



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:40 AM UTC

PDB ID : 3X0B / pdb_00003x0b
Title : Crystal structure of PIP4KIIBETA I368A 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 : 2.60 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

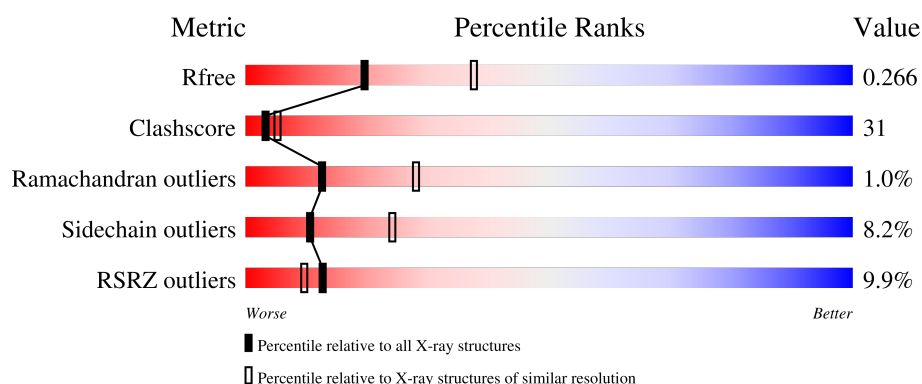
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	
1	B	393	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5273 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.

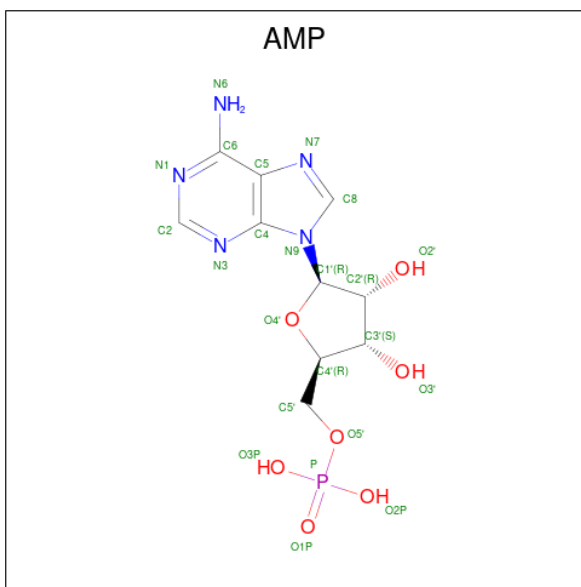
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2614	1663	446	491	14			
1	B	301	Total	C	N	O	S	0	0	0
			2485	1590	429	453	13			

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	368	ALA	ILE	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	368	ALA	ILE	engineered mutation	UNP P78356

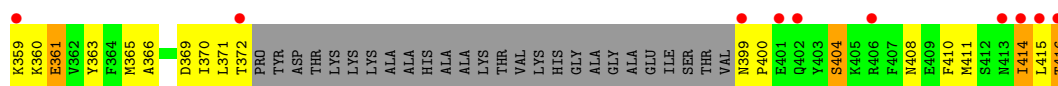
- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	13	Total	O	0	0
			13	13		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.58Å 182.14Å 107.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.99 – 2.60 52.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (52.99-2.60) 98.0 (52.99-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.282 (Not available) , 0.266	Depositor DCC
R_{free} test set	1620 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.8	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	0.92	EDS
Total number of atoms	5273	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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	0.58	0/2666	0.92	5/3585 (0.1%)
1	B	0.59	1/2536 (0.0%)	0.92	9/3407 (0.3%)
All	All	0.59	1/5202 (0.0%)	0.92	14/6992 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	HIS	C-N	-9.63	1.21	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	SER	CA-C-O	7.77	128.98	120.82
1	B	35	LEU	N-CA-C	-7.64	100.45	110.53
1	A	138	ARG	N-CA-C	6.52	119.21	111.71
1	B	213	ARG	N-CA-CB	-6.21	99.99	110.99
1	A	127	ILE	CA-C-N	-6.07	110.78	121.70
1	A	127	ILE	C-N-CA	-6.07	110.78	121.70
1	B	213	ARG	N-CA-C	6.06	118.37	108.55
1	A	125	ALA	CA-C-N	5.87	125.88	119.89
1	A	125	ALA	C-N-CA	5.87	125.88	119.89
1	B	214	LYS	N-CA-C	5.86	117.95	108.41
1	B	139	PHE	N-CA-C	5.41	117.02	107.61
1	B	139	PHE	N-CA-CB	-5.37	102.49	110.71
1	B	404	SER	N-CA-C	5.15	116.58	111.07
1	B	212	HIS	O-C-N	-5.07	116.34	122.48

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	2614	0	2584	161	0
1	B	2485	0	2469	166	0
2	A	69	36	36	3	0
2	B	23	12	12	6	0
3	A	21	0	0	1	0
3	B	13	0	0	0	0
All	All	5225	48	5101	314	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 31.

