



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:26 PM BST

PDB ID : 3X05
Title : Crystal structure of PIP4KIIBETA T201M complex with AMP
Authors : Takeuchi, K.; Lo, Y.H.; Sumita, K.; Senda, M.; Terakawa, J.; Dimitoris, A.; Locasale, J.W.; Sasaki, M.; Yoshino, H.; Zhang, Y.; Kahoud, E.R.; Takano, T.; Yokota, T.; Emerling, B.; Asara, J.A.; Ishida, T.; Shimada, I.; Daikoku, T.; Cantley, L.C.; Senda, T.; Sasaki, A.T.
Deposited on : 2014-10-09
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

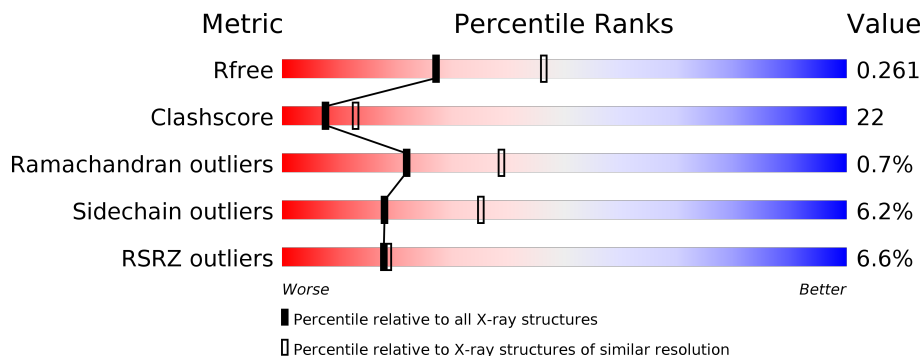
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	393	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 55% 24% • 19%</p>
1	B	393	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 47%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">8% 47% 27% • 23%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5301 atoms, of which 48 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.

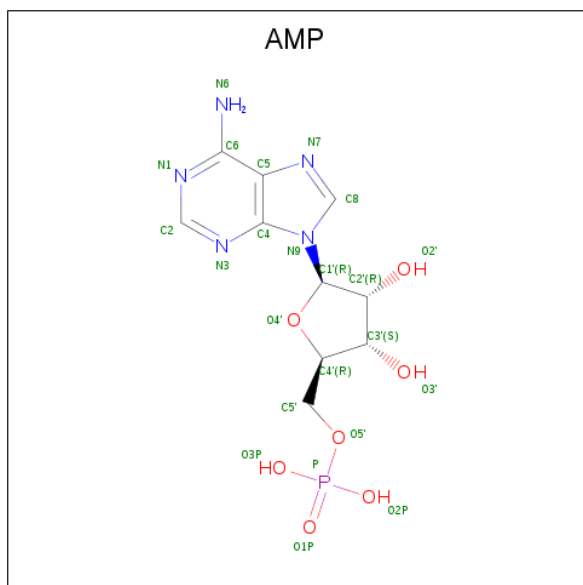
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2623	1670	444	494	15	0	0	0
1	B	303	2498	1599	426	459	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP P78356
A	25	PRO	-	EXPRESSION TAG	UNP P78356
A	26	ASN	-	EXPRESSION TAG	UNP P78356
A	27	CYS	-	EXPRESSION TAG	UNP P78356
A	28	ALA	-	EXPRESSION TAG	UNP P78356
A	29	PRO	-	EXPRESSION TAG	UNP P78356
A	30	GLY	-	EXPRESSION TAG	UNP P78356
A	201	MET	THR	ENGINEERED MUTATION	UNP P78356
B	24	GLY	-	EXPRESSION TAG	UNP P78356
B	25	PRO	-	EXPRESSION TAG	UNP P78356
B	26	ASN	-	EXPRESSION TAG	UNP P78356
B	27	CYS	-	EXPRESSION TAG	UNP P78356
B	28	ALA	-	EXPRESSION TAG	UNP P78356
B	29	PRO	-	EXPRESSION TAG	UNP P78356
B	30	GLY	-	EXPRESSION TAG	UNP P78356
B	201	MET	THR	ENGINEERED MUTATION	UNP P78356

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	B	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	B	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

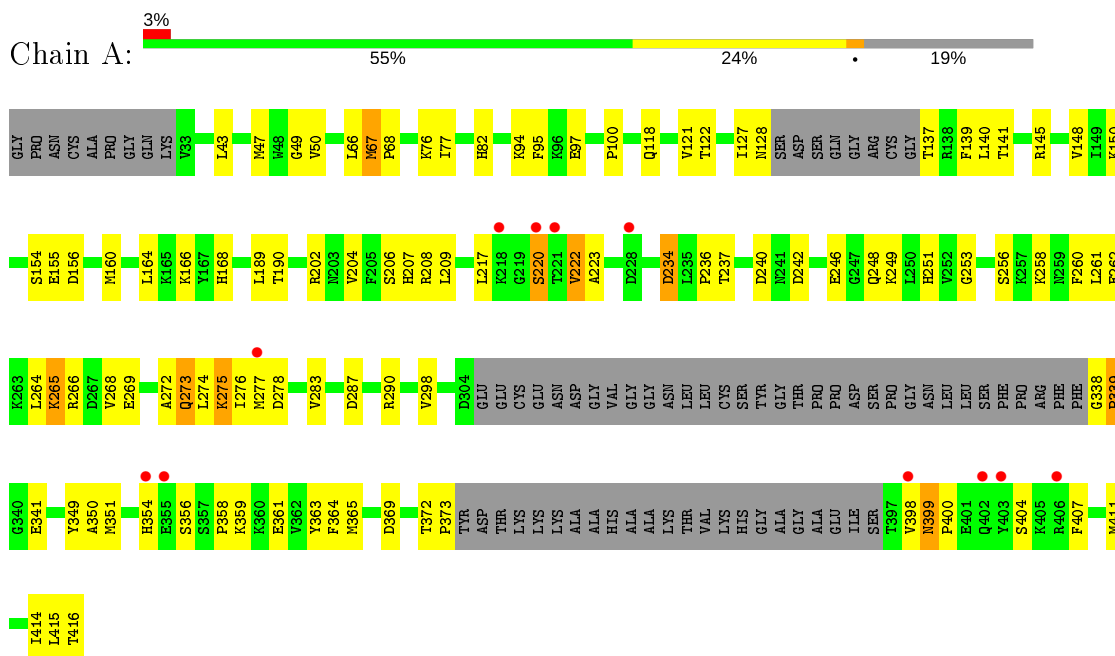
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	24	Total	O	0	0
			24	24		

