



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:55 AM UTC

PDB ID : 3X01 / pdb_00003x01
Title : Crystal structure of PIP4KIIBETA 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 : 2.15 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](#) ①) 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

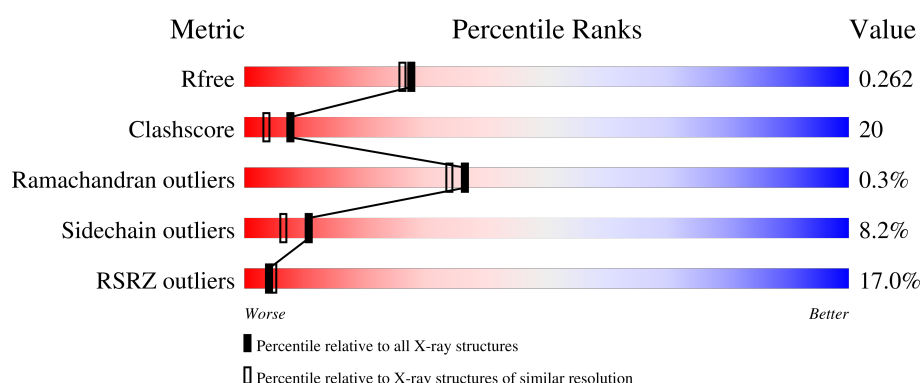
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	393	13% 53% 22% 5% 20%
1	B	393	13% 50% 22% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5309 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
1	A	315	Total	C	N	O	S	0	0	0
			2595	1651	442	488	14			
1	B	298	Total	C	N	O	S	0	0	0
			2468	1583	423	449	13			

There are 14 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
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

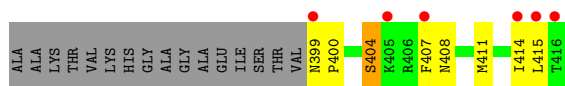
- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	51	Total	O	0	0
			51	51		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.39Å 181.79Å 107.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 2.15 48.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.40-2.15) 98.0 (48.40-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.246 , 0.279 0.233 , 0.262	Depositor DCC
R_{free} test set	2845 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 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	5309	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 3.67% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	6/2647 (0.2%)	0.84	3/3556 (0.1%)
1	B	0.66	2/2519 (0.1%)	0.83	1/3382 (0.0%)
All	All	0.73	8/5166 (0.2%)	0.84	4/6938 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	SER	C-O	-8.55	1.12	1.23
1	A	107	ARG	C-O	-6.79	1.16	1.24
1	B	207	HIS	CG-ND1	-6.53	1.31	1.38
1	B	207	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	280	SER	N-CA	-5.52	1.38	1.45
1	A	203	ASN	C-O	-5.44	1.17	1.23
1	A	280	SER	CA-C	-5.20	1.46	1.52
1	A	231	LYS	CA-C	-5.12	1.45	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	LEU	N-CA-C	-9.13	99.18	110.41
1	A	371	LEU	N-CA-C	-8.67	95.90	109.07
1	A	280	SER	N-CA-C	5.98	118.50	109.41
1	A	231	LYS	N-CA-C	-5.80	105.46	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2595	0	2565	108	0
1	B	2468	0	2449	104	0
2	A	69	36	36	5	0
2	B	23	12	12	0	0
3	A	55	0	0	2	0
3	B	51	0	0	1	0
All	All	5261	48	5062	206	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 20.