All (314) 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:215:TYR:CE2	1:B:243:PHE:HD1	1.34	1.44
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.20	1.25
1:B:215:TYR:CE2	1:B:243:PHE:CD1	2.23	1.25
1:B:252:VAL:CG1	1:B:256:SER:HB2	1.67	1.25
1:B:215:TYR:HE2	1:B:243:PHE:CD1	1.57	1.23
1:B:204:VAL:HG22	2:B:501:AMP:C2	1.78	1.16
1:A:42:ILE:HD12	1:A:42:ILE:H	1.08	1.16
1:B:243:PHE:HE2	1:B:414:ILE:CG2	1.53	1.14
1:B:411:MET:O	1:B:414:ILE:HG13	1.47	1.11
1:B:252:VAL:HG11	1:B:256:SER:HB2	1.28	1.10
1:A:398:VAL:HG13	1:A:399:ASN:N	1.69	1.08
1:B:243:PHE:CE2	1:B:414:ILE:HG21	1.87	1.07
1:B:248:GLN:O	1:B:249:LYS:HD2	1.55	1.06
1:A:398:VAL:HG22	1:A:399:ASN:HD22	1.20	1.04
1:B:204:VAL:CG2	2:B:501:AMP:C2	2.43	1.02
1:B:243:PHE:CE2	1:B:414:ILE:HG22	1.91	0.98
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.42	0.98
1:A:294:GLU:O	1:A:298:VAL:HG23	1.63	0.97
1:A:338:GLY:HA3	1:A:341:GLU:OE1	1.64	0.97
1:A:398:VAL:HG22	1:A:399:ASN:ND2	1.80	0.96
1:A:398:VAL:HG22	1:A:399:ASN:H	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:TYR:CD2	1:B:243:PHE:CD1	2.54	0.94
1:B:283:VAL:HG22	1:B:365:MET:HG2	1.50	0.92
1:B:215:TYR:CD2	1:B:243:PHE:HD1	1.85	0.92
1:B:94:LYS:HB2	1:B:190:THR:HB	1.51	0.90
1:B:416:THR:HG23	1:B:416:THR:O	1.71	0.90
1:A:268:VAL:HG12	1:A:404:SER:HB2	1.55	0.88
1:B:216:ASP:O	1:B:217:LEU:HD23	1.73	0.88
1:A:67:MET:HA	1:A:67:MET:CE	2.03	0.87
1:B:216:ASP:C	1:B:217:LEU:HD23	2.00	0.86
1:A:399:ASN:HD22	1:A:399:ASN:H	1.22	0.86
1:B:204:VAL:HG21	1:B:282:LEU:HD23	1.57	0.84
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.59	0.83
1:A:242:ASP:O	1:A:246:GLU:HG2	1.77	0.82
1:B:110:PHE:CE2	1:B:182:GLN:HG2	2.13	0.82
1:A:217:LEU:HD13	1:A:414:ILE:CD1	2.10	0.82
1:B:236:PRO:HG2	1:B:238:PHE:HE1	1.42	0.81
1:B:118:GLN:O	1:B:122:THR:HB	1.81	0.81
1:A:399:ASN:HB2	1:A:400:PRO:CD	2.10	0.81
1:A:42:ILE:H	1:A:42:ILE:CD1	1.84	0.80
1:B:359:LYS:O	1:B:361:GLU:HG2	1.82	0.80
1:B:248:GLN:O	1:B:249:LYS:CD	2.30	0.79
1:A:371:LEU:O	1:A:372:THR:CB	2.30	0.79
1:B:247:GLY:O	1:B:249:LYS:HD3	1.83	0.79
1:B:243:PHE:CZ	1:B:414:ILE:HG22	2.18	0.79
1:A:67:MET:HA	1:A:67:MET:HE2	1.63	0.78
1:B:416:THR:O	1:B:416:THR:CG2	2.30	0.78
1:A:399:ASN:ND2	1:A:402:GLN:HB2	1.99	0.78
1:A:401:GLU:O	1:A:405:LYS:HD3	1.83	0.78
1:B:243:PHE:CZ	1:B:414:ILE:CG2	2.65	0.78
1:A:398:VAL:HG21	1:A:402:GLN:CB	2.14	0.76
1:B:34:LYS:HE2	1:B:122:THR:CG2	2.14	0.76
1:B:248:GLN:C	1:B:249:LYS:HD2	2.10	0.76
1:B:411:MET:O	1:B:414:ILE:CG1	2.30	0.76
1:A:160:MET:HG2	1:A:371:LEU:HD21	1.70	0.74
1:B:160:MET:HE2	1:B:371:LEU:HD21	1.67	0.74
1:B:204:VAL:CG1	1:B:366:ALA:HB3	2.18	0.74
1:A:77:ILE:HD11	1:B:77:ILE:CD1	2.17	0.74
1:A:128:ASN:CB	1:A:140:LEU:HD23	2.18	0.73
1:A:398:VAL:CG1	1:A:399:ASN:N	2.40	0.73
1:B:415:LEU:O	1:B:416:THR:HB	1.87	0.73
1:A:96:LYS:NZ	2:A:503:AMP:O3P	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:CG2	1:A:370:ILE:O	2.34	0.73
1:A:399:ASN:ND2	1:A:402:GLN:OE1	2.20	0.73
1:A:398:VAL:HG22	1:A:399:ASN:N	2.04	0.72
1:A:77:ILE:CD1	1:B:77:ILE:HD11	2.19	0.72
1:A:371:LEU:O	1:A:372:THR:HB	1.87	0.72
1:A:398:VAL:HG13	1:A:399:ASN:H	1.53	0.72
1:B:252:VAL:HG12	1:B:252:VAL:O	1.88	0.71
1:A:42:ILE:HD12	1:A:42:ILE:N	1.94	0.71
1:A:65:MET:HE2	1:A:67:MET:HE1	1.72	0.70
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.27	0.70
1:B:224:ARG:C	1:B:225:GLU:HG3	2.14	0.70
1:B:225:GLU:HB3	1:B:242:ASP:OD1	1.91	0.70
1:A:268:VAL:HG12	1:A:404:SER:CB	2.22	0.69
1:B:252:VAL:CG1	1:B:256:SER:CB	2.61	0.69
1:A:65:MET:HE2	1:A:67:MET:CE	2.22	0.69
1:A:40:GLU:HB3	1:A:42:ILE:HD13	1.74	0.69
1:B:217:LEU:HB3	1:B:411:MET:HE1	1.75	0.69
1:B:208:ARG:HG3	1:B:209:LEU:N	2.06	0.69
1:B:283:VAL:HG22	1:B:365:MET:CG	2.24	0.68
1:B:240:ASP:OD2	1:B:410:PHE:HE1	1.76	0.68
1:B:252:VAL:HG13	1:B:256:SER:HB2	1.71	0.68
1:A:256:SER:HB3	1:A:351:MET:CE	2.25	0.67
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.32	0.67
1:B:217:LEU:CB	1:B:411:MET:HE1	2.24	0.66
1:B:248:GLN:C	1:B:249:LYS:CD	2.69	0.66
1:B:40:GLU:CD	1:B:138:ARG:HH22	2.04	0.65
1:A:399:ASN:HB2	1:A:400:PRO:HD2	1.79	0.65
1:B:243:PHE:CZ	1:B:414:ILE:HG21	2.30	0.65
1:A:399:ASN:HD21	1:A:402:GLN:HB2	1.61	0.64
1:A:128:ASN:HB2	1:A:140:LEU:HD23	1.78	0.64
1:A:67:MET:HA	1:A:67:MET:HE3	1.80	0.64
1:A:248:GLN:HG3	1:A:249:LYS:N	2.13	0.63
1:B:260:PHE:HB2	1:B:351:MET:HE1	1.79	0.63
1:B:277:MET:SD	1:B:400:PRO:HG3	2.37	0.63
1:B:281:LEU:HD12	1:B:366:ALA:O	1.98	0.63
1:B:236:PRO:HG2	1:B:238:PHE:CE1	2.30	0.63
1:A:128:ASN:HB3	1:A:140:LEU:HD23	1.81	0.63
1:A:67:MET:HE2	1:A:68:PRO:HD3	1.80	0.63
1:B:189:LEU:HD12	1:B:189:LEU:N	2.13	0.63
1:B:179:LEU:HG	1:B:263:LYS:HG2	1.81	0.62
1:B:268:VAL:HG13	1:B:279:TYR:OH	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:OD1	1:B:290:ARG:HB2	1.99	0.62
1:B:49:GLY:HA3	1:B:95:PHE:CE1	2.35	0.62
1:A:127:ILE:HG22	1:A:128:ASN:N	2.13	0.62