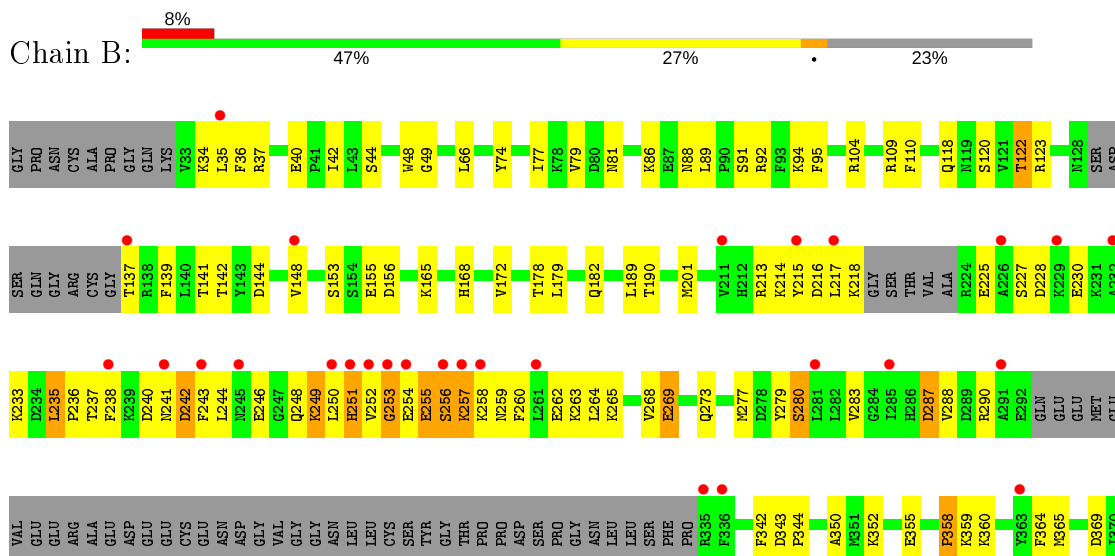
3 Residue-property plots

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: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



L371	T372	PRO	TYR	ASP	THR	LYS	LYS	LYS	ALA	ALA	HIS	ALA	ALA	LYS	THR	VAL	LYS	HIS	GLY	ALA	GLY	ALA	ALA	GLU	ILE	SER	THR	VAL	N399	P400	E401	Q402	Y403	S404	F405	R406	F407	F410	M411	S412	N413	I414	L415	T416
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.70Å 181.54Å 107.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.35 – 2.50 93.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (54.35-2.50) 98.8 (93.26-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.226 , 0.273 0.214 , 0.261	Depositor DCC
R_{free} test set	1834 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5301	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

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	0.48	0/2677	0.58	0/3604
1	B	0.43	0/2551	0.56	0/3430
All	All	0.45	0/5228	0.57	0/7034

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2623	0	2588	97	0
1	B	2498	0	2475	134	0
2	A	46	24	24	4	0
2	B	46	24	24	1	0
3	A	16	0	0	0	0
3	B	24	0	0	0	0
All	All	5253	48	5111	226	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 22.