All (206) 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:138:ARG:HH11	1:B:138:ARG:CG	1.60	1.14
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.16	1.13
1:A:256:SER:HB3	1:A:351:MET:HE2	1.32	1.11
1:A:77:ILE:HD11	1:B:77:ILE:CD1	1.79	1.11
1:A:77:ILE:CD1	1:B:77:ILE:HD11	1.81	1.09
1:B:138:ARG:HH11	1:B:138:ARG:HG2	0.97	1.08
1:A:256:SER:HB3	1:A:351:MET:CE	1.93	0.98
1:B:37:ARG:HH11	1:B:37:ARG:HG2	1.25	0.97
1:A:372:THR:O	1:A:372:THR:HG22	1.63	0.96
1:A:268:VAL:HG12	1:A:404:SER:HB2	1.47	0.95
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.48	0.94
1:B:250:LEU:HD22	1:B:363:TYR:CD2	2.06	0.89
1:B:138:ARG:HG2	1:B:138:ARG:NH1	1.77	0.88
1:B:217:LEU:HB3	1:B:411:MET:HE1	1.56	0.87
1:B:268:VAL:HG13	1:B:404:SER:HB2	1.56	0.87
1:A:129:SER:OG	1:A:138:ARG:CG	2.23	0.85
1:B:337:PHE:CD1	1:B:337:PHE:O	2.30	0.85
1:B:260:PHE:CD2	1:B:415:LEU:HD11	2.12	0.84
1:A:229:LYS:O	1:A:232:ALA:HB3	1.80	0.81
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.10	0.81
1:A:127:ILE:CG2	1:A:128:ASN:N	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLU:HG3	1:B:241:ASN:HB2	1.62	0.81
1:A:141:THR:HG22	1:A:142:THR:O	1.81	0.80
1:A:343:ASP:OD2	1:A:345:SER:HB3	1.82	0.80
1:A:357:SER:OG	1:A:358:PRO:HD2	1.82	0.80
1:B:138:ARG:NH1	1:B:138:ARG:CB	2.48	0.77
1:A:234:ASP:O	1:A:236:PRO:HD3	1.86	0.76
1:B:337:PHE:O	1:B:337:PHE:HD1	1.69	0.75
1:A:218:LYS:HG2	1:A:403:TYR:OH	1.87	0.74
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.01	0.74
1:B:138:ARG:CG	1:B:138:ARG:NH1	2.30	0.74
1:A:32:LYS:HG3	1:A:33:VAL:N	2.02	0.74
1:A:67:MET:HA	1:A:67:MET:HE2	1.70	0.74
1:B:287:ASP:OD1	1:B:290:ARG:HB2	1.88	0.74
1:A:227:SER:O	1:A:231:LYS:HG3	1.88	0.74
1:B:253:GLY:O	1:B:256:SER:N	2.22	0.73
1:B:138:ARG:HH11	1:B:138:ARG:CB	2.02	0.73
1:B:213:ARG:HH12	1:B:246:GLU:HG3	1.54	0.73
1:B:258:LYS:O	1:B:262:GLU:HG2	1.90	0.72
1:A:268:VAL:CG1	1:A:404:SER:HB2	2.19	0.72
1:B:268:VAL:CG1	1:B:404:SER:HB2	2.21	0.70
1:B:288:VAL:HG21	1:B:360:LYS:HG2	1.73	0.70
1:A:127:ILE:HG22	1:A:128:ASN:N	2.06	0.70
1:A:372:THR:O	1:A:372:THR:CG2	2.34	0.70
1:A:109:ARG:CZ	1:A:172:VAL:HG22	2.22	0.70
1:A:127:ILE:HG22	1:A:128:ASN:HB2	1.73	0.70
1:A:32:LYS:HG3	1:A:33:VAL:H	1.58	0.69
1:A:208:ARG:HH11	1:A:208:ARG:HB3	1.57	0.69
1:B:213:ARG:NH1	1:B:246:GLU:HG3	2.07	0.69
1:B:233:LYS:O	1:B:236:PRO:HD3	1.91	0.68
1:A:129:SER:OG	1:A:138:ARG:HG3	1.93	0.68
1:A:338:GLY:HA3	1:A:341:GLU:OE1	1.93	0.67
1:A:218:LYS:HD2	1:A:224:ARG:CZ	2.25	0.67
1:A:407:PHE:CD2	1:A:407:PHE:C	2.72	0.67
1:A:241:ASN:O	1:A:245:ASN:HB2	1.97	0.65
1:B:37:ARG:HG2	1:B:37:ARG:NH1	2.06	0.65
1:B:243:PHE:CE2	1:B:414:ILE:HG22	2.31	0.65
1:B:234:ASP:OD1	1:B:234:ASP:N	2.30	0.64
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.13	0.64
1:A:65:MET:HE2	1:A:67:MET:CE	2.28	0.64
1:B:250:LEU:CD2	1:B:363:TYR:CD2	2.81	0.63
1:A:141:THR:HG23	1:A:145:ARG:HA	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HG22	1:A:128:ASN:CB	2.28	0.63
1:A:407:PHE:CD2	1:A:407:PHE:O	2.52	0.62
1:A:129:SER:OG	1:A:138:ARG:HG2	1.98	0.62
1:A:32:LYS:NZ	1:A:32:LYS:HB2	2.15	0.62
1:B:260:PHE:HD2	1:B:415:LEU:HD11	1.60	0.61
1:A:415:LEU:O	1:A:416:THR:HG23	2.00	0.61
1:A:274:LEU:O	1:A:275:LYS:HB2	1.99	0.61
3:A:632:HOH:O	1:B:56:GLU:HG2	1.99	0.61
1:A:67:MET:HA	1:A:67:MET:CE	2.29	0.60
1:B:250:LEU:HD22	1:B:363:TYR:CE2	2.35	0.60
1:A:208:ARG:HH11	1:A:208:ARG:CB	2.14	0.60
1:A:217:LEU:CD1	1:A:414:ILE:CD1	2.78	0.60
1:B:118:GLN:O	1:B:122:THR:HB	2.02	0.60
1:A:242:ASP:O	1:A:246:GLU:HG2	2.01	0.60
1:B:257:LYS:HG3	1:B:258:LYS:N	2.16	0.60
1:B:411:MET:O	1:B:414:ILE:HG12	2.01	0.60
1:A:219:GLY:N	1:A:240:ASP:OD2	2.34	0.60
1:A:141:THR:CG2	1:A:145:ARG:HA	2.31	0.59
1:B:250:LEU:CD2	1:B:363:TYR:CE2	2.85	0.59
1:B:214:LYS:HE3	1:B:237:THR:OG1	2.02	0.59
1:B:182:GLN:O	1:B:201:THR:HG22	2.03	0.59
1:B:231:LYS:HE3	1:B:238:PHE:HE2	1.67	0.59
1:A:119:ASN:HB3	1:A:123:ARG:NH1	2.18	0.58
1:B:230:GLU:O	1:B:233:LYS:HG3	2.04	0.58
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.69	0.58
1:A:407:PHE:O	1:A:411:MET:HG2	2.04	0.57
1:A:230:GLU:O	1:A:233:LYS:HG3	2.05	0.57
1:B:265:LYS:HG3	1:B:408:ASN:HD21	1.70	0.56
1:A:216:ASP:O	1:A:224:ARG:NH2	2.38	0.56
1:B:37:ARG:CG	1:B:37:ARG:NH1	2.65	0.56
1:A:65:MET:HE2	1:A:67:MET:HE3	1.86	0.56
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.36	0.55
1:B:267:ASP:O	1:B:270:PHE:HB3	2.06	0.55
1:A:249:LYS:C	1:A:250:LEU:HD23	2.32	0.55
1:B:225:GLU:HG3	1:B:241:ASN:CB	2.35	0.55
1:B:144:ASP:OD2	1:B:146:ARG:HD2	2.07	0.54
1:A:248:GLN:O	1:A:249:LYS:HG2	2.08	0.54
1:A:139:PHE:HZ	2:A:501:AMP:C4	2.25	0.54
1:B:283:VAL:HG22	1:B:365:MET:HG2	1.89	0.54
1:A:46:LEU:HD21	1:A:149:ILE:HD13	1.90	0.53
1:B:213:ARG:HH12	1:B:246:GLU:CG	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:MET:O	1:B:278:ASP:HB2	2.08	0.53
