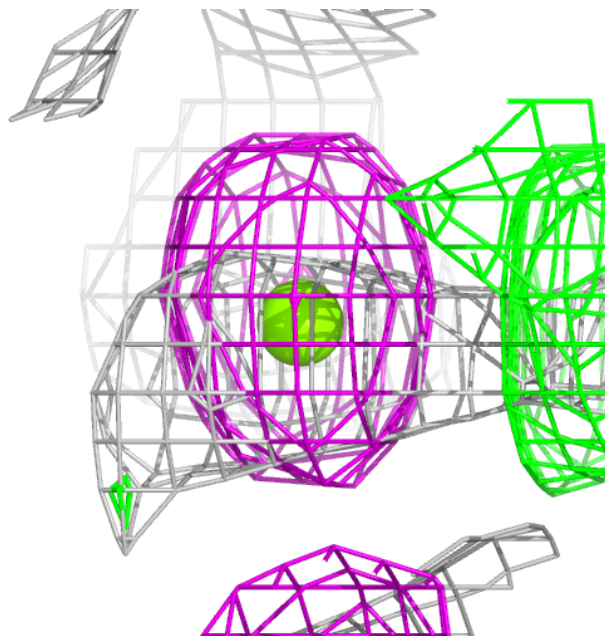
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	D	402	1/1	0.69	0.41	30,30,30,30	0
2	AMP	B	401	23/23	0.71	0.14	72,92,121,131	0
3	MG	B	402	1/1	0.73	0.43	30,30,30,30	0
2	AMP	D	401	23/23	0.81	0.14	72,91,109,113	0
2	AMP	C	401	23/23	0.82	0.13	50,66,94,100	0
3	MG	C	402	1/1	0.82	0.29	30,30,30,30	0
2	AMP	A	401	23/23	0.85	0.13	46,68,109,117	0
3	MG	C	403	1/1	0.90	0.35	30,30,30,30	0
3	MG	A	402	1/1	0.91	0.30	30,30,30,30	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.

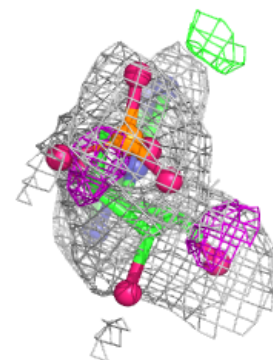
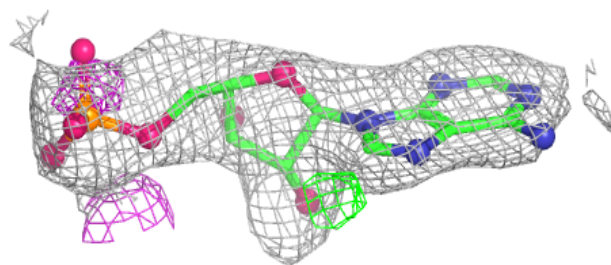
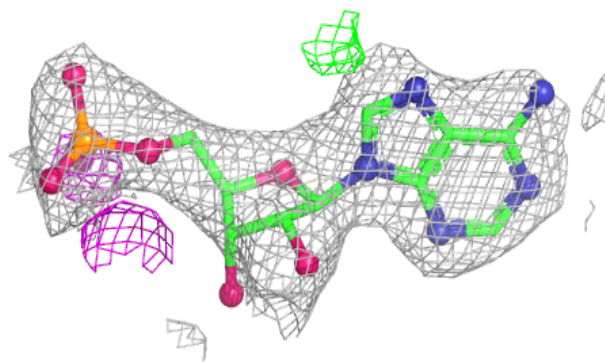
Electron density around MG D 402:

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



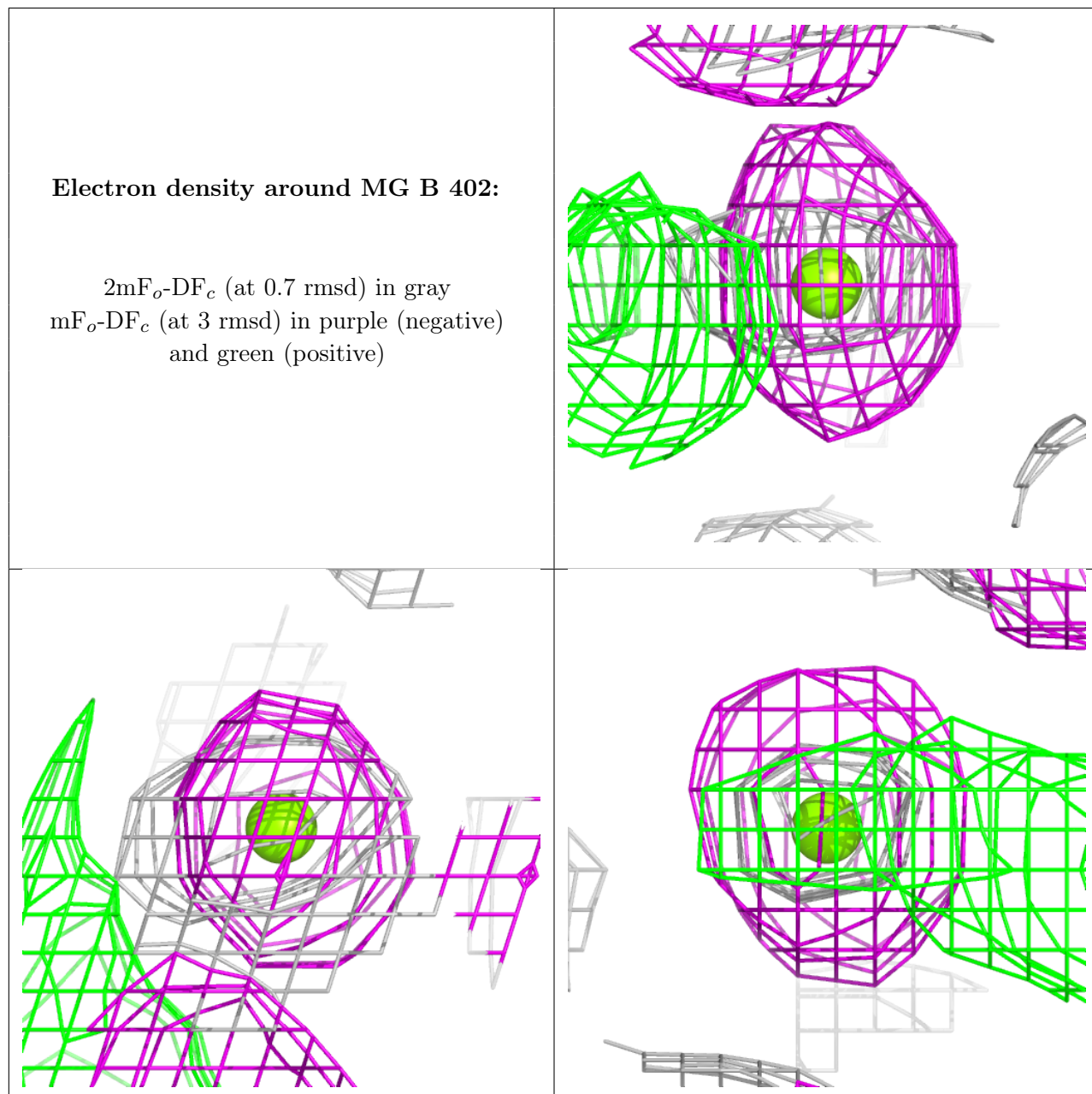
Electron density around AMP B 401:

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and green (positive)



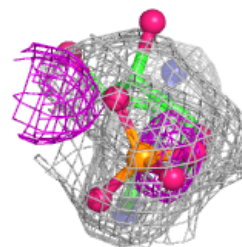
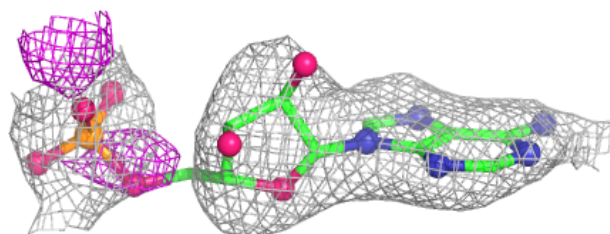
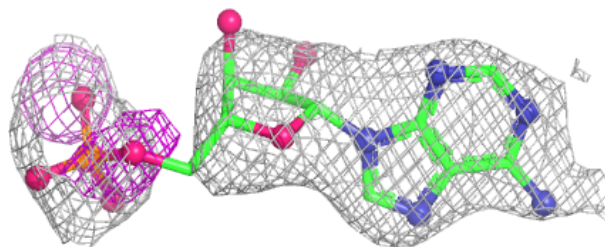
Electron density around MG B 402:

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

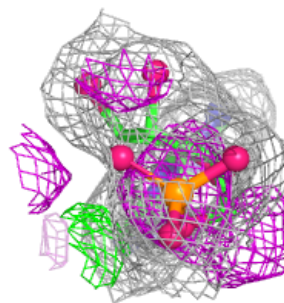
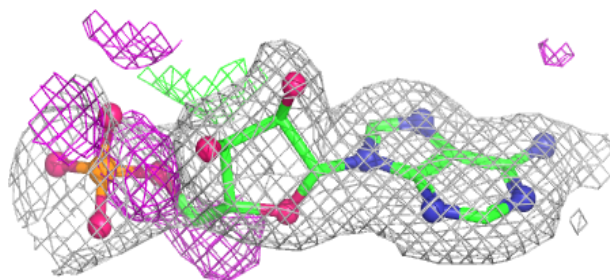
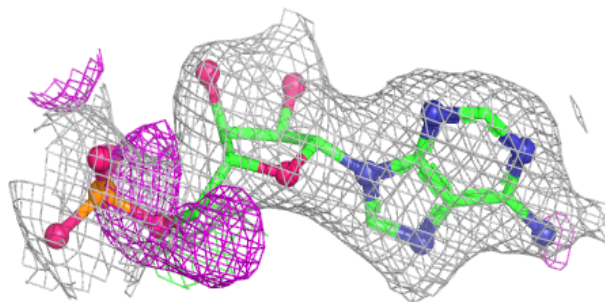


Electron density around AMP D 401:

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

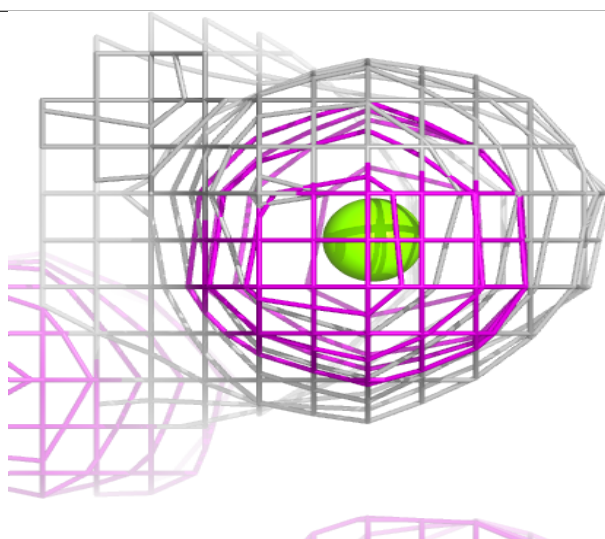
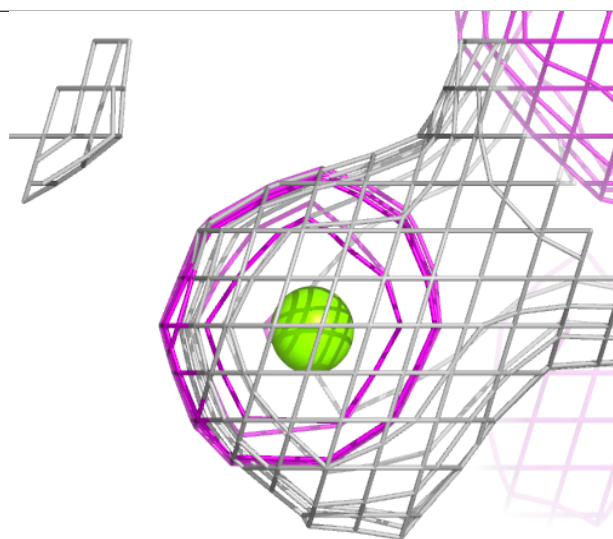
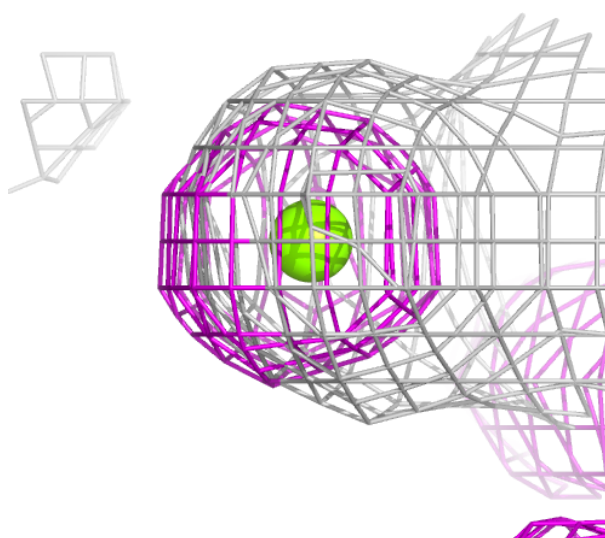
**Electron density around AMP C 401:**