All (226) 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:77:ILE:CD1	1:B:77:ILE:HD11	1.81	1.10
1:B:399:ASN:HB3	1:B:400:PRO:HD3	1.34	1.06
1:A:77:ILE:HD11	1:B:77:ILE:CD1	1.85	1.06
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.06	1.05
1:A:268:VAL:HG12	1:A:404:SER:HB2	1.42	1.01
1:A:253:GLY:N	1:A:354:HIS:HD2	1.61	0.98
1:B:287:ASP:OD1	1:B:359:LYS:HE3	1.65	0.96
1:B:268:VAL:HG12	1:B:404:SER:HB2	1.48	0.96
1:B:268:VAL:CG1	1:B:404:SER:HB2	1.98	0.93
1:B:225:GLU:HG3	1:B:241:ASN:HB2	1.51	0.92
1:B:230:GLU:HA	1:B:233:LYS:HZ3	1.32	0.91
1:A:415:LEU:O	1:A:416:THR:HG23	1.71	0.89
1:A:137:THR:O	1:A:137:THR:HG23	1.70	0.88
1:B:371:LEU:O	1:B:372:THR:HG22	1.72	0.88
1:A:264:LEU:HD11	1:A:407:PHE:HE1	1.40	0.86
1:A:67:MET:HA	1:A:67:MET:HE2	1.55	0.86
1:B:258:LYS:O	1:B:262:GLU:HG2	1.76	0.86
1:A:248:GLN:HG3	1:A:249:LYS:H	1.42	0.84
1:B:277:MET:SD	1:B:400:PRO:HG3	2.18	0.83
1:B:269:GLU:O	1:B:273:GLN:HG3	1.79	0.83
1:A:265:LYS:HG3	1:A:266:ARG:N	1.92	0.83
1:A:258:LYS:HE3	1:A:262:GLU:OE2	1.80	0.82
1:B:251:HIS:CD2	1:B:358:PRO:HD2	2.13	0.82
1:B:371:LEU:O	1:B:372:THR:CB	2.30	0.80
1:A:248:GLN:HG3	1:A:249:LYS:N	1.96	0.80
1:B:371:LEU:O	1:B:372:THR:CG2	2.29	0.79
1:B:110:PHE:CE1	1:B:182:GLN:HG2	2.19	0.78
1:A:242:ASP:O	1:A:246:GLU:HG2	1.84	0.77
1:A:256:SER:HB3	1:A:351:MET:CE	2.14	0.77
1:A:268:VAL:CG1	1:A:404:SER:HB2	2.14	0.77
1:B:249:LYS:HB2	1:B:251:HIS:CE1	2.20	0.76
1:B:399:ASN:HB3	1:B:400:PRO:CD	2.14	0.76
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.67	0.76
1:B:37:ARG:HG2	1:B:37:ARG:HH11	1.52	0.75
1:B:42:ILE:HD11	1:B:189:LEU:HD22	1.68	0.75
1:A:253:GLY:N	1:A:354:HIS:CD2	2.53	0.72
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.19	0.71
1:B:268:VAL:CG1	1:B:404:SER:CB	2.68	0.71
1:B:242:ASP:O	1:B:246:GLU:HG3	1.91	0.71
1:B:371:LEU:O	1:B:372:THR:HB	1.90	0.71
1:A:248:GLN:O	1:A:249:LYS:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HB2	1:A:190:THR:HB	1.74	0.70
1:B:283:VAL:HG22	1:B:365:MET:HG2	1.74	0.69
1:A:67:MET:HA	1:A:67:MET:CE	2.24	0.68
1:A:256:SER:HB3	1:A:351:MET:HE2	1.74	0.68
1:A:66:LEU:O	1:A:67:MET:HE3	1.94	0.68
1:A:207:HIS:CE1	1:A:208:ARG:CG	2.78	0.67
1:B:81:ASN:O	1:B:91:SER:HB3	1.93	0.67
1:B:118:GLN:O	1:B:122:THR:HB	1.96	0.65
1:B:213:ARG:HH12	1:B:246:GLU:CD	2.00	0.65
1:A:273:GLN:HG3	1:A:274:LEU:N	2.12	0.64
1:B:249:LYS:HD2	1:B:249:LYS:H	1.64	0.63
1:B:230:GLU:HA	1:B:233:LYS:NZ	2.13	0.62
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.64	0.62
1:B:213:ARG:NH1	1:B:246:GLU:OE1	2.33	0.61
1:B:213:ARG:HA	1:B:235:LEU:HD21	1.82	0.61
1:B:399:ASN:O	1:B:402:GLN:N	2.33	0.61
1:A:137:THR:O	1:A:137:THR:CG2	2.42	0.60
1:B:249:LYS:O	1:B:250:LEU:HD12	2.01	0.60
1:B:156:ASP:OD1	1:B:372:THR:HG23	2.02	0.59
1:B:179:LEU:HG	1:B:263:LYS:HD2	1.84	0.59
1:B:94:LYS:HB2	1:B:190:THR:HB	1.83	0.59
1:A:208:ARG:NH2	1:A:341:GLU:O	2.36	0.59
1:B:411:MET:O	1:B:414:ILE:HG12	2.03	0.58
1:A:264:LEU:HD11	1:A:407:PHE:CE1	2.29	0.58
1:A:207:HIS:CD2	1:A:208:ARG:HG2	2.38	0.58
1:A:372:THR:HG23	1:A:373:PRO:HD2	1.86	0.58
1:A:274:LEU:O	1:A:275:LYS:HB2	2.04	0.58
1:B:399:ASN:CB	1:B:400:PRO:HD3	2.22	0.58
1:A:220:SER:HB3	1:A:222:VAL:HG23	1.85	0.57
1:B:37:ARG:HG2	1:B:37:ARG:NH1	2.20	0.57
1:A:265:LYS:HG3	1:A:266:ARG:H	1.67	0.57
1:B:42:ILE:CD1	1:B:189:LEU:HD22	2.35	0.57
1:A:253:GLY:CA	1:A:354:HIS:HD2	2.17	0.57
1:B:371:LEU:C	1:B:372:THR:HG22	2.25	0.57
1:B:248:GLN:HG3	1:B:249:LYS:N	2.20	0.56
1:A:222:VAL:HG12	1:A:223:ALA:H	1.70	0.56
1:B:79:VAL:O	1:B:92:ARG:HA	2.05	0.56
1:A:234:ASP:O	1:A:236:PRO:HD3	2.05	0.56
1:A:166:LYS:CD	1:A:274:LEU:HD21	2.36	0.56
1:A:253:GLY:H	1:A:354:HIS:HD2	1.50	0.56
1:A:155:GLU:N	1:A:155:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:O	1:B:253:GLY:C	2.44	0.56
1:A:399:ASN:ND2	1:A:400:PRO:HD2	2.21	0.55
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.35	0.55
1:B:399:ASN:O	1:B:403:TYR:N	2.38	0.55
1:A:399:ASN:HD22	1:A:400:PRO:HD2	1.72	0.55
1:B:236:PRO:HG2	1:B:238:PHE:CZ	2.41	0.55
1:A:127:ILE:O	1:A:128:ASN:HB3	2.06	0.55
1:B:230:GLU:HG3	1:B:233:LYS:HZ1	1.72	0.55
1:B:256:SER:O	1:B:260:PHE:CB	2.55	0.55
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.89	0.54
1:B:42:ILE:CD1	1:B:189:LEU:CD2	2.85	0.54
1:A:207:HIS:NE2	1:A:208:ARG:HG2	2.23	0.54
1:B:110:PHE:CZ	1:B:182:GLN:HG2	2.43	0.54
1:B:42:ILE:HD11	1:B:189:LEU:CD2	2.36	0.54
1:B:407:PHE:O	1:B:411:MET:HG2	2.08	0.54
1:B:237:THR:HG22	1:B:237:THR:O	2.06	0.53
1:B:42:ILE:HD12	1:B:189:LEU:HD23	1.91	0.53
1:B:249:LYS:HB2	1:B:251:HIS:HE1	1.72	0.53
1:B:139:PHE:CZ	1:B:148:VAL:CG1	2.92	0.53
1:B:225:GLU:CG	1:B:241:ASN:HB2	2.32	0.53
1:B:66:LEU:HD12	1:B:168:HIS:CE1	2.44	0.53
1:B:189:LEU:N	1:B:189:LEU:HD12	2.24	0.52
1:A:268:VAL:CG1	1:A:404:SER:CB	2.87	0.52
1:B:251:HIS:HD2	1:B:358:PRO:HD2	1.70	0.52
1:A:268:VAL:CG1	1:A:404:SER:HA	2.40	0.52
1:A:399:ASN:ND2	1:A:400:PRO:CD	2.73	0.52
1:A:82:HIS:HB2	1:B:74:TYR:CZ	2.45	0.52
1:B:342:PHE:CE1	1:B:350:ALA:HB3	2.44	0.52
1:A:251:HIS:HB3	1:A:354:HIS:CE1	2.45	0.52
1:B:139:PHE:CZ	1:B:148:VAL:HG11	2.44	0.52
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.38	0.52
1:B:355:GLU:OE1	1:B:355:GLU:HA	2.09	0.51
1:B:230:GLU:HG3	1:B:233:LYS:NZ	2.25	0.51
