Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:22 pm BST

PDB ID	:	3X0B
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 following versions of software and data (see references ⓘ) were used in the production of this report:

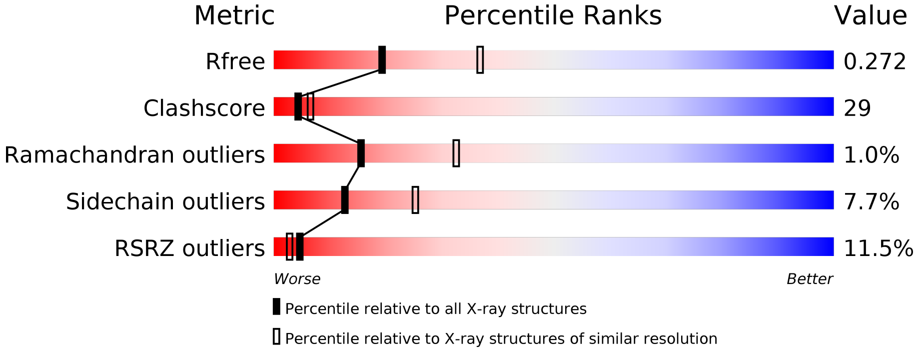
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

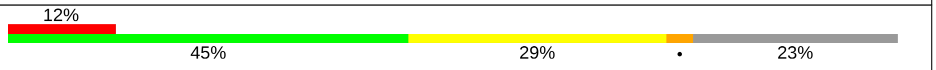
The reported resolution of this entry is 2.60 Å.

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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 <=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.

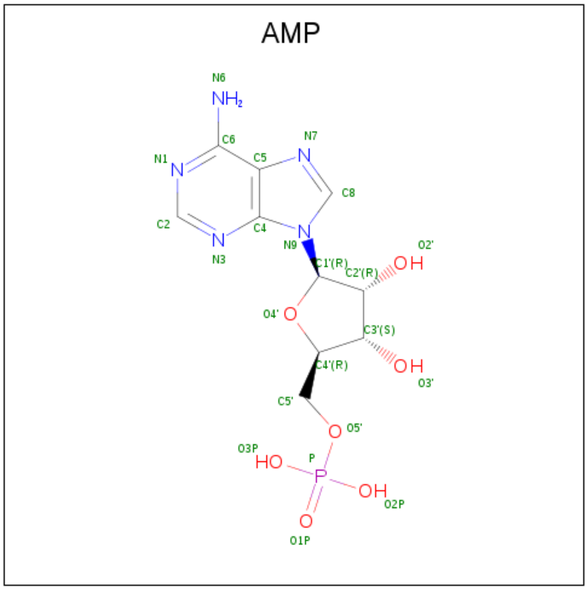
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total 2614	C 1663	N 446	O 491	S 14	0	0	0
1	B	301	Total 2485	C 1590	N 429	O 453	S 13	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	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 (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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.

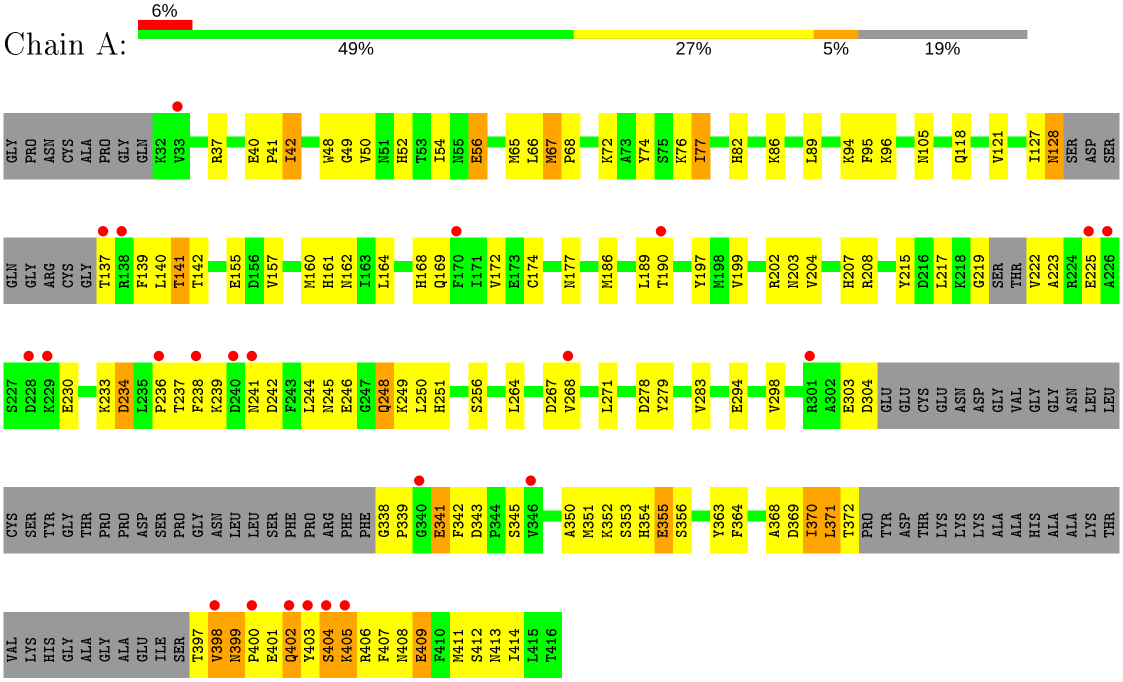
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.