1:A:217:LEU:CD1	1:A:414:ILE:CD1	2.76	0.62
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.30	0.61
1:B:264:LEU:HD12	1:B:264:LEU:O	2.00	0.61
1:A:342:PHE:CE1	1:A:352:LYS:HG3	2.36	0.61
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.30	0.61
1:A:268:VAL:CG1	1:A:404:SER:HA	2.31	0.60
1:A:399:ASN:N	1:A:399:ASN:HD22	1.93	0.60
1:A:370:ILE:O	1:A:370:ILE:HG22	2.01	0.60
1:A:398:VAL:CG1	1:A:399:ASN:H	2.12	0.60
1:B:204:VAL:HG22	2:B:501:AMP:H2	1.58	0.60
1:B:240:ASP:HB3	1:B:410:PHE:CE1	2.37	0.60
1:A:56:GLU:HG2	3:A:608:HOH:O	2.02	0.59
1:A:208:ARG:NH1	1:A:208:ARG:HB2	2.17	0.59
1:A:398:VAL:CG2	1:A:399:ASN:HD22	2.07	0.59
1:B:285:ILE:HD13	1:B:363:TYR:HD2	1.67	0.59
1:B:371:LEU:O	1:B:372:THR:HB	2.02	0.59
1:A:74:TYR:CE2	1:B:82:HIS:CB	2.85	0.59
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.84	0.59
1:A:222:VAL:HG23	1:A:223:ALA:N	2.15	0.59
1:B:34:LYS:HE2	1:B:122:THR:HG21	1.81	0.59
1:A:207:HIS:CE1	1:A:208:ARG:HG3	2.38	0.58
1:B:204:VAL:HG12	1:B:366:ALA:HB3	1.85	0.58
1:A:160:MET:CG	1:A:371:LEU:HD21	2.33	0.58
1:A:268:VAL:HG13	1:A:279:TYR:OH	2.02	0.58
1:B:40:GLU:OE1	1:B:138:ARG:NH2	2.37	0.57
1:A:398:VAL:HG21	1:A:402:GLN:HB2	1.86	0.57
1:A:398:VAL:CG2	1:A:399:ASN:H	1.94	0.57
1:A:230:GLU:O	1:A:233:LYS:HG3	2.05	0.56
1:A:155:GLU:CD	1:A:155:GLU:H	2.14	0.56
1:A:234:ASP:OD1	1:A:234:ASP:N	2.35	0.56
1:A:399:ASN:CB	1:A:400:PRO:CD	2.83	0.56
1:B:285:ILE:HD13	1:B:363:TYR:CD2	2.40	0.56
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.25	0.56
1:A:236:PRO:HB2	1:A:238:PHE:CE1	2.41	0.56
1:B:79:VAL:O	1:B:92:ARG:HA	2.06	0.56
1:B:139:PHE:C	1:B:139:PHE:CD2	2.84	0.56
1:A:250:LEU:HD22	1:A:363:TYR:CE2	2.41	0.55
1:A:128:ASN:C	1:A:128:ASN:ND2	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLY:HA3	1:A:406:ARG:HD3	1.88	0.55
1:B:204:VAL:HG23	2:B:501:AMP:N1	2.21	0.55
1:A:342:PHE:HE1	1:A:352:LYS:HG3	1.69	0.55
1:A:398:VAL:HG21	1:A:402:GLN:CG	2.37	0.55
1:A:234:ASP:C	1:A:236:PRO:HD3	2.32	0.54
1:A:234:ASP:O	1:A:236:PRO:HD3	2.08	0.54
1:B:371:LEU:O	1:B:372:THR:CB	2.55	0.54
1:A:82:HIS:HB2	1:B:74:TYR:CZ	2.43	0.54
1:A:74:TYR:CE2	1:B:82:HIS:HB3	2.44	0.53
1:B:252:VAL:CG1	1:B:252:VAL:O	2.56	0.53
1:A:141:THR:CG2	1:A:142:THR:O	2.56	0.53
1:A:264:LEU:HD11	1:A:407:PHE:HE2	1.73	0.53
1:B:157:VAL:HG13	1:B:186:MET:HE3	1.90	0.53
1:A:208:ARG:HB2	1:A:208:ARG:CZ	2.38	0.53
1:A:370:ILE:O	1:A:370:ILE:HG23	2.07	0.53
1:B:225:GLU:HA	1:B:239:LYS:HB2	1.91	0.53
1:A:74:TYR:CD2	1:B:82:HIS:HB3	2.44	0.52
1:A:278:ASP:HA	1:A:403:TYR:CZ	2.44	0.52
1:A:369:ASP:OD2	2:A:501:AMP:H4'	2.09	0.52
1:B:215:TYR:CE2	1:B:243:PHE:CE1	2.92	0.52
1:A:354:HIS:C	1:A:356:SER:H	2.17	0.52
1:B:248:GLN:OE1	1:B:249:LYS:N	2.43	0.52
1:A:399:ASN:HB2	1:A:400:PRO:HD3	1.92	0.52
1:A:411:MET:O	1:A:412:SER:C	2.52	0.52
1:A:268:VAL:HG11	1:A:404:SER:HA	1.91	0.52
1:A:398:VAL:CG2	1:A:399:ASN:ND2	2.66	0.52
1:B:246:GLU:C	1:B:248:GLN:N	2.68	0.51
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.93	0.51
1:B:240:ASP:OD2	1:B:410:PHE:CE1	2.62	0.51
1:B:277:MET:O	1:B:278:ASP:HB2	2.10	0.51
1:A:74:TYR:CZ	1:B:82:HIS:HB2	2.46	0.51
1:A:354:HIS:ND1	1:A:355:GLU:N	2.59	0.51
1:A:155:GLU:CD	1:A:155:GLU:N	2.68	0.51
1:A:128:ASN:HB3	1:A:140:LEU:CD2	2.41	0.50
1:A:41:PRO:HD2	1:A:42:ILE:HD12	1.94	0.50
1:A:67:MET:CE	1:A:67:MET:CA	2.83	0.50
1:B:215:TYR:HD2	1:B:243:PHE:CD1	2.21	0.50
1:A:241:ASN:O	1:A:245:ASN:HB2	2.12	0.50
1:A:370:ILE:HG22	1:A:371:LEU:HD13	1.93	0.50
1:B:354:HIS:CD2	1:B:355:GLU:H	2.30	0.50
1:B:246:GLU:C	1:B:248:GLN:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:VAL:HG12	1:B:404:SER:CB	2.42	0.50
1:B:337:PHE:O	1:B:338:GLY:O	2.30	0.50
1:A:368:ALA:O	1:A:369:ASP:HB2	2.11	0.49
1:B:208:ARG:CG	1:B:209:LEU:N	2.75	0.49
1:A:141:THR:HG23	1:A:142:THR:O	2.13	0.49
1:A:160:MET:O	1:A:164:LEU:HB2	2.12	0.49
1:A:215:TYR:HB2	1:A:283:VAL:HB	1.94	0.49
1:A:256:SER:HB3	1:A:351:MET:HE2	1.94	0.49
1:A:371:LEU:O	1:A:372:THR:OG1	2.30	0.49
1:B:240:ASP:HB3	1:B:410:PHE:CZ	2.47	0.49
1:A:42:ILE:CD1	1:A:42:ILE:N	2.64	0.49
1:B:215:TYR:HE2	1:B:243:PHE:CE1	2.24	0.49
1:A:77:ILE:HG12	1:B:77:ILE:HD11	1.93	0.49
1:A:350:ALA:HB2	1:A:364:PHE:CE2	2.48	0.49
1:B:217:LEU:HB2	1:B:411:MET:HE1	1.95	0.49
1:B:399:ASN:HB3	1:B:400:PRO:HD3	1.94	0.49
1:A:67:MET:HE2	1:A:68:PRO:CD	2.43	0.49
1:A:127:ILE:HG22	1:A:128:ASN:H	1.78	0.49
1:A:398:VAL:CG2	1:A:402:GLN:HB2	2.43	0.49
1:B:369:ASP:CG	2:B:501:AMP:O3'	2.56	0.49
1:A:267:ASP:O	1:A:271:LEU:HG	2.12	0.48
1:B:138:ARG:CB	1:B:151:THR:HB	2.43	0.48
1:B:337:PHE:O	1:B:338:GLY:C	2.54	0.48
1:B:208:ARG:HG3	1:B:209:LEU:HD23	1.96	0.48
1:A:40:GLU:O	1:A:41:PRO:C	2.56	0.48
1:B:245:ASN:C	1:B:247:GLY:H	2.22	0.48
1:B:138:ARG:HB2	1:B:151:THR:HB	1.95	0.48
1:A:407:PHE:CZ	1:A:411:MET:HE3	2.49	0.47
1:B:234:ASP:OD1	1:B:234:ASP:N	2.48	0.47
1:B:267:ASP:O	1:B:270:PHE:HB3	2.13	0.47
1:B:66:LEU:HD12	1:B:168:HIS:CE1	2.49	0.47