1:A:407:PHE:O	1:A:411:MET:HG2	2.10	0.51
1:B:288:VAL:HG23	1:B:360:LYS:O	2.11	0.51
1:B:40:GLU:OE1	1:B:137:THR:HG21	2.11	0.51
1:B:287:ASP:CG	1:B:359:LYS:HE3	2.29	0.51
1:A:166:LYS:HD2	1:A:274:LEU:HD21	1.92	0.51
1:A:369:ASP:OD1	2:A:501:AMP:O1P	2.29	0.51
1:B:215:TYR:HD2	1:B:243:PHE:HB2	1.76	0.50
1:B:37:ARG:HG3	1:B:88:ASN:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LYS:HD2	1:B:249:LYS:N	2.26	0.50
1:B:277:MET:SD	1:B:400:PRO:CG	2.97	0.50
1:B:215:TYR:HB3	1:B:217:LEU:HD21	1.93	0.49
1:B:252:VAL:HG13	1:B:352:LYS:O	2.12	0.49
1:B:399:ASN:HA	1:B:402:GLN:OE1	2.12	0.49
1:A:207:HIS:CE1	1:A:208:ARG:HG2	2.47	0.49
1:B:250:LEU:HB2	1:B:414:ILE:O	2.12	0.49
1:B:216:ASP:OD1	1:B:280:SER:HB3	2.12	0.49
1:A:141:THR:CG2	1:A:145:ARG:HA	2.43	0.49
1:A:207:HIS:CE1	1:A:208:ARG:HG3	2.47	0.48
1:A:49:GLY:HA3	1:A:95:PHE:CE1	2.49	0.48
1:B:360:LYS:HE2	1:B:360:LYS:HB2	1.47	0.48
1:A:66:LEU:HD12	1:A:168:HIS:CE1	2.49	0.48
1:A:204:VAL:HG23	2:A:501:AMP:C6	2.49	0.48
1:A:204:VAL:HA	1:A:349:TYR:CD2	2.48	0.48
1:B:213:ARG:HG2	1:B:238:PHE:HE2	1.78	0.48
1:B:35:LEU:O	1:B:37:ARG:N	2.45	0.48
1:B:213:ARG:CG	1:B:238:PHE:HE2	2.27	0.48
1:A:150:LYS:NZ	2:A:501:AMP:O2P	2.28	0.47
1:B:369:ASP:OD2	2:B:501:AMP:O2P	2.31	0.47
1:A:339:PRO:HD2	1:A:341:GLU:CD	2.35	0.47
1:B:264:LEU:HD12	1:B:264:LEU:O	2.14	0.47
1:B:230:GLU:CG	1:B:233:LYS:NZ	2.77	0.47
1:A:137:THR:HG22	1:A:140:LEU:HD21	1.96	0.47
1:A:276:ILE:HG22	1:A:277:MET:N	2.30	0.47
1:B:257:LYS:HG2	1:B:258:LYS:N	2.30	0.47
1:A:166:LYS:HD3	1:A:274:LEU:HD21	1.97	0.47
1:B:34:LYS:NZ	1:B:122:THR:HG21	2.29	0.46
1:A:277:MET:O	1:A:278:ASP:HB2	2.15	0.46
1:B:248:GLN:HG3	1:B:249:LYS:H	1.80	0.46
1:A:361:GLU:OE1	1:A:363:TYR:OH	2.21	0.46
1:A:399:ASN:CG	1:A:400:PRO:N	2.68	0.46
1:B:153:SER:O	1:B:156:ASP:HB2	2.16	0.46
1:A:67:MET:HE2	1:A:68:PRO:HD3	1.96	0.46
1:B:179:LEU:HG	1:B:263:LYS:CD	2.46	0.46
1:B:213:ARG:HG2	1:B:238:PHE:CE2	2.51	0.46
1:B:268:VAL:HG12	1:B:404:SER:CB	2.30	0.46
1:A:189:LEU:N	1:A:189:LEU:HD12	2.31	0.46
1:A:160:MET:O	1:A:164:LEU:HB2	2.15	0.46
1:B:277:MET:HA	1:B:279:TYR:CE2	2.51	0.46
1:B:287:ASP:OD2	1:B:290:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:NH1	1:B:172:VAL:HG22	2.31	0.45
1:B:242:ASP:N	1:B:242:ASP:OD1	2.49	0.45
1:B:256:SER:O	1:B:260:PHE:HB2	2.16	0.45
1:B:120:SER:O	1:B:142:THR:HB	2.16	0.45
1:B:37:ARG:CG	1:B:37:ARG:HH11	2.25	0.45
1:A:265:LYS:HB2	1:A:265:LYS:HE2	1.71	0.45
1:A:350:ALA:HA	1:A:363:TYR:O	2.16	0.45
1:B:238:PHE:HB3	1:B:242:ASP:HB2	1.98	0.45
1:B:243:PHE:HE2	1:B:414:ILE:CG2	2.28	0.45
1:A:269:GLU:O	1:A:272:ALA:HB3	2.17	0.45
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.99	0.45
1:A:237:THR:HG22	1:A:237:THR:O	2.16	0.44
1:A:338:GLY:HA3	1:A:341:GLU:HB2	1.99	0.44
1:B:218:LYS:HD3	1:B:403:TYR:OH	2.17	0.44
1:A:43:LEU:O	1:A:47:MET:HG3	2.18	0.44
1:A:207:HIS:CE1	1:A:208:ARG:HD3	2.52	0.44
1:A:273:GLN:HG3	1:A:274:LEU:H	1.82	0.44
1:B:243:PHE:CE2	1:B:414:ILE:CG2	3.00	0.44
1:B:243:PHE:CE1	1:B:248:GLN:HB3	2.52	0.44
1:B:251:HIS:NE2	1:B:358:PRO:HD2	2.32	0.44
1:B:399:ASN:O	1:B:402:GLN:HB2	2.17	0.44
1:A:206:SER:HB2	1:A:364:PHE:CE2	2.53	0.44
1:B:141:THR:HG22	1:B:148:VAL:HG22	2.00	0.44
1:A:253:GLY:CA	1:A:354:HIS:CD2	3.00	0.43
1:B:364:PHE:O	1:B:365:MET:HG3	2.17	0.43
1:B:36:PHE:O	1:B:44:SER:OG	2.29	0.43
1:A:156:ASP:OD1	1:A:372:THR:O	2.36	0.43
1:A:415:LEU:O	1:A:416:THR:CG2	2.56	0.43
1:B:230:GLU:CG	1:B:233:LYS:HZ3	2.31	0.43
1:B:37:ARG:CG	1:B:37:ARG:NH1	2.81	0.43
1:B:48:TRP:HB2	1:B:89:LEU:HD21	1.99	0.43
1:A:398:VAL:HG12	1:A:399:ASN:N	2.34	0.43
1:B:253:GLY:O	1:B:254:GLU:C	2.57	0.43
1:B:256:SER:O	1:B:260:PHE:HB3	2.19	0.43
1:B:255:GLU:O	1:B:259:ASN:HB2	2.18	0.43
1:B:49:GLY:HA3	1:B:95:PHE:CE1	2.54	0.43
1:A:209:LEU:HD12	1:A:364:PHE:HZ	1.83	0.43
1:A:268:VAL:CG1	1:A:404:SER:CA	2.97	0.43
1:B:236:PRO:CG	1:B:238:PHE:CZ	3.02	0.42
1:B:401:GLU:O	1:B:404:SER:OG	2.31	0.42
1:B:251:HIS:CD2	1:B:358:PRO:CD	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLN:O	1:B:201:MET:HA	2.19	0.42
1:B:155:GLU:CD	1:B:155:GLU:H	2.21	0.42
1:B:216:ASP:OD1	1:B:280:SER:CB	2.68	0.42
1:A:118:GLN:O	1:A:122:THR:HG23	2.20	0.42
1:A:276:ILE:CG2	1:A:277:MET:N	2.83	0.42
1:A:97:GLU:CD	1:A:100:PRO:HB3	2.40	0.42
1:B:42:ILE:HD12	1:B:189:LEU:CD2	2.49	0.41
1:B:139:PHE:CZ	1:B:148:VAL:HG13	2.55	0.41
1:B:227:SER:OG	1:B:228:ASP:N	2.53	0.41
1:B:410:PHE:C	1:B:410:PHE:CD1	2.94	0.41
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.80	0.41
1:B:343:ASP:HA	1:B:344:PRO:HD2	1.89	0.41
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.91	0.41
1:B:144:ASP:OD1	1:B:144:ASP:C	2.59	0.41
1:A:139:PHE:CZ	1:A:148:VAL:CG1	3.04	0.41
1:A:260:PHE:CD2	1:A:415:LEU:HD11	2.56	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.91	0.41
1:A:139:PHE:CZ	1:A:148:VAL:HG11	2.56	0.40
1:B:252:VAL:O	1:B:253:GLY:O	2.39	0.40
1:A:204:VAL:HG23	2:A:501:AMP:N6	2.36	0.40
1:A:50:VAL:HG21	1:A:121:VAL:HG11	2.03	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	312/393 (79%)	298 (96%)	12 (4%)	2 (1%)	25	43
1	B	293/393 (75%)	281 (96%)	10 (3%)	2 (1%)	22	39
All	All	605/786 (77%)	579 (96%)	22 (4%)	4 (1%)	22	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PRO
1	A	358	PRO
1	B	253	GLY
1	B	358	PRO