1:B:208:ARG:NH2	1:B:337:PHE:CG	2.77	0.53
1:B:231:LYS:HE3	1:B:238:PHE:CE2	2.44	0.53
1:B:238:PHE:HD2	1:B:242:ASP:OD2	1.91	0.53
1:A:268:VAL:HG12	1:A:404:SER:CB	2.32	0.53
1:B:227:SER:OG	1:B:230:GLU:HB2	2.09	0.53
1:A:268:VAL:CG1	1:A:404:SER:CB	2.87	0.53
1:B:217:LEU:CB	1:B:411:MET:HE1	2.32	0.53
1:A:234:ASP:C	1:A:236:PRO:HD3	2.34	0.52
1:A:127:ILE:HG23	1:A:128:ASN:N	2.22	0.52
1:B:238:PHE:HB3	1:B:242:ASP:HB2	1.92	0.52
1:B:288:VAL:CG2	1:B:360:LYS:HG2	2.39	0.52
1:B:86:LYS:HE2	1:B:91:SER:OG	2.09	0.52
1:A:229:LYS:O	1:A:232:ALA:CB	2.54	0.52
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.91	0.51
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.40	0.51
1:B:240:ASP:O	1:B:244:LEU:HG	2.11	0.51
1:A:370:ILE:O	1:A:370:ILE:HG13	2.10	0.51
1:A:69:ASP:O	1:A:72:LYS:HG2	2.12	0.50
1:B:281:LEU:HD12	1:B:366:ALA:O	2.12	0.50
1:B:268:VAL:CG1	1:B:404:SER:CB	2.90	0.50
1:B:257:LYS:CG	1:B:258:LYS:N	2.74	0.50
1:A:43:LEU:HD21	1:A:140:LEU:HD11	1.95	0.49
1:B:264:LEU:HD21	1:B:411:MET:HB2	1.93	0.49
1:B:224:ARG:NH2	1:B:239:LYS:HE2	2.27	0.49
1:B:231:LYS:CE	1:B:238:PHE:HE2	2.25	0.49
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.93	0.49
1:B:86:LYS:NZ	3:B:638:HOH:O	2.36	0.49
1:A:65:MET:HE2	1:A:67:MET:HE1	1.94	0.49
1:A:69:ASP:HA	1:A:72:LYS:HD3	1.95	0.49
1:A:231:LYS:HA	1:A:236:PRO:HB3	1.95	0.49
1:B:251:HIS:C	1:B:252:VAL:CG1	2.86	0.49
1:B:287:ASP:OD1	1:B:290:ARG:CB	2.60	0.49
1:A:415:LEU:O	1:A:416:THR:CG2	2.60	0.49
1:B:260:PHE:HD2	1:B:415:LEU:CD1	2.25	0.49
1:B:94:LYS:HB2	1:B:190:THR:HB	1.94	0.48
1:A:358:PRO:HG2	1:A:359:LYS:H	1.78	0.48
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.69	0.48
1:A:354:HIS:O	1:A:355:GLU:C	2.55	0.48
1:B:138:ARG:NH1	1:B:138:ARG:HB3	2.26	0.48
1:B:42:ILE:HD11	1:B:189:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HH21	1:B:239:LYS:NZ	2.12	0.48
1:B:230:GLU:O	1:B:236:PRO:HB3	2.12	0.48
1:B:139:PHE:O	1:B:139:PHE:CD1	2.67	0.48
1:B:208:ARG:NH2	1:B:337:PHE:CD1	2.82	0.48
1:A:264:LEU:HD11	1:A:407:PHE:HE2	1.78	0.47
1:B:242:ASP:N	1:B:242:ASP:OD1	2.47	0.47
1:B:218:LYS:HG3	1:B:224:ARG:NH1	2.29	0.47
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.50	0.47
1:A:233:LYS:HG3	1:A:233:LYS:H	1.52	0.46
1:A:139:PHE:CE1	2:A:501:AMP:C8	3.04	0.45
1:B:360:LYS:HE3	1:B:360:LYS:HB2	1.70	0.45
1:A:129:SER:OG	1:A:138:ARG:CD	2.65	0.45
1:A:139:PHE:CZ	2:A:501:AMP:C4	3.04	0.45
1:B:54:ILE:HG21	1:B:118:GLN:HB2	1.99	0.45
1:A:298:VAL:HG12	1:A:299:GLU:N	2.31	0.45
1:B:399:ASN:HB3	1:B:400:PRO:HD3	2.00	0.44
1:B:34:LYS:HE2	1:B:122:THR:CG2	2.47	0.44
1:B:215:TYR:CE1	1:B:243:PHE:HD1	2.36	0.44
1:B:225:GLU:HB3	1:B:242:ASP:OD1	2.18	0.43
1:B:230:GLU:C	1:B:232:ALA:N	2.76	0.43
1:A:361:GLU:OE1	1:A:363:TYR:OH	2.32	0.43
1:A:343:ASP:C	1:A:345:SER:N	2.75	0.43
1:A:407:PHE:C	1:A:407:PHE:HD2	2.25	0.43
1:B:138:ARG:CB	1:B:138:ARG:CZ	2.93	0.43
1:A:251:HIS:HA	1:A:416:THR:C	2.44	0.43
1:A:263:LYS:O	1:A:264:LEU:C	2.61	0.43
1:B:34:LYS:HE2	1:B:122:THR:HG23	1.99	0.43
1:B:165:LYS:HE2	1:B:165:LYS:HB2	1.90	0.43
1:A:86:LYS:HG2	3:A:609:HOH:O	2.19	0.43
1:A:343:ASP:C	1:A:345:SER:H	2.27	0.43
1:A:77:ILE:HD11	1:B:77:ILE:CG1	2.47	0.42
1:A:33:VAL:HG13	1:B:59:ASN:HA	2.02	0.42
1:A:243:PHE:C	1:A:243:PHE:CD2	2.97	0.42
1:B:260:PHE:CD2	1:B:415:LEU:CD1	2.94	0.42
1:A:74:TYR:CE1	1:A:76:LYS:HD3	2.54	0.42
1:B:215:TYR:CD1	1:B:243:PHE:HD1	2.36	0.42
1:B:179:LEU:HG	1:B:263:LYS:HG2	2.01	0.42
1:B:224:ARG:NH1	1:B:240:ASP:OD1	2.52	0.42
1:A:140:LEU:HB2	1:A:149:ILE:HB	2.00	0.42
1:B:87:GLU:OE1	1:B:87:GLU:HA	2.19	0.42
1:B:230:GLU:C	1:B:232:ALA:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HE3	1:A:262:GLU:OE2	2.19	0.42
1:A:127:ILE:HD13	1:A:127:ILE:HA	1.69	0.42
1:A:295:GLU:O	1:A:298:VAL:HB	2.20	0.42
1:A:32:LYS:HB2	1:A:32:LYS:HZ2	1.83	0.41
1:A:139:PHE:HE1	2:A:501:AMP:C8	2.38	0.41
1:A:160:MET:O	1:A:164:LEU:HB2	2.19	0.41
1:A:159:GLU:OE2	1:A:371:LEU:HA	2.21	0.41
1:A:354:HIS:ND1	1:A:355:GLU:N	2.69	0.41
1:A:206:SER:C	1:A:208:ARG:N	2.79	0.41
1:A:415:LEU:C	1:A:416:THR:HG23	2.46	0.41
1:B:407:PHE:O	1:B:411:MET:HG2	2.20	0.41
1:A:239:LYS:O	1:A:242:ASP:HB2	2.20	0.41
1:A:204:VAL:HG23	2:A:501:AMP:C6	2.55	0.41
1:A:355:GLU:H	1:A:355:GLU:HG2	1.49	0.40
1:B:364:PHE:C	1:B:365:MET:HG3	2.46	0.40
1:A:206:SER:C	1:A:208:ARG:H	2.29	0.40
1:A:268:VAL:HG13	1:A:279:TYR:OH	2.21	0.40
1:B:124:SER:HB3	1:B:143:TYR:CG	2.56	0.40
1:B:167:TYR:O	1:B:171:ILE:HG12	2.21	0.40
1:A:268:VAL:CG1	1:A:404:SER:HA	2.51	0.40
1:B:250:LEU:HD23	1:B:363:TYR:CE2	2.57	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	305/393 (78%)	295 (97%)	8 (3%)	2 (1%)	18	13
1	B	282/393 (72%)	274 (97%)	8 (3%)	0	100	100
All	All	587/786 (75%)	569 (97%)	16 (3%)	2 (0%)	36	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PRO
1	A	358	PRO