1:B:159:GLU:OE2	1:B:159:GLU:HA	2.15	0.47
1:B:257:LYS:O	1:B:261:LEU:HG	2.15	0.47
1:B:97:GLU:OE1	1:B:100:PRO:HB3	2.15	0.47
1:B:240:ASP:HB3	1:B:410:PHE:HE1	1.80	0.47
1:B:365:MET:HE3	1:B:365:MET:HB2	1.78	0.47
1:A:66:LEU:O	1:A:67:MET:HE3	2.15	0.46
1:A:161:HIS:O	1:A:162:ASN:C	2.59	0.46
1:B:179:LEU:HD12	1:B:264:LEU:HB2	1.97	0.46
1:B:214:LYS:C	1:B:215:TYR:HD1	2.22	0.46
1:B:246:GLU:O	1:B:248:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLU:C	1:B:357:SER:H	2.24	0.46
1:A:139:PHE:CD1	1:A:139:PHE:C	2.94	0.46
1:A:168:HIS:O	1:A:172:VAL:HG23	2.15	0.46
1:B:410:PHE:CD2	1:B:410:PHE:O	2.68	0.46
1:B:40:GLU:CD	1:B:138:ARG:NH2	2.73	0.46
1:A:74:TYR:CE2	1:B:82:HIS:HB2	2.51	0.46
1:B:189:LEU:N	1:B:189:LEU:CD1	2.77	0.46
1:B:215:TYR:N	1:B:215:TYR:CD1	2.81	0.46
1:A:160:MET:CE	1:A:164:LEU:HD13	2.45	0.46
1:A:94:LYS:HB2	1:A:190:THR:HB	1.98	0.46
1:B:40:GLU:H	1:B:40:GLU:HG2	1.57	0.46
1:B:110:PHE:CZ	1:B:182:GLN:HG2	2.51	0.46
1:B:215:TYR:HB3	1:B:217:LEU:HD21	1.98	0.46
1:A:174:CYS:O	1:A:177:ASN:HB2	2.16	0.45
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.51	0.45
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.83	0.45
1:A:54:ILE:HG21	1:A:118:GLN:HB2	1.97	0.45
1:A:56:GLU:CD	1:B:48:TRP:HE1	2.24	0.45
1:B:139:PHE:HD2	1:B:139:PHE:O	2.00	0.45
1:A:406:ARG:O	1:A:407:PHE:C	2.60	0.45
1:B:157:VAL:HG13	1:B:186:MET:CE	2.47	0.45
1:A:65:MET:HE2	1:A:67:MET:HE3	1.99	0.45
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.17	0.44
1:A:225:GLU:HA	1:A:239:LYS:HB2	1.99	0.44
1:A:371:LEU:HA	1:A:371:LEU:HD12	1.55	0.44
1:B:165:LYS:HE2	1:B:165:LYS:HB2	1.77	0.44
1:B:268:VAL:HG12	1:B:404:SER:HB2	1.99	0.44
1:A:105:ASN:OD1	1:A:168:HIS:NE2	2.35	0.44
1:A:127:ILE:CG2	1:A:128:ASN:N	2.80	0.44
1:B:240:ASP:O	1:B:244:LEU:HD12	2.17	0.44
1:B:224:ARG:HH21	1:B:239:LYS:NZ	2.15	0.44
1:B:34:LYS:CE	1:B:122:THR:HG21	2.48	0.44
1:B:233:LYS:O	1:B:236:PRO:HD3	2.18	0.43
1:B:236:PRO:CG	1:B:238:PHE:HE1	2.23	0.43
1:A:208:ARG:CZ	1:A:208:ARG:CB	2.96	0.43
1:A:52:HIS:NE2	1:A:77:ILE:HD13	2.33	0.43
1:A:50:VAL:HG21	1:A:121:VAL:HG11	2.00	0.43
1:A:405:LYS:HD2	1:A:405:LYS:N	2.32	0.43
1:B:43:LEU:HD21	1:B:140:LEU:HD11	2.00	0.43
1:A:251:HIS:O	1:A:353:SER:HA	2.18	0.43
1:A:354:HIS:CD2	1:A:356:SER:OG	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD12	1:A:370:ILE:HA	1.52	0.43
1:A:409:GLU:O	1:A:413:ASN:ND2	2.52	0.43
1:B:81:ASN:O	1:B:91:SER:HB3	2.18	0.43
1:B:215:TYR:HD1	1:B:215:TYR:N	2.17	0.43
1:B:236:PRO:CG	1:B:238:PHE:CE1	3.01	0.43
1:A:189:LEU:N	1:A:189:LEU:HD12	2.33	0.43
1:B:74:TYR:CE1	1:B:76:LYS:HD3	2.54	0.43
1:A:48:TRP:HB2	1:A:89:LEU:HD21	2.00	0.43
1:A:77:ILE:HD12	1:B:79:VAL:HG22	2.01	0.43
1:A:343:ASP:OD2	1:A:345:SER:OG	2.35	0.43
1:A:404:SER:O	1:A:408:ASN:HB2	2.19	0.43
1:B:49:GLY:HA3	1:B:95:PHE:CZ	2.54	0.43
1:B:160:MET:HE1	1:B:183:PHE:CE2	2.55	0.42
1:B:205:PHE:HZ	1:B:214:LYS:HG3	1.84	0.42
1:A:354:HIS:C	1:A:356:SER:N	2.77	0.42
1:B:64:VAL:HG23	1:B:65:MET:HG2	2.01	0.42
1:A:237:THR:O	1:A:237:THR:HG22	2.20	0.41
1:B:181:PRO:HG2	1:B:370:ILE:HG12	2.02	0.41
1:A:302:ALA:O	1:A:303:GLU:C	2.62	0.41
1:A:54:ILE:HD13	1:A:54:ILE:HA	1.92	0.41
1:A:202:ARG:HG3	1:A:203:ASN:N	2.35	0.41
1:B:204:VAL:HG11	1:B:366:ALA:HB3	1.99	0.41
1:B:399:ASN:N	1:B:400:PRO:CD	2.83	0.41
1:B:404:SER:O	1:B:408:ASN:HB2	2.21	0.41
1:A:204:VAL:HG23	2:A:501:AMP:C2	2.55	0.41
1:A:350:ALA:HA	1:A:363:TYR:O	2.21	0.41
1:B:96:LYS:HE2	1:B:98:TYR:CE2	2.55	0.41
1:A:74:TYR:CD1	1:A:74:TYR:C	2.98	0.41
1:A:126:PRO:C	1:A:127:ILE:HD13	2.46	0.41
1:A:41:PRO:HD2	1:A:42:ILE:CD1	2.50	0.41
1:A:256:SER:HB3	1:A:351:MET:HE1	2.01	0.41
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.51	0.41
1:B:125:ALA:HA	1:B:126:PRO:HD3	1.96	0.41
1:B:268:VAL:CG1	1:B:404:SER:HA	2.50	0.41
1:B:343:ASP:HA	1:B:344:PRO:HD2	1.91	0.41
1:B:371:LEU:HD12	1:B:371:LEU:HA	1.88	0.41
1:B:411:MET:HA	1:B:414:ILE:HD11	2.03	0.41
1:A:169:GLN:O	1:A:172:VAL:HB	2.21	0.41
1:A:49:GLY:HA3	1:A:95:PHE:CE1	2.56	0.40
1:B:40:GLU:HG3	1:B:43:LEU:HG	2.03	0.40
1:A:250:LEU:HD22	1:A:363:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASP:OD1	1:B:92:ARG:CZ	2.69	0.40
1:B:224:ARG:NH1	1:B:240:ASP:OD1	2.52	0.40
1:A:398:VAL:HG13	1:A:399:ASN:O	2.20	0.40
1:B:188:ARG:C	1:B:189:LEU:HD12	2.46	0.40
1:B:45:VAL:HG12	1:B:189:LEU:HD23	2.04	0.40
1:B:204:VAL:CG2	2:B:501:AMP:N1	2.73	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	308/393 (78%)	290 (94%)	16 (5%)	2 (1%)	21	42
1	B	287/393 (73%)	267 (93%)	16 (6%)	4 (1%)	9	19
All	All	595/786 (76%)	557 (94%)	32 (5%)	6 (1%)	12	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLY
1	A	339	PRO
1	B	247	GLY
1	B	356	SER
1	A	355	GLU
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	294/351 (84%)	268 (91%)	26 (9%)	9	21
1	B	279/351 (80%)	258 (92%)	21 (8%)	12	28
All	All	573/702 (82%)	526 (92%)	47 (8%)	10	24