5.3.2 Protein sidechains [i](#)

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	296/352 (84%)	281 (95%)	15 (5%)	24	45
1	B	281/352 (80%)	260 (92%)	21 (8%)	13	26
All	All	577/704 (82%)	541 (94%)	36 (6%)	18	35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	MET
1	A	76	LYS
1	A	154	SER
1	A	202	ARG
1	A	220	SER
1	A	222	VAL
1	A	234	ASP
1	A	240	ASP
1	A	265	LYS
1	A	273	GLN
1	A	275	LYS
1	A	298	VAL
1	A	356	SER
1	A	359	LYS
1	A	399	ASN
1	B	86	LYS
1	B	104	ARG
1	B	122	THR
1	B	123	ARG

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Mol	Chain	Res	Type
1	B	165	LYS
1	B	178	THR
1	B	214	LYS
1	B	235	LEU
1	B	240	ASP
1	B	242	ASP
1	B	249	LYS
1	B	251	HIS
1	B	255	GLU
1	B	256	SER
1	B	257	LYS
1	B	265	LYS
1	B	269	GLU
1	B	280	SER
1	B	287	ASP
1	B	406	ARG
1	B	416	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	251	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	AMP	B	502	-	22,25,25	0.84	1 (4%)	25,38,38	1.33	3 (12%)
2	AMP	A	501	-	22,25,25	0.86	1 (4%)	25,38,38	1.24	3 (12%)
2	AMP	A	502	-	22,25,25	0.95	1 (4%)	25,38,38	1.33	3 (12%)
2	AMP	B	501	-	22,25,25	0.99	1 (4%)	25,38,38	1.50	4 (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
2	AMP	B	502	-	-	3/6/26/26	0/3/3/3
2	AMP	A	501	-	-	0/6/26/26	0/3/3/3
2	AMP	A	502	-	-	4/6/26/26	0/3/3/3
2	AMP	B	501	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AMP	C5-C4	2.46	1.47	1.40
2	B	501	AMP	C5-C4	2.42	1.47	1.40
2	A	502	AMP	C5-C4	2.29	1.47	1.40
2	B	502	AMP	C5-C4	2.25	1.46	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	AMP	N3-C2-N1	-3.75	122.81	128.68
2	B	501	AMP	N3-C2-N1	-3.68	122.92	128.68
2	A	501	AMP	N3-C2-N1	-3.54	123.15	128.68
2	A	502	AMP	N3-C2-N1	-3.49	123.23	128.68
2	B	501	AMP	C3'-C2'-C1'	3.48	106.21	100.98
2	A	502	AMP	O3P-P-O5'	-2.74	99.43	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	C4-C5-N7	-2.73	106.55	109.40
2	A	502	AMP	C4-C5-N7	-2.59	106.70	109.40
2	B	502	AMP	C4-C5-N7	-2.51	106.78	109.40
2	A	501	AMP	O3P-P-O5'	-2.27	100.70	106.73
2	A	501	AMP	C4-C5-N7	-2.17	107.14	109.40
2	B	502	AMP	C2-N1-C6	2.07	122.30	118.75
2	B	501	AMP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

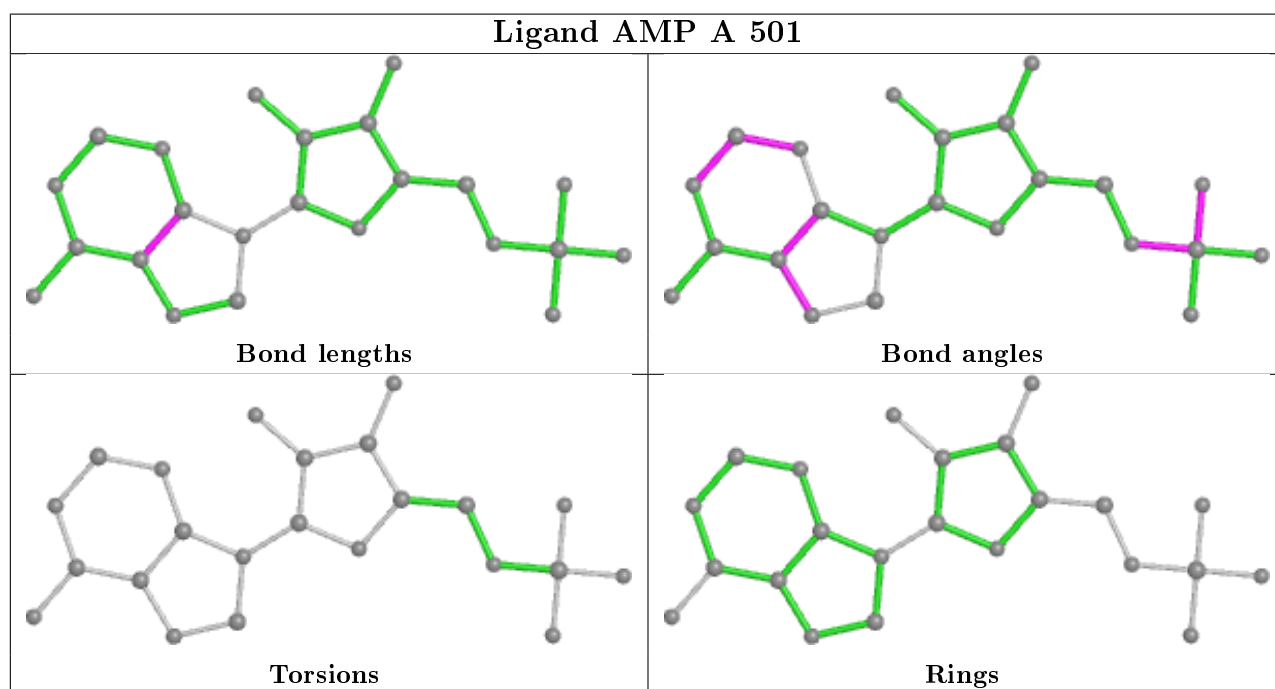
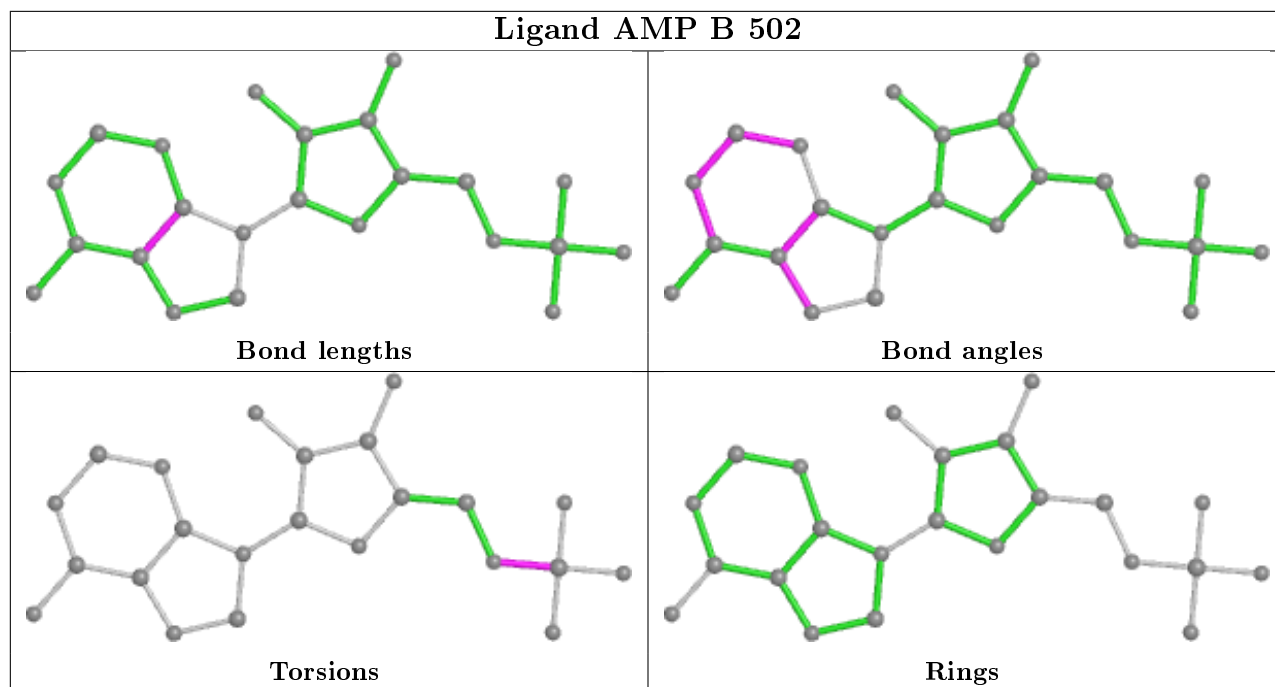
Mol	Chain	Res	Type	Atoms
2	B	502	AMP	C5'-O5'-P-O2P
2	A	502	AMP	C5'-O5'-P-O1P
2	A	502	AMP	C5'-O5'-P-O2P
2	A	502	AMP	C5'-O5'-P-O3P
2	B	502	AMP	C5'-O5'-P-O1P
2	B	502	AMP	C5'-O5'-P-O3P
2	A	502	AMP	O4'-C4'-C5'-O5'