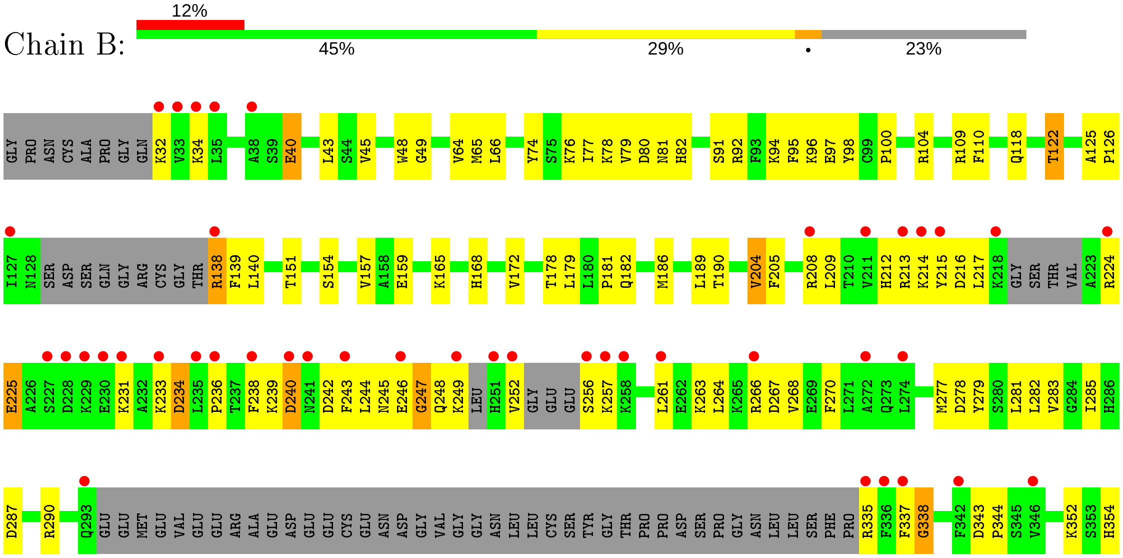
- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta

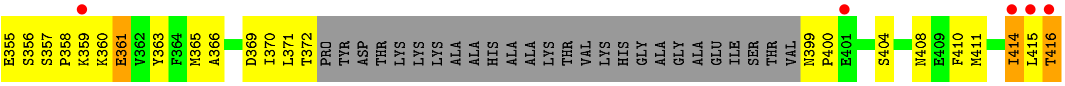
Chain A:



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

Chain B:




E355
S356
S357
P358
K359
K360
E361
V362
Y363
F364
M365
A366
D369
I370
L371
T372
PRO
TYR
ASP
THR
LYS
LYS
LYS
ALA
ALA
HIS
ALA
ALA
LYS
THR
VAL
LYS
HIS
GLY
ALA
GLY
ALA
GLU
ILE
SER
THR
VAL
N399
P400
E401
S404
N408
E409
F410
M411
I414
L415
T416

4 Data and refinement statistics (i)

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 93.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (52.99-2.60) 98.0 (93.27-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.282 0.238 , 0.272	Depositor DCC
R_{free} test set	1620 reflections (5.00%)	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 , 68.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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	0.93	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/2666	0.61	0/3585
1	B	0.47	1/2536 (0.0%)	0.62	1/3407 (0.0%)
All	All	0.47	1/5202 (0.0%)	0.61	1/6992 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	HIS	C-N	-5.49	1.21	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	213	ARG	N-CA-CB	-5.89	99.99	110.60

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	2614	0	2584	155	0
1	B	2485	0	2468	157	0
2	A	69	36	36	3	0
2	B	23	12	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	0	1	0
3	B	13	0	0	0	0
All	All	5225	48	5100	299	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 29.