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	293/352 (83%)	267 (91%)	26 (9%)	9	5
1	B	278/352 (79%)	257 (92%)	21 (8%)	12	8
All	All	571/704 (81%)	524 (92%)	47 (8%)	10	6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	67	MET
1	A	127	ILE
1	A	128	ASN
1	A	141	THR
1	A	202	ARG
1	A	206	SER
1	A	208	ARG
1	A	220	SER
1	A	225	GLU
1	A	233	LYS
1	A	251	HIS
1	A	275	LYS
1	A	295	GLU
1	A	298	VAL
1	A	345	SER
1	A	348	VAL
1	A	351	MET
1	A	355	GLU
1	A	360	LYS
1	A	371	LEU

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Mol	Chain	Res	Type
1	A	402	GLN
1	A	406	ARG
1	A	407	PHE
1	A	409	GLU
1	A	414	ILE
1	B	32	LYS
1	B	37	ARG
1	B	104	ARG
1	B	115	GLN
1	B	122	THR
1	B	123	ARG
1	B	138	ARG
1	B	150	LYS
1	B	155	GLU
1	B	201	THR
1	B	208	ARG
1	B	230	GLU
1	B	231	LYS
1	B	234	ASP
1	B	242	ASP
1	B	246	GLU
1	B	252	VAL
1	B	268	VAL
1	B	280	SER
1	B	360	LYS
1	B	404	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	259	ASN
1	A	408	ASN
1	B	115	GLN
1	B	408	ASN

5.3.3 RNA ⓘ

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](#)

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	A	501	-	25,25,25	1.96	6 (24%)	37,38,38	1.91	9 (24%)
2	AMP	A	502	-	25,25,25	1.36	4 (16%)	37,38,38	1.95	10 (27%)
2	AMP	A	503	-	25,25,25	1.45	4 (16%)	37,38,38	1.94	11 (29%)
2	AMP	B	501	-	25,25,25	1.79	3 (12%)	37,38,38	2.19	8 (21%)

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	A	502	-	-	3/10/26/26	0/3/3/3
2	AMP	A	503	-	-	1/10/26/26	0/3/3/3
2	AMP	B	501	-	-	5/10/26/26	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	AMP	C5-C4	4.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AMP	C5-N7	-4.48	1.30	1.39
2	A	501	AMP	C5-N7	-4.47	1.30	1.39
2	A	501	AMP	C4-N9	-4.39	1.28	1.37
2	A	502	AMP	C5-C4	4.17	1.46	1.39
2	B	501	AMP	C8-N9	-4.14	1.30	1.37
2	A	501	AMP	C8-N9	-3.88	1.31	1.37
2	B	501	AMP	C4-N9	-3.80	1.29	1.37
2	A	503	AMP	C8-N7	3.12	1.37	1.31
2	A	502	AMP	C8-N7	2.55	1.36	1.31
2	A	503	AMP	C5-C6	2.47	1.47	1.41
2	A	502	AMP	C5-C6	2.46	1.47	1.41
2	A	502	AMP	C5-N7	-2.38	1.34	1.39
2	A	503	AMP	C5-N7	-2.23	1.35	1.39
2	A	501	AMP	C2'-C3'	-2.07	1.47	1.53
2	A	501	AMP	O4'-C4'	-2.05	1.40	1.45
2	A	501	AMP	C6-N1	-2.05	1.30	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	C5-C4-N3	-6.31	118.02	126.72
2	A	502	AMP	C5-C4-N3	-5.76	118.79	126.72
2	B	501	AMP	N3-C4-N9	5.58	136.66	127.17
2	A	503	AMP	C5-C4-N3	-5.46	119.20	126.72
2	A	501	AMP	C5-C4-N3	-5.17	119.60	126.72
2	B	501	AMP	C2-N3-C4	4.40	122.58	111.83
2	A	502	AMP	N3-C4-N9	4.36	134.58	127.17
2	B	501	AMP	N3-C2-N1	-4.24	122.17	128.58
2	A	503	AMP	N3-C4-N9	4.11	134.16	127.17
2	A	503	AMP	N3-C2-N1	-3.96	122.59	128.58
2	A	501	AMP	N3-C4-N9	3.94	133.87	127.17
2	B	501	AMP	C4-N9-C8	3.73	109.65	105.74
2	A	502	AMP	N3-C2-N1	-3.72	122.95	128.58
2	A	502	AMP	C2-N3-C4	3.71	120.88	111.83
2	A	503	AMP	C2-N3-C4	3.65	120.74	111.83
2	A	502	AMP	C4-C5-N7	-3.54	106.53	110.58
2	A	503	AMP	C4-C5-N7	-3.40	106.69	110.58
2	A	501	AMP	C2-N3-C4	3.30	119.88	111.83
2	A	501	AMP	C4-C5-N7	-3.07	107.07	110.58
2	A	501	AMP	O5'-P-O1P	-2.95	98.47	106.44
2	A	501	AMP	N3-C2-N1	-2.86	124.26	128.58
2	A	502	AMP	C4-N9-C8	2.81	108.68	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	AMP	C2-N1-C6	2.78	123.30	118.73
2	A	502	AMP	C5-N7-C8	2.72	107.72	103.45
2	A	501	AMP	C4-N9-C8	2.63	108.50	105.74
2	A	503	AMP	C5-N7-C8	2.61	107.55	103.45
2	B	501	AMP	C4-C5-N7	-2.60	107.61	110.58
2	A	503	AMP	C4-N9-C8	2.59	108.46	105.74
2	B	501	AMP	N9-C8-N7	-2.48	110.42	113.94
2	A	502	AMP	N9-C8-N7	-2.47	110.43	113.94
2	A	503	AMP	O3P-P-O5'	-2.45	100.28	106.67
2	A	503	AMP	N9-C8-N7	-2.32	110.64	113.94
2	A	502	AMP	C2-N1-C6	2.30	122.51	118.73
2	B	501	AMP	C5-N7-C8	2.25	106.99	103.45
2	A	502	AMP	O3P-P-O5'	-2.16	101.03	106.67
2	A	501	AMP	C6-C5-N7	2.15	136.24	132.09
2	A	501	AMP	C3'-C2'-C1'	2.09	105.41	101.46
2	A	503	AMP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	501	AMP	C5'-O5'-P-O1P
2	B	501	AMP	C5'-O5'-P-O2P
2	B	501	AMP	C5'-O5'-P-O3P
2	B	501	AMP	O4'-C4'-C5'-O5'
2	A	503	AMP	C5'-O5'-P-O1P
2	B	501	AMP	C3'-C4'-C5'-O5'