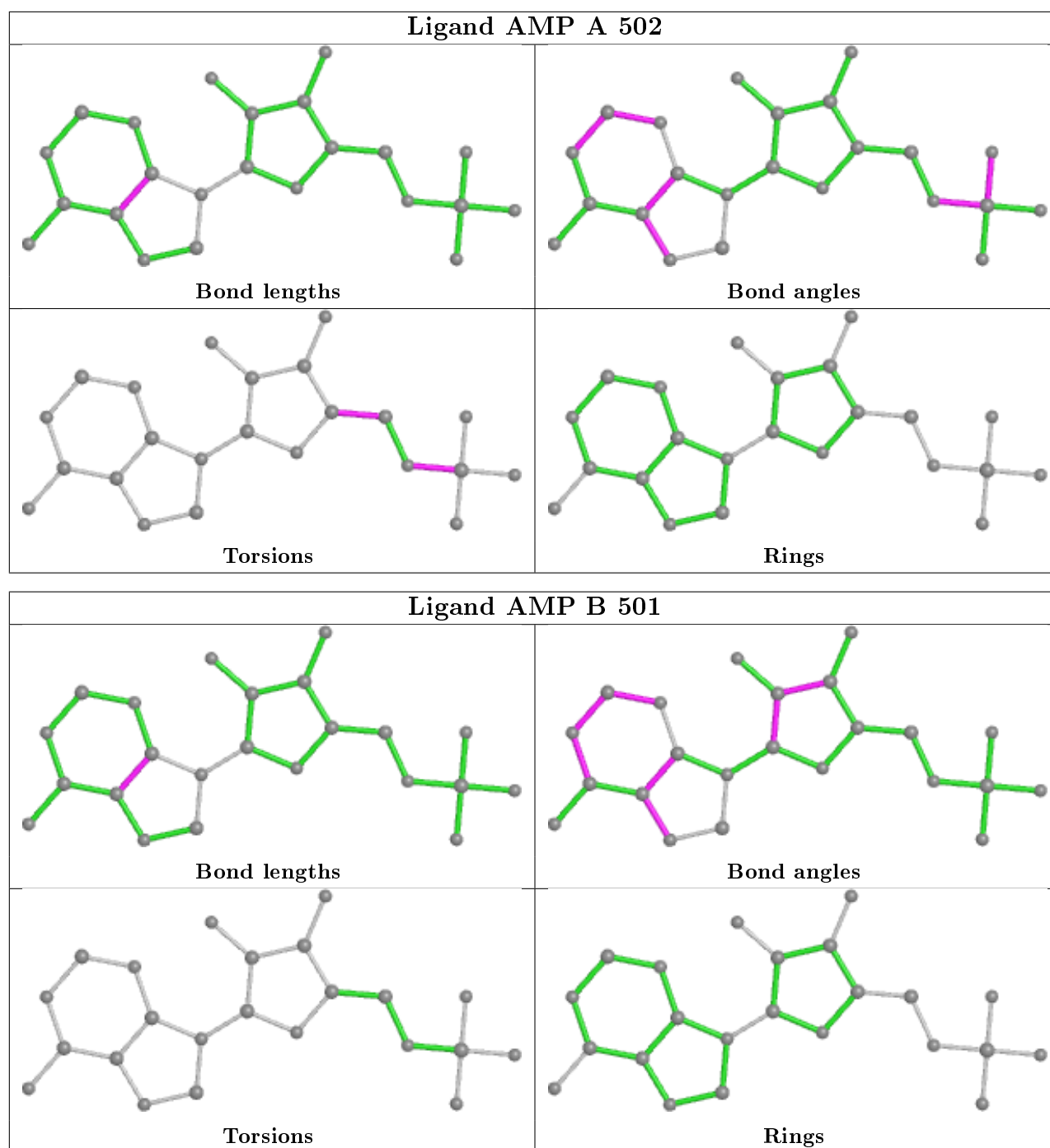
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	4	0
2	B	501	AMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/393 (81%)	0.62	11 (3%) 45 48	25, 66, 119, 146	0
1	B	303/393 (77%)	0.81	30 (9%) 7 7	25, 72, 138, 166	0
All	All	623/786 (79%)	0.71	41 (6%) 18 19	25, 69, 130, 166	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	THR	7.5
1	A	402	GLN	5.8
1	B	254	GLU	5.7
1	B	250	LEU	5.1
1	B	215	TYR	4.7
1	B	253	GLY	4.0
1	B	137	THR	3.8
1	A	220	SER	3.8
1	A	406	ARG	3.8
1	B	245	ASN	3.4
1	B	336	PHE	3.3
1	B	363	TYR	3.3
1	A	228	ASP	3.1
1	B	232	ALA	3.0
1	A	355	GLU	3.0
1	B	238	PHE	3.0
1	B	241	ASN	2.9
1	B	229	LYS	2.8
1	B	256	SER	2.8
1	A	354	HIS	2.8
1	B	211	VAL	2.6
1	B	291	ALA	2.6
1	B	261	LEU	2.5
1	B	251	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	217	LEU	2.5
1	B	281	LEU	2.4
1	B	413	ASN	2.4
1	B	257	LYS	2.3
1	B	226	ALA	2.3
1	A	218	LYS	2.3
1	B	285	ILE	2.3
1	A	398	VAL	2.3
1	B	407	PHE	2.2
1	B	252	VAL	2.2
1	A	277	MET	2.1
1	B	148	VAL	2.1
1	B	243	PHE	2.1
1	B	258	LYS	2.1
1	B	335	ARG	2.1
1	A	403	TYR	2.1
1	B	35	LEU	2.1

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 monosaccharides in this entry.