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

Mol	Chain	Res	Type
1	A	37	ARG
1	A	42	ILE
1	A	56	GLU
1	A	67	MET
1	A	72	LYS
1	A	76	LYS
1	A	77	ILE
1	A	86	LYS
1	A	128	ASN
1	A	137	THR
1	A	141	THR
1	A	234	ASP
1	A	303	GLU
1	A	304	ASP
1	A	341	GLU
1	A	348	VAL
1	A	360	LYS
1	A	370	ILE
1	A	371	LEU
1	A	397	THR
1	A	398	VAL
1	A	399	ASN
1	A	402	GLN
1	A	404	SER
1	A	406	ARG
1	A	409	GLU
1	B	40	GLU
1	B	45	VAL
1	B	104	ARG
1	B	122	THR
1	B	123	ARG
1	B	138	ARG
1	B	154	SER

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Mol	Chain	Res	Type
1	B	155	GLU
1	B	178	THR
1	B	204	VAL
1	B	225	GLU
1	B	231	LYS
1	B	248	GLN
1	B	251	HIS
1	B	266	ARG
1	B	335	ARG
1	B	352	LYS
1	B	360	LYS
1	B	361	GLU
1	B	414	ILE
1	B	416	THR

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	128	ASN
1	A	207	HIS
1	A	259	ASN
1	A	399	ASN
1	A	413	ASN

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](#)

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	502	-	25,25,25	2.28	10 (40%)	37,38,38	2.04	9 (24%)
2	AMP	A	501	-	25,25,25	1.44	4 (16%)	37,38,38	2.07	12 (32%)
2	AMP	B	501	-	25,25,25	1.51	5 (20%)	37,38,38	2.25	13 (35%)
2	AMP	A	503	-	25,25,25	2.18	7 (28%)	37,38,38	2.11	10 (27%)

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	502	-	-	3/10/26/26	0/3/3/3
2	AMP	A	501	-	-	3/10/26/26	0/3/3/3
2	AMP	B	501	-	-	5/10/26/26	0/3/3/3
2	AMP	A	503	-	-	4/10/26/26	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	AMP	C5-N7	-5.32	1.29	1.39
2	A	502	AMP	C5-N7	-4.74	1.30	1.39
2	A	502	AMP	C8-N9	-4.35	1.30	1.37
2	A	502	AMP	C4-N9	-4.32	1.28	1.37
2	A	503	AMP	C8-N9	-4.32	1.30	1.37
2	A	503	AMP	C4-N9	-4.18	1.29	1.37
2	A	501	AMP	C5-N7	-3.42	1.32	1.39
2	B	501	AMP	C8-N9	-3.34	1.31	1.37
2	B	501	AMP	C5-C4	3.31	1.45	1.39
2	A	502	AMP	P-O3P	-3.27	1.42	1.54
2	A	501	AMP	C5-C4	3.26	1.44	1.39
2	B	501	AMP	C5-N7	-3.25	1.33	1.39
2	A	503	AMP	P-O2P	-3.18	1.43	1.54
2	A	502	AMP	P-O2P	-3.07	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AMP	C4-N9	-2.85	1.31	1.37
2	B	501	AMP	C4-N9	-2.80	1.31	1.37
2	A	503	AMP	P-O3P	-2.62	1.45	1.54
2	A	502	AMP	O4'-C4'	-2.58	1.39	1.45
2	A	501	AMP	C8-N9	-2.53	1.33	1.37
2	A	502	AMP	P-O1P	-2.41	1.43	1.50
2	A	502	AMP	C2'-C3'	-2.37	1.47	1.53
2	A	502	AMP	P-O5'	-2.21	1.53	1.60
2	A	503	AMP	C6-N1	-2.16	1.29	1.35
2	A	503	AMP	P-O5'	-2.09	1.53	1.60
2	A	502	AMP	C3'-C4'	-2.02	1.47	1.53
2	B	501	AMP	C5-C6	2.01	1.46	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	AMP	C5-C4-N3	-6.92	117.19	126.72
2	B	501	AMP	C5-C4-N3	-6.00	118.45	126.72
2	A	501	AMP	C5-C4-N3	-5.87	118.64	126.72
2	A	502	AMP	C5-C4-N3	-5.80	118.74	126.72
2	B	501	AMP	N3-C4-N9	5.16	135.94	127.17
2	A	503	AMP	N3-C4-N9	4.75	135.25	127.17
2	A	501	AMP	N3-C4-N9	4.65	135.08	127.17
2	A	502	AMP	N3-C4-N9	4.63	135.04	127.17
2	A	502	AMP	C2-N3-C4	4.05	121.72	111.83
2	A	502	AMP	N3-C2-N1	-4.01	122.52	128.58
2	B	501	AMP	C4-N9-C8	3.99	109.93	105.74
2	B	501	AMP	C2-N3-C4	3.90	121.35	111.83
2	A	503	AMP	C2-N3-C4	3.70	120.87	111.83
2	A	501	AMP	C2-N3-C4	3.70	120.86	111.83
2	B	501	AMP	N3-C2-N1	-3.67	123.02	128.58
2	A	501	AMP	N3-C2-N1	-3.65	123.05	128.58
2	B	501	AMP	C4-C5-N7	-3.56	106.51	110.58
2	A	503	AMP	C4-C5-N7	-3.55	106.53	110.58
2	A	501	AMP	C4-C5-N7	-3.25	106.86	110.58
2	A	502	AMP	C4-N9-C8	3.16	109.05	105.74
2	A	502	AMP	C4-C5-N7	-3.11	107.02	110.58
2	A	501	AMP	O3P-P-O5'	-3.10	98.58	106.67
2	B	501	AMP	O3P-P-O5'	-2.98	98.90	106.67
2	A	503	AMP	N3-C2-N1	-2.84	124.29	128.58
2	A	503	AMP	O3P-P-O1P	2.82	121.83	110.83
2	B	501	AMP	C5-N7-C8	2.81	107.87	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	N9-C8-N7	-2.72	110.07	113.94
2	A	501	AMP	C4-N9-C8	2.66	108.54	105.74
2	B	501	AMP	O3P-P-O2P	2.63	117.65	107.80
2	A	503	AMP	O4'-C1'-C2'	-2.51	101.25	106.62
2	A	503	AMP	C2'-C1'-N9	-2.48	107.14	113.30
2	A	501	AMP	C5-N7-C8	2.47	107.34	103.45
2	A	502	AMP	C2'-C1'-N9	-2.40	107.33	113.30
2	A	503	AMP	O4'-C1'-N9	2.28	112.47	108.09
2	A	502	AMP	N9-C8-N7	-2.22	110.79	113.94
2	A	502	AMP	C5-N7-C8	2.20	106.90	103.45
2	A	501	AMP	O3P-P-O2P	2.16	115.91	107.80
2	A	503	AMP	C5-N7-C8	2.14	106.81	103.45
2	B	501	AMP	C2-N1-C6	2.12	122.21	118.73
2	A	501	AMP	N9-C8-N7	-2.08	110.98	113.94
2	A	501	AMP	C2-N1-C6	2.08	122.15	118.73
2	B	501	AMP	C1'-N9-C8	-2.06	122.53	127.09
2	A	501	AMP	C6-C5-N7	2.03	136.00	132.09
2	B	501	AMP	C2'-C1'-N9	-2.02	108.28	113.30

There are no chirality outliers.

All (15) torsion outliers are listed below:

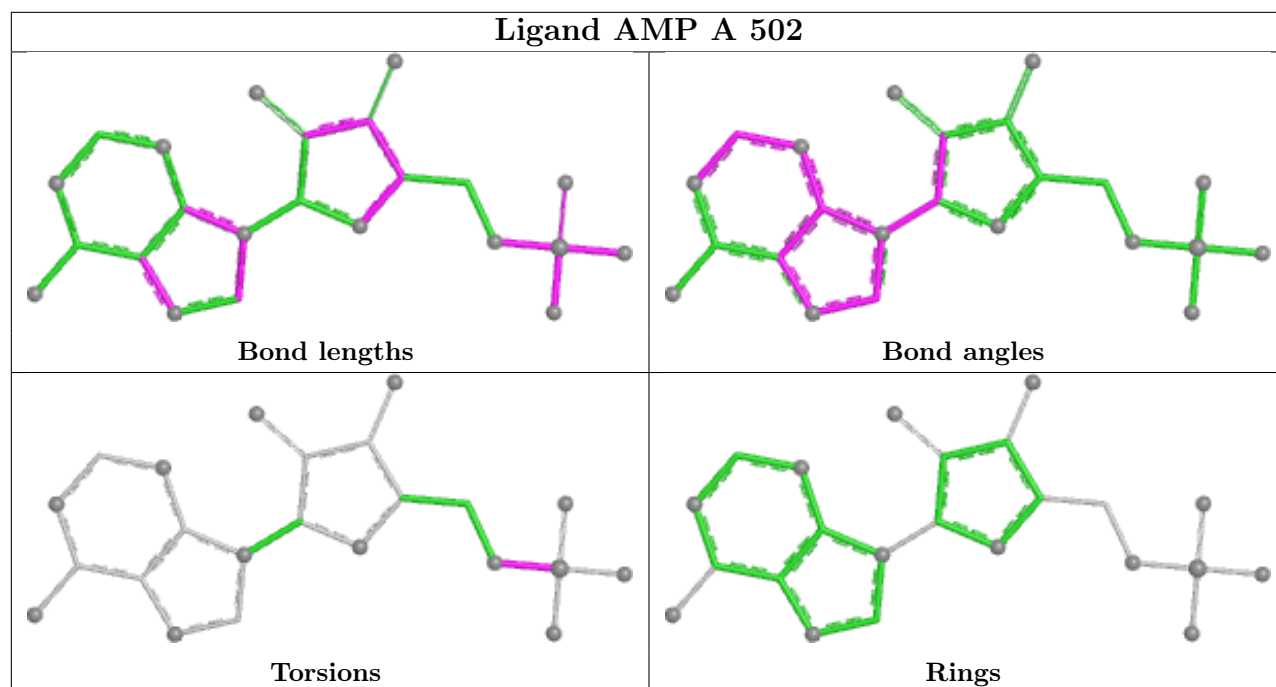
Mol	Chain	Res	Type	Atoms
2	A	501	AMP	C5'-O5'-P-O1P
2	A	501	AMP	C5'-O5'-P-O2P
2	A	501	AMP	C5'-O5'-P-O3P
2	A	502	AMP	C5'-O5'-P-O2P
2	A	502	AMP	C5'-O5'-P-O3P
2	A	503	AMP	C5'-O5'-P-O1P
2	A	503	AMP	C5'-O5'-P-O2P
2	A	503	AMP	C5'-O5'-P-O3P
2	B	501	AMP	C5'-O5'-P-O1P
2	B	501	AMP	C5'-O5'-P-O2P
2	B	501	AMP	C5'-O5'-P-O3P
2	B	501	AMP	C3'-C4'-C5'-O5'
2	A	503	AMP	O4'-C4'-C5'-O5'
2	B	501	AMP	O4'-C4'-C5'-O5'
2	A	502	AMP	C5'-O5'-P-O1P

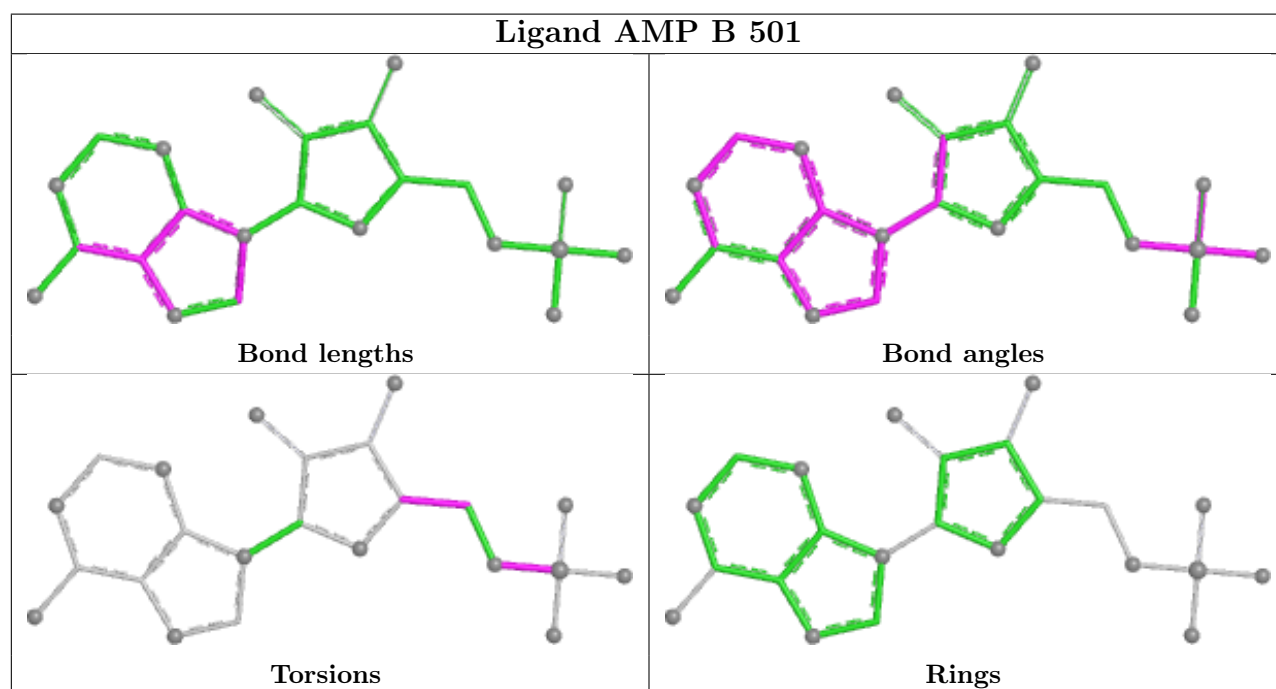
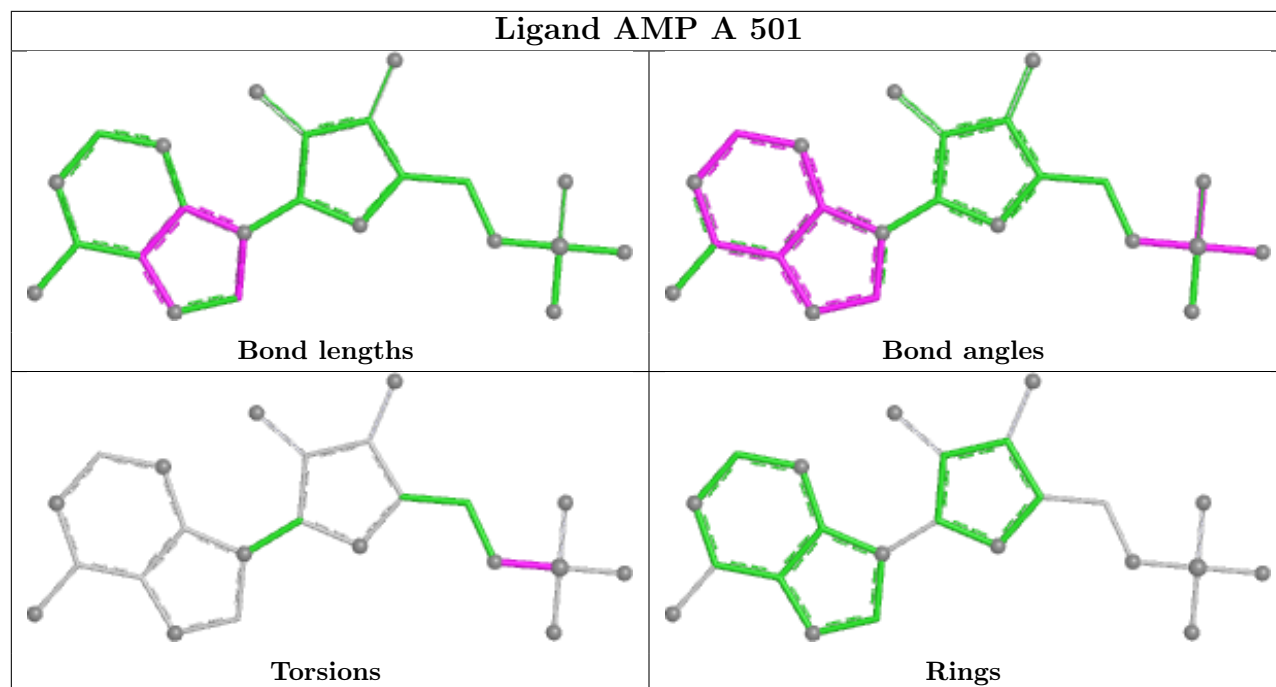
There are no ring outliers.