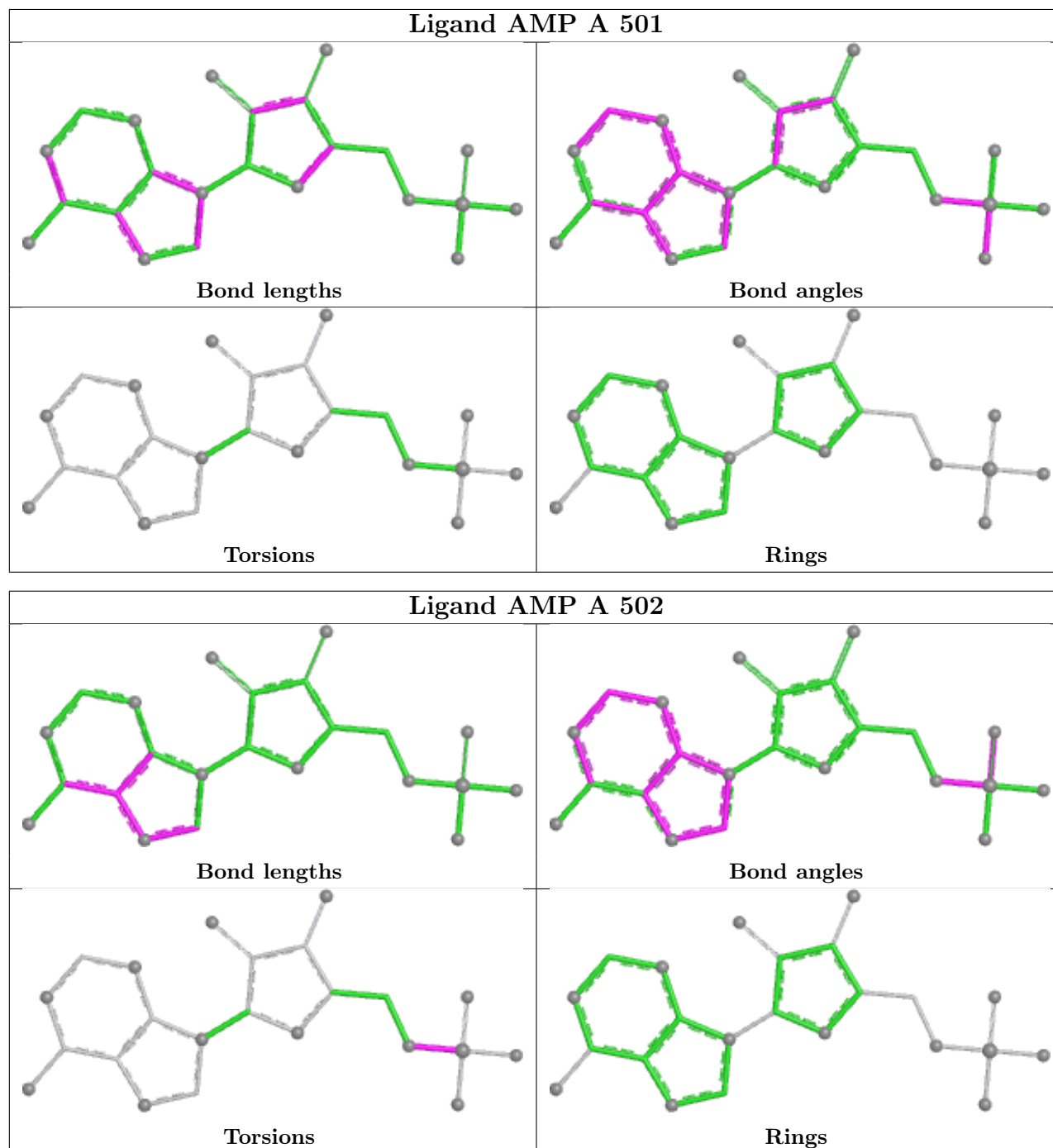
There are no ring outliers.