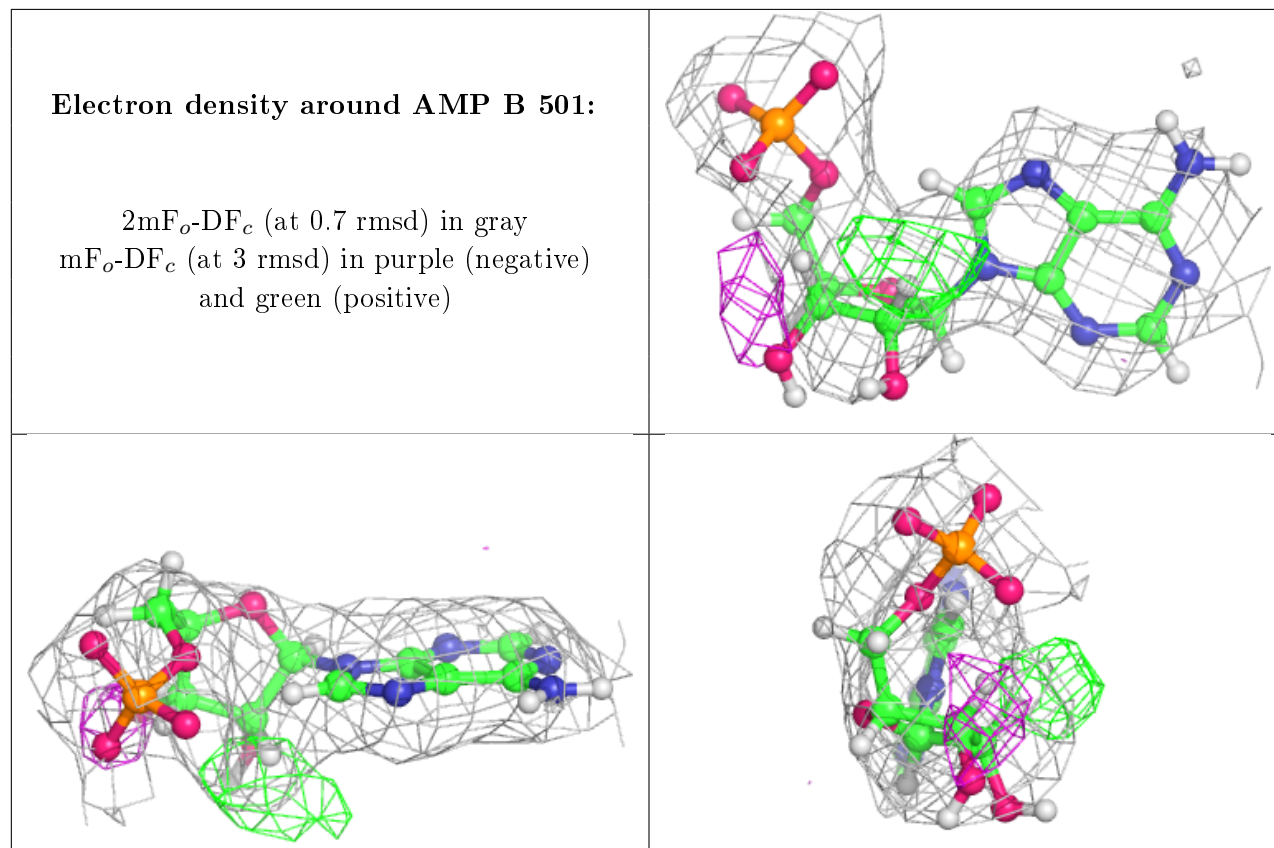
6.4 Ligands [i](#)

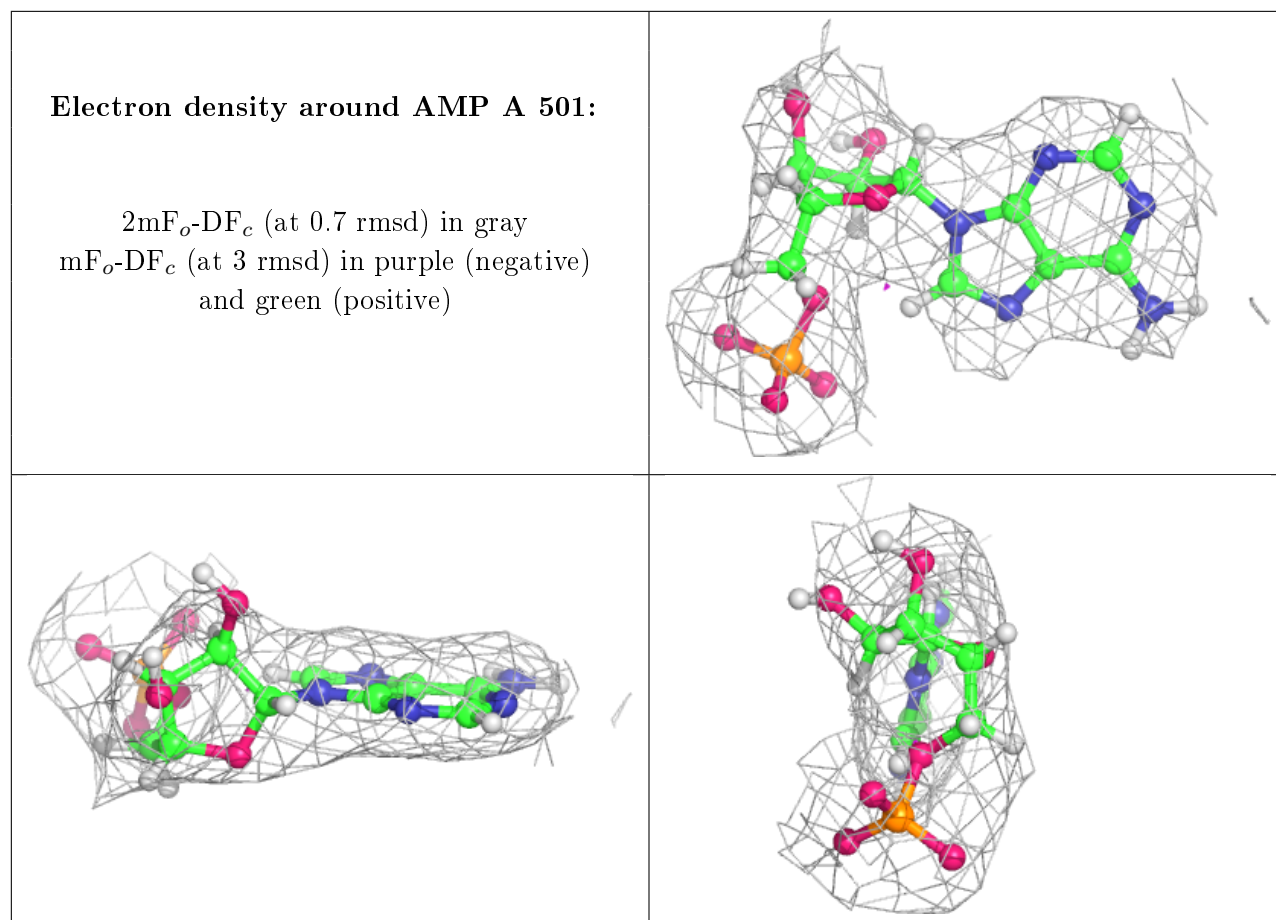
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AMP	B	501	23/23	0.84	0.20	78,100,131,134	0
2	AMP	A	501	23/23	0.95	0.15	46,91,118,119	0
2	AMP	A	502	23/23	0.97	0.16	49,72,90,92	0
2	AMP	B	502	23/23	0.97	0.18	40,52,63,66	0