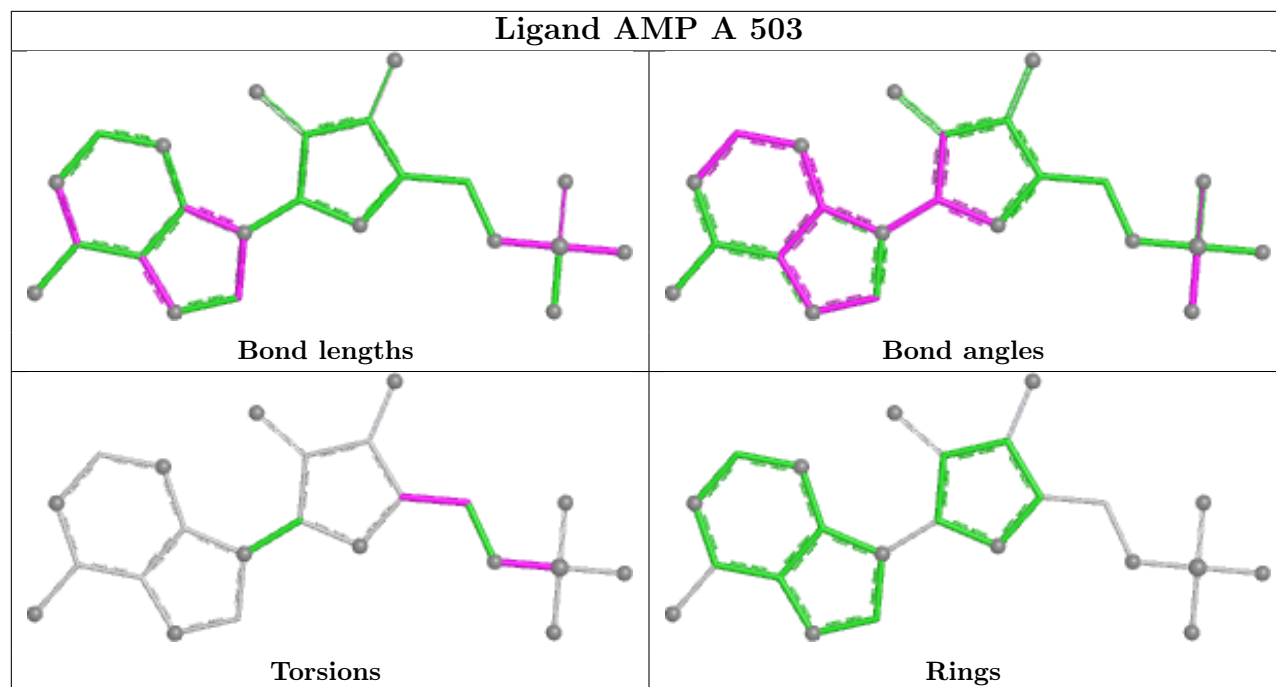
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	2	0
2	B	501	AMP	6	0
2	A	503	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	318/393 (80%)	0.62	23 (7%) 21 17	25, 70, 122, 146	0
1	B	301/393 (76%)	0.82	38 (12%) 8 6	24, 74, 138, 178	0
All	All	619/786 (78%)	0.72	61 (9%) 13 10	24, 72, 133, 178	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	GLN	7.5
1	B	416	THR	6.7
1	B	359	LYS	6.7
1	A	398	VAL	6.4
1	B	256	SER	6.3
1	B	251	HIS	5.9
1	A	138	ARG	5.8
1	A	128	ASN	5.7
1	A	137	THR	5.7
1	B	415	LEU	5.6
1	B	252	VAL	5.5
1	B	247	GLY	5.2
1	B	414	ILE	5.2
1	B	138	ARG	5.0
1	B	208	ARG	4.9
1	A	397	THR	4.5
1	B	249	LYS	4.4
1	A	372	THR	4.2
1	A	371	LEU	4.1
1	B	336	PHE	4.0
1	B	337	PHE	4.0
1	A	219	GLY	3.8
1	A	222	VAL	3.7
1	B	245	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	223	ALA	3.4
1	A	354	HIS	3.4
1	B	338	GLY	3.3
1	B	214	LYS	3.3
1	A	38	ALA	3.1
1	B	233	LYS	3.1
1	B	399	ASN	3.0
1	B	261	LEU	3.0
1	A	404	SER	2.9
1	B	406	ARG	2.8
1	B	258	LYS	2.8
1	B	35	LEU	2.7
1	B	413	ASN	2.7
1	B	128	ASN	2.6
1	B	257	LYS	2.6
1	B	401	GLU	2.5
1	A	33	VAL	2.5
1	A	40	GLU	2.4
1	A	339	PRO	2.4
1	A	32	LYS	2.3
1	B	229	LYS	2.3
1	A	228	ASP	2.3
1	A	405	LYS	2.2
1	B	259	ASN	2.2
1	B	402	GLN	2.2
1	A	297	GLU	2.2
1	B	33	VAL	2.2
1	B	248	GLN	2.2
1	B	354	HIS	2.2
1	B	242	ASP	2.1
1	A	402	GLN	2.1
1	B	335	ARG	2.1
1	B	372	THR	2.1
1	B	339	PRO	2.1
1	A	55	ASN	2.0
1	A	369	ASP	2.0
1	A	406	ARG	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](#)

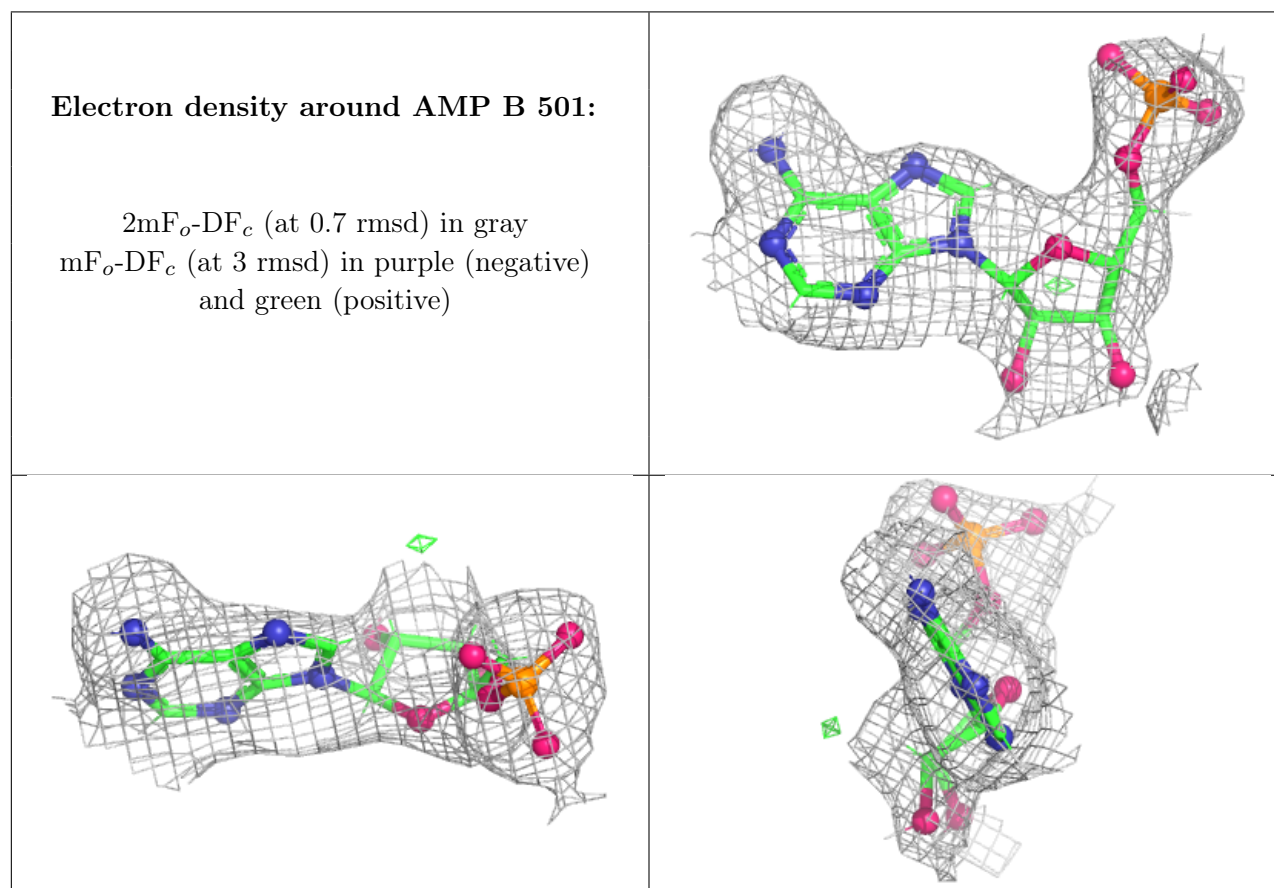
There are no oligosaccharides in this entry.