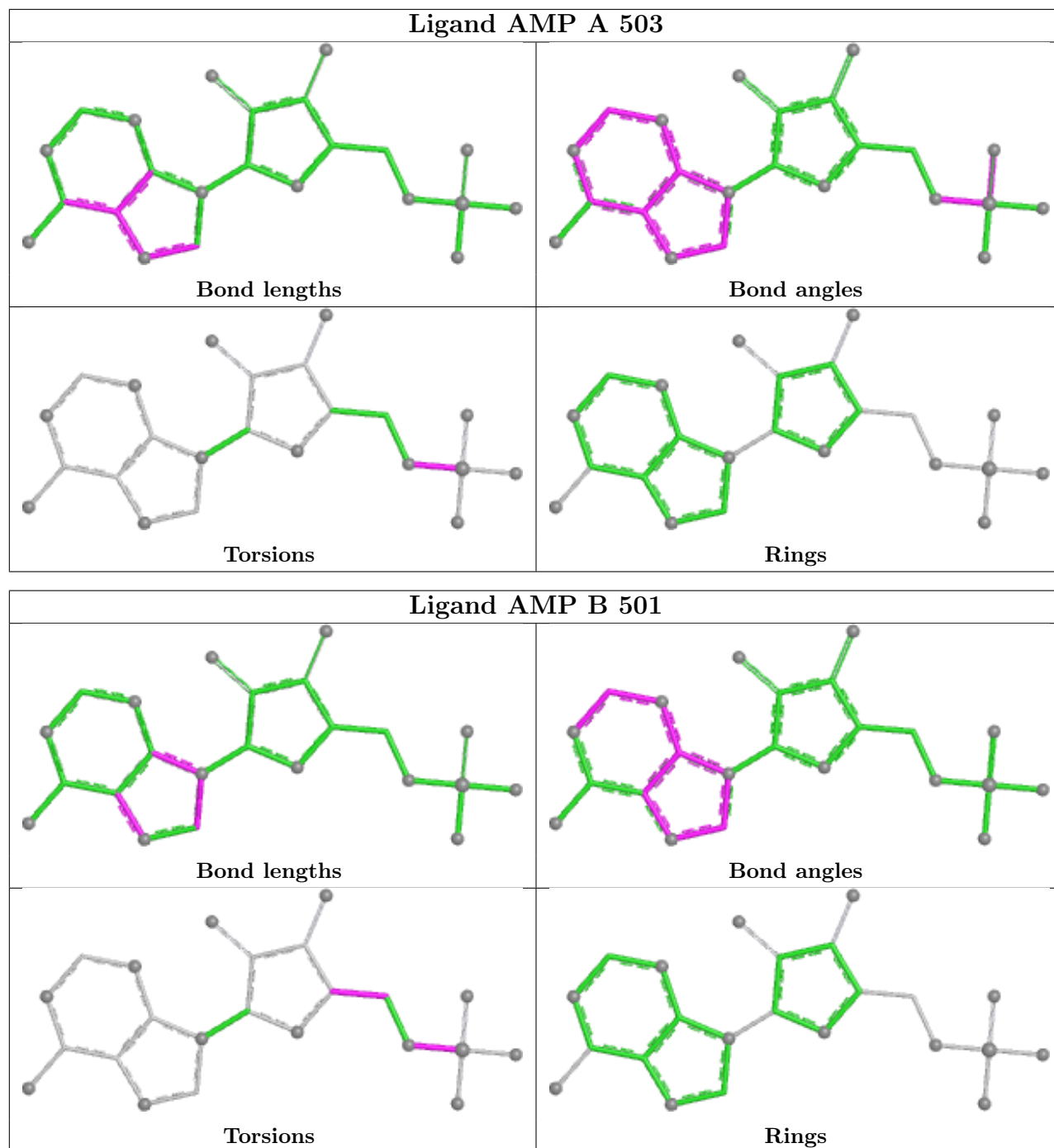
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	5	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	315/393 (80%)	0.97	53 (16%)  	30, 61, 111, 138	0
1	B	298/393 (75%)	1.03	51 (17%)  	32, 66, 128, 144	0
All	All	613/786 (77%)	1.00	104 (16%)  	30, 62, 122, 144	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	THR	10.8
1	B	337	PHE	8.3
1	A	220	SER	7.2
1	B	253	GLY	6.9
1	B	247	GLY	6.8
1	B	336	PHE	6.6
1	B	236	PRO	6.6
1	A	233	LYS	5.7
1	B	138	ARG	5.4
1	A	129	SER	5.2
1	B	338	GLY	5.1
1	A	138	ARG	4.8
1	A	416	THR	4.7
1	A	339	PRO	4.4
1	B	335	ARG	4.2
1	A	372	THR	4.2
1	B	139	PHE	4.2
1	A	356	SER	4.1
1	A	354	HIS	4.1
1	B	339	PRO	4.1
1	A	338	GLY	4.0
1	A	400	PRO	3.9
1	A	407	PHE	3.8
1	A	208	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	33	VAL	3.8
1	A	358	PRO	3.7
1	A	219	GLY	3.7
1	B	208	ARG	3.7
1	B	416	THR	3.6
1	B	358	PRO	3.5
1	B	238	PHE	3.4
1	B	356	SER	3.4
1	B	226	ALA	3.4
1	B	244	LEU	3.4
1	B	348	VAL	3.4
1	A	128	ASN	3.3
1	A	246	GLU	3.3
1	B	235	LEU	3.3
1	B	371	LEU	3.3
1	B	278	ASP	3.2
1	B	291	ALA	3.1
1	B	246	GLU	3.1
1	B	252	VAL	3.0
1	A	357	SER	3.0
1	A	405	LYS	3.0
1	A	304	ASP	3.0
1	B	272	ALA	3.0
1	A	232	ALA	2.9
1	B	357	SER	2.9
1	B	128	ASN	2.8
1	B	259	ASN	2.8
1	B	192	ASP	2.8
1	A	139	PHE	2.8
1	A	64	VAL	2.8
1	A	32	LYS	2.8
1	B	227	SER	2.8
1	A	355	GLU	2.8
1	A	302	ALA	2.8
1	A	172	VAL	2.8
1	B	288	VAL	2.8
1	A	244	LEU	2.7
1	B	250	LEU	2.7
1	B	245	ASN	2.7
1	B	399	ASN	2.7
1	A	247	GLY	2.6
1	A	277	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	227	SER	2.6
1	B	127	ILE	2.6
1	B	237	THR	2.6
1	B	258	LYS	2.5
1	A	344	PRO	2.4
1	B	232	ALA	2.4
1	A	371	LEU	2.4
1	B	415	LEU	2.4
1	B	251	HIS	2.4
1	B	243	PHE	2.4
1	B	229	LYS	2.3
1	A	225	GLU	2.3
1	A	401	GLU	2.3
1	B	405	LYS	2.3
1	A	413	ASN	2.3
1	A	409	GLU	2.3
1	B	354	HIS	2.3
1	A	250	LEU	2.2
1	A	175	HIS	2.2
1	A	404	SER	2.2
1	B	234	ASP	2.2
1	A	234	ASP	2.2
1	B	287	ASP	2.2
1	A	403	TYR	2.2
1	A	228	ASP	2.1
1	A	230	GLU	2.1
1	A	402	GLN	2.1
1	B	225	GLU	2.1
1	B	248	GLN	2.1
1	A	251	HIS	2.1
1	B	414	ILE	2.1
1	A	410	PHE	2.1
1	A	272	ALA	2.1
1	A	406	ARG	2.1
1	A	278	ASP	2.0
1	A	298	VAL	2.0
1	B	407	PHE	2.0
1	B	231	LYS	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 [i](#)