The following is a graphical depiction of the model fit to experimental electron density of all

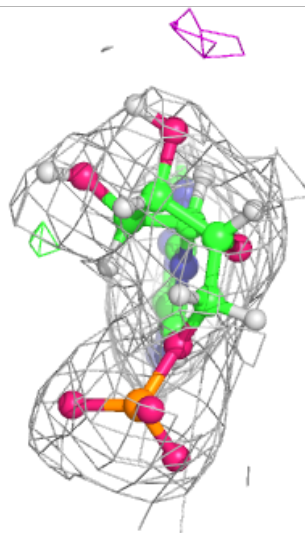
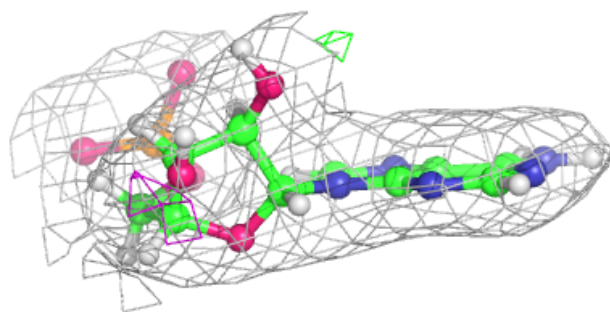
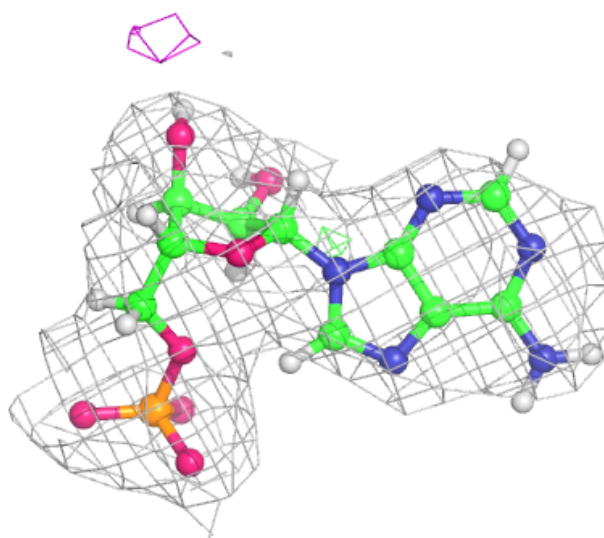
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

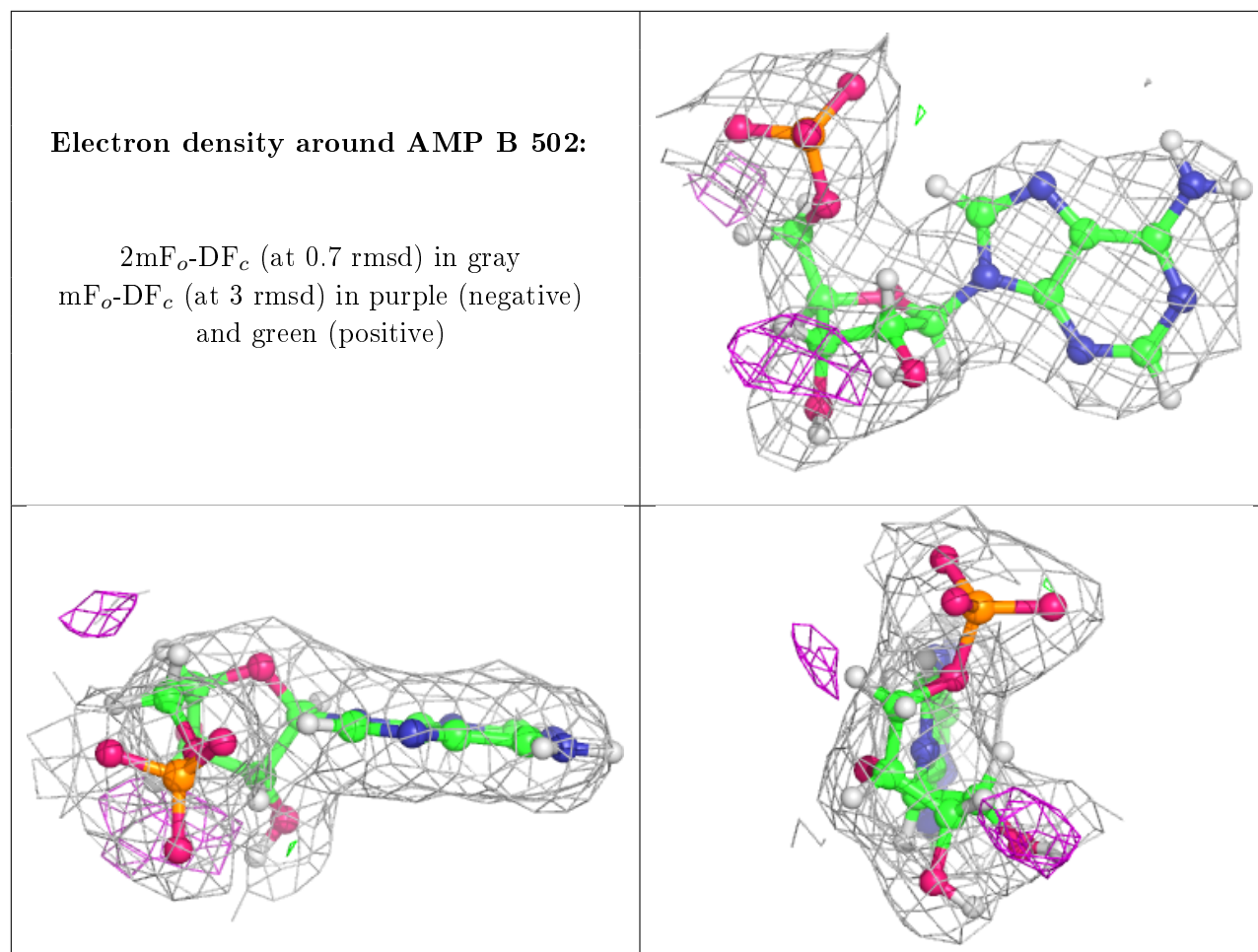




Electron density around AMP A 502:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.