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.

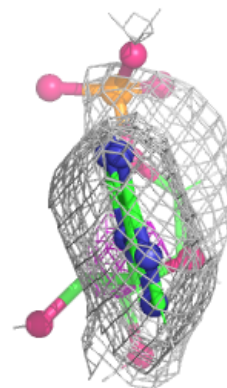
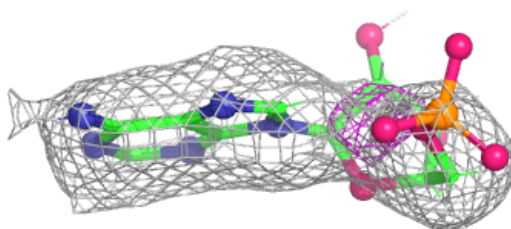
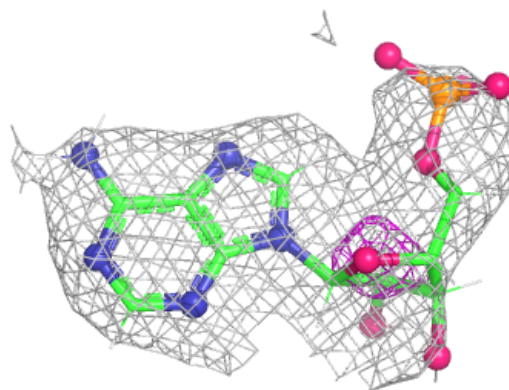
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AMP	B	501	23/23	0.78	0.14	103,136,166,169	0
2	AMP	A	501	23/23	0.84	0.12	67,142,195,197	0
2	AMP	A	502	23/23	0.93	0.09	50,67,80,90	0
2	AMP	A	503	23/23	0.94	0.09	43,68,85,90	0

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.



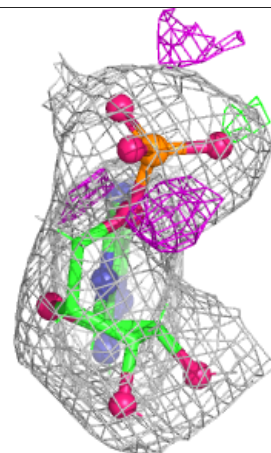
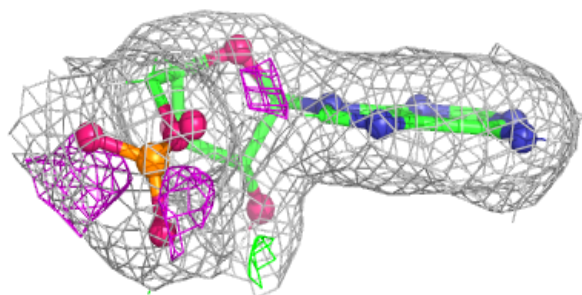
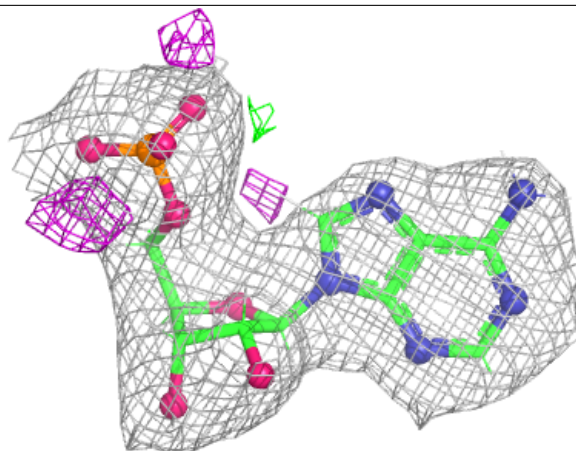
Electron density around AMP A 501:

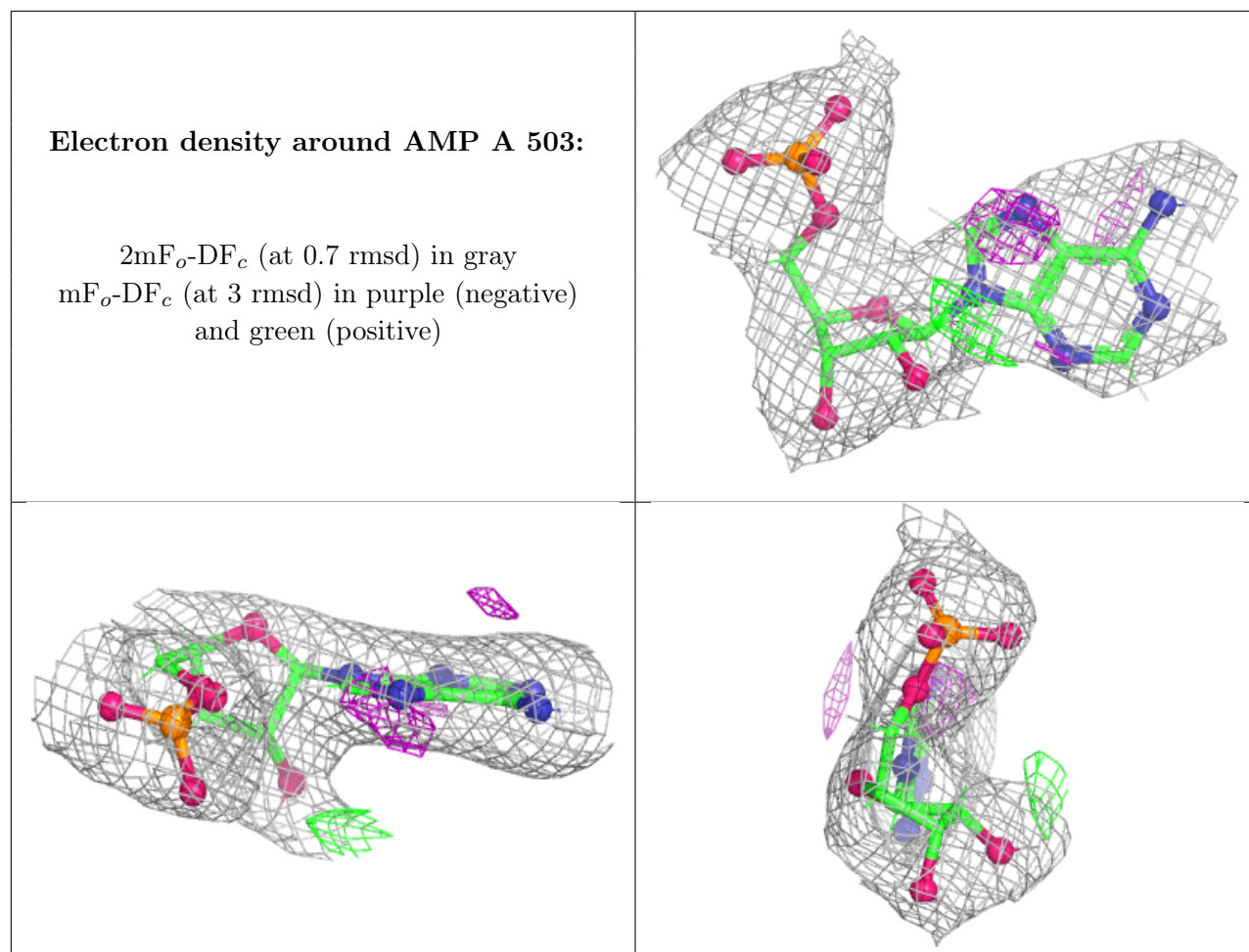
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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.