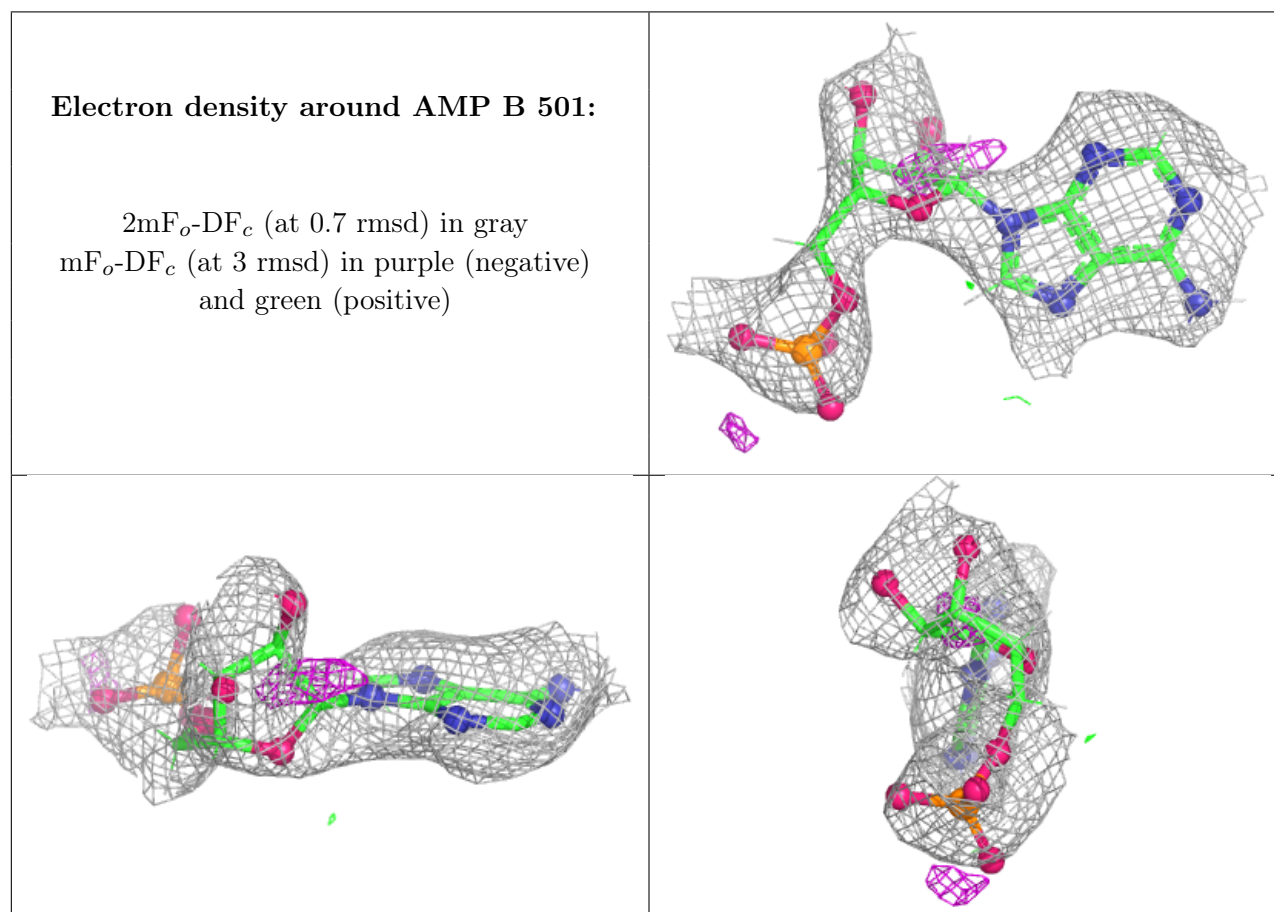
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

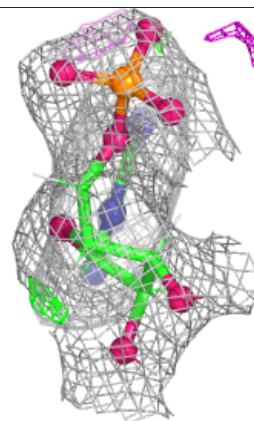
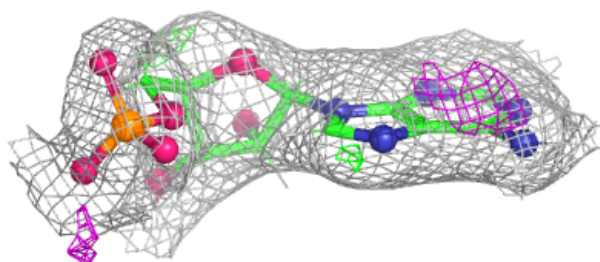
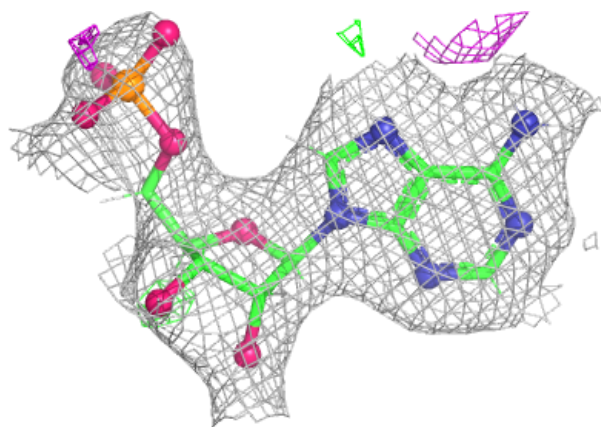
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	B	501	23/23	0.84	0.14	72,99,141,144	0
2	AMP	A	501	23/23	0.90	0.11	45,94,156,157	0
2	AMP	A	502	23/23	0.95	0.10	42,53,66,73	0
2	AMP	A	503	23/23	0.97	0.07	33,45,56,56	0

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.