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



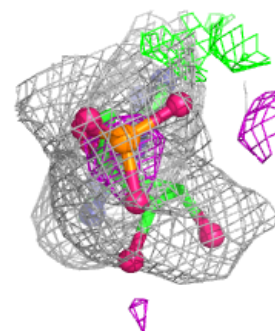
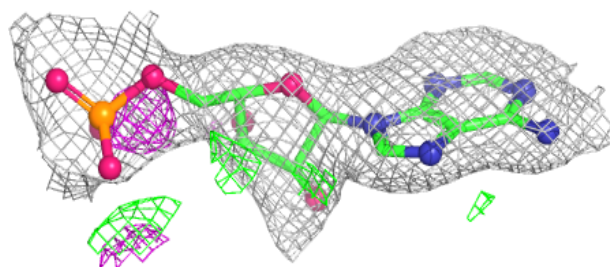
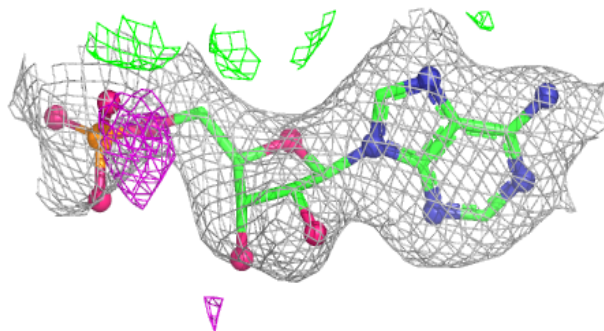
Electron density around MG C 402:

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



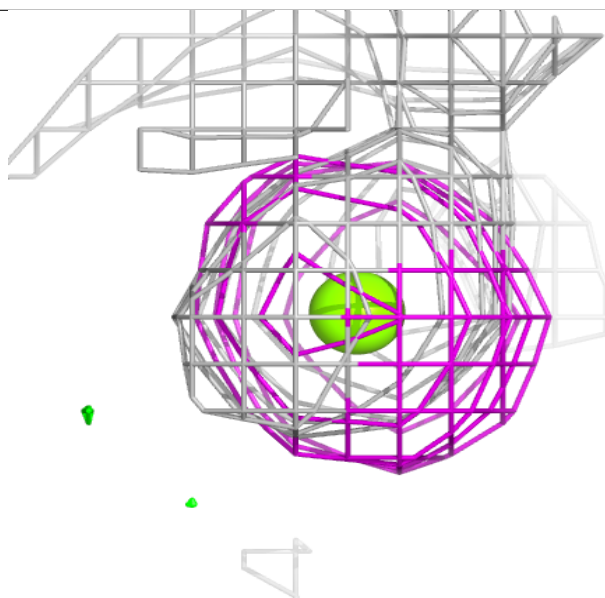
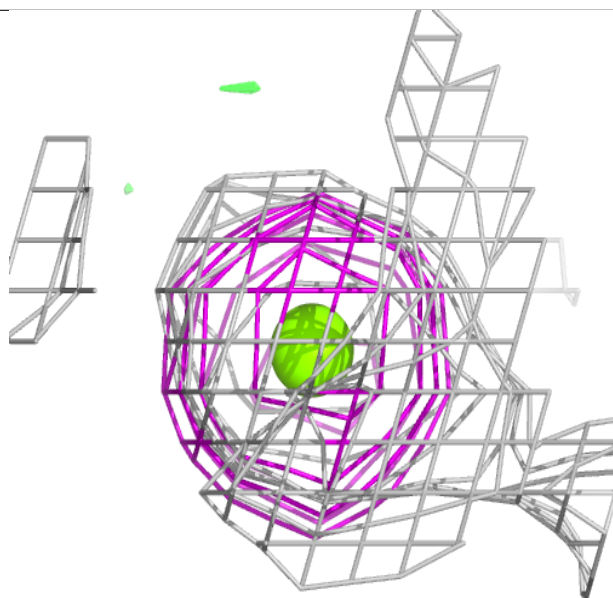
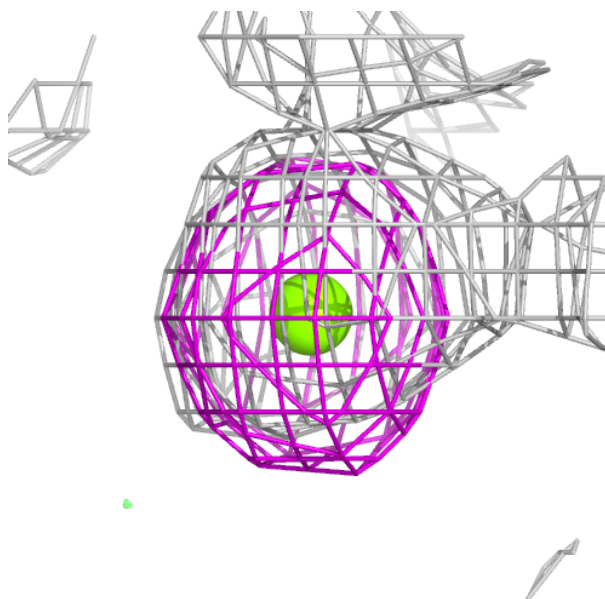
Electron density around AMP A 401:

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and green (positive)



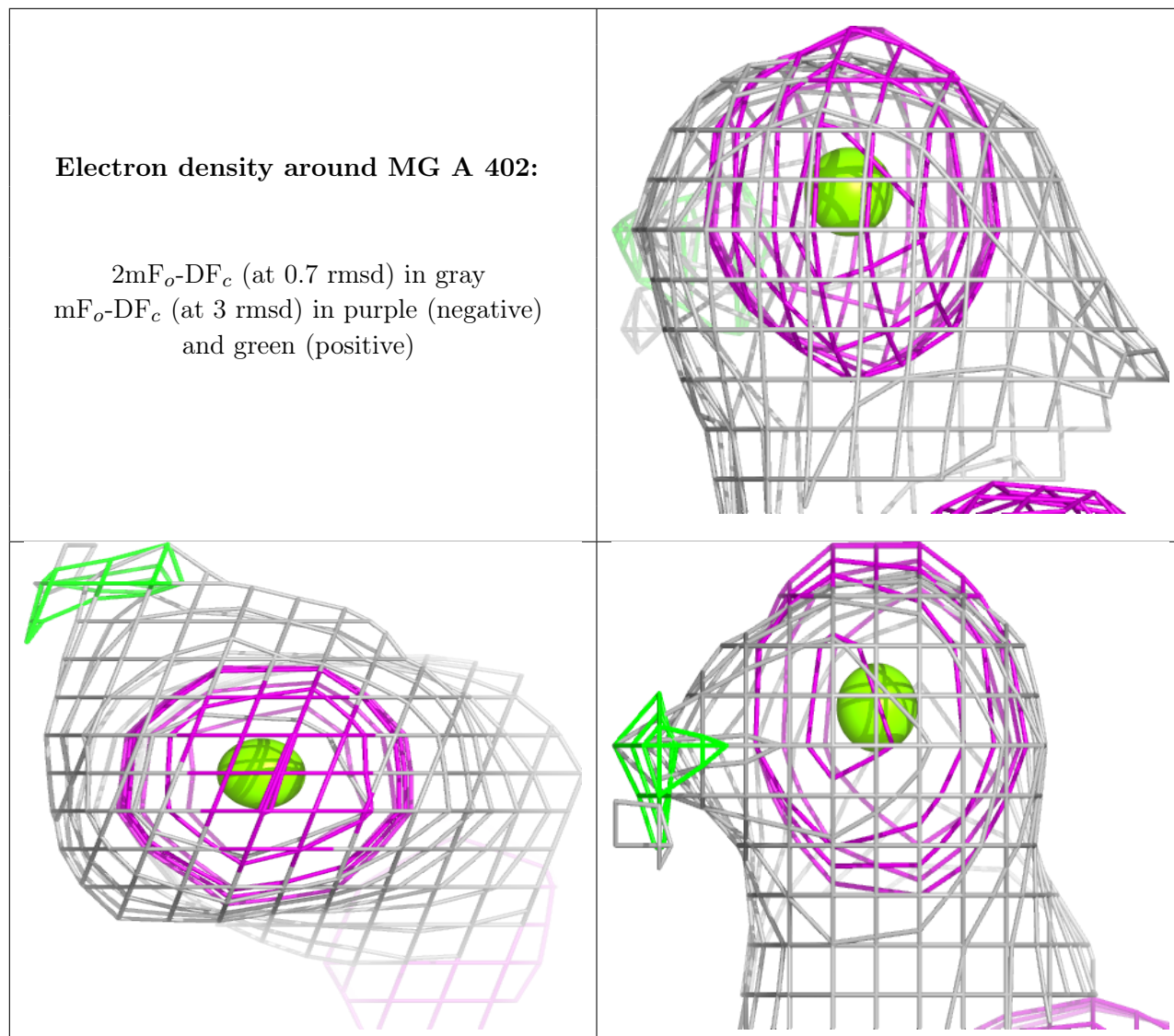
Electron density around MG C 403:

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



Electron density around MG A 402:

$2mF_o-DF_c$ (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.