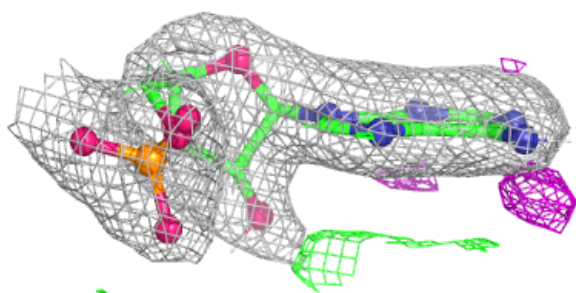
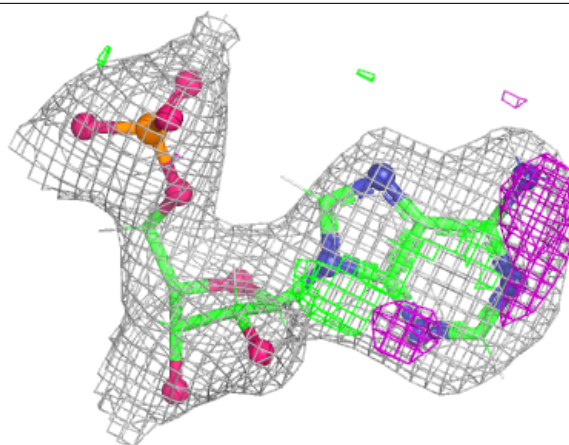
Electron density around AMP A 501:

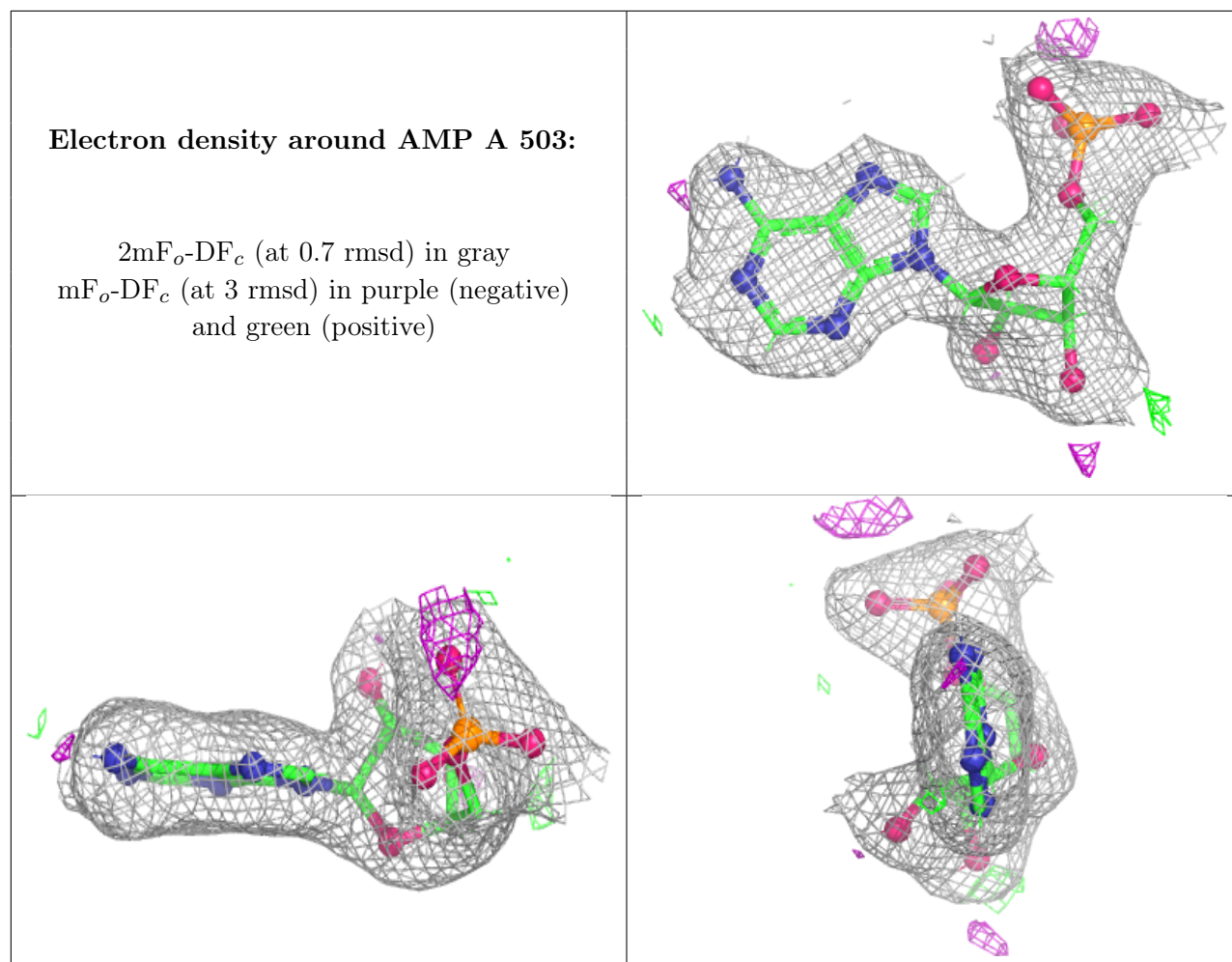
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.