All (299) 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:H	1:A:42:ILE:HD12	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
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:O	1:B:416:THR:HG23	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:A:399:ASN:H	1:A:399:ASN:HD22	1.22	0.86
1:B:204:VAL:HG21	1:B:282:LEU:HD23	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:ASP:C	1:B:217:LEU:HD23	2.00	0.81
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:CD1	1:A:42:ILE:H	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:B:416:THR:CG2	1:B:416:THR:O	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:67:MET:HA	1:A:67:MET:HE2	1.64	0.77
1:A:398:VAL:HG21	1:A:402:GLN:CB	2.14	0.76
1:A:370:ILE:O	1:A:370:ILE:CG2	2.34	0.76
1:B:34:LYS:HE2	1:B:122:THR:CG2	2.14	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: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:399:ASN:ND2	1:A:402:GLN:OE1	2.20	0.73
1:A:96:LYS:NZ	2:A:503:AMP:O3P	2.22	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:248:GLN:C	1:B:249:LYS:HD2	2.10	0.71
1:B:252:VAL:HG12	1:B:252:VAL:O	1.88	0.71
1:A:42:ILE:N	1:A:42:ILE:HD12	1.94	0.71
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:CG1	1:B:256:SER:CB	2.61	0.69
1:B:208:ARG:HG3	1:B:209:LEU:N	2.06	0.69
1:A:40:GLU:HB3	1:A:42:ILE:HD13	1.74	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:A:67:MET:HA	1:A:67:MET:HE3	1.79	0.65
1:B:224:ARG:C	1:B:225:GLU:HG3	2.14	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:127:ILE:HG22	1:A:128:ASN:N	2.13	0.64
1:A:248:GLN:HG3	1:A:249:LYS:N	2.13	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:B:189:LEU:N	1:B:189:LEU:HD12	2.13	0.63
1:A:67:MET:HE2	1:A:68:PRO:HD3	1.81	0.62
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
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:217:LEU:CD1	1:A:414:ILE:CD1	2.76	0.62
1:B:264:LEU:HD12	1:B:264:LEU:O	2.00	0.61
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.30	0.61
1:A:342:PHE:CE1	1:A:352:LYS:HG3	2.36	0.61
1:B:248:GLN:C	1:B:249:LYS:CD	2.69	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:HD22	1:A:399:ASN:N	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:40:GLU:CD	1:B:138:ARG:HH22	2.04	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: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

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:56:GLU:HG2	3:A:608:HOH:O	2.02	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: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:A:74:TYR:CE2	1:B:82:HIS:CB	2.85	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: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:A:256:SER:HB3	1:A:351:MET:HE2	1.88	0.56
1:B:79:VAL:O	1:B:92:ARG:HA	2.06	0.56
1:A:250:LEU:HD22	1:A:363:TYR:CE2	2.41	0.55
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: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: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: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:A:74:TYR:CD2	1:B:82:HIS:HB3	2.44	0.52
1:B:215:TYR:CE2	1:B:243:PHE:CE1	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:GLU:H	1:A:155:GLU:CD	2.14	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: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:B:78:LYS:HD2	1:B:94:LYS:HE2	1.93	0.51
1:A:354:HIS:ND1	1:A:355:GLU:N	2.59	0.51
1:A:74:TYR:CZ	1:B:82:HIS:HB2	2.46	0.51
1:B:139:PHE:C	1:B:139:PHE:CD2	2.84	0.51
1:A:128:ASN:C	1:A:128:ASN:ND2	2.63	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:234:ASP:C	1:A:236:PRO:HD3	2.32	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:337:PHE:O	1:B:338:GLY:O	2.30	0.50
1:B:268:VAL:HG12	1:B:404:SER:CB	2.42	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: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:350:ALA:HB2	1:A:364:PHE:CE2	2.48	0.49
1:A:77:ILE:HG12	1:B:77:ILE:HD11	1.93	0.49
1:B:399:ASN:HB3	1:B:400:PRO:HD3	1.94	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: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:A:67:MET:HE2	1:A:68:PRO:CD	2.43	0.48
1:B:208:ARG:HG3	1:B:209:LEU:HD23	1.96	0.48
1:B:138:ARG:HB2	1:B:151:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:411:MET:O	1:A:412:SER:C	2.52	0.47
1:A:66:LEU:O	1:A:67:MET:HE3	2.15	0.47
1:B:159:GLU:HA	1:B:159:GLU:OE2	2.15	0.47
1:B:66:LEU:HD12	1:B:168:HIS:CE1	2.49	0.47
1:B:257:LYS:O	1:B:261:LEU:HG	2.15	0.47
1:B:246:GLU:C	1:B:248:GLN:N	2.68	0.47
1:B:240:ASP:HB3	1:B:410:PHE:HE1	1.80	0.47
1:B:97:GLU:OE1	1:B:100:PRO:HB3	2.15	0.47
1:A:354:HIS:C	1:A:356:SER:H	2.17	0.46
1:B:179:LEU:HD12	1:B:264:LEU:HB2	1.97	0.46
1:B:246:GLU:O	1:B:248:GLN:N	2.48	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:A:155:GLU:N	1:A:155:GLU:CD	2.68	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:74:TYR:CE2	1:B:82:HIS:HB2	2.51	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:HA	1:A:244:LEU:HD23	1.83	0.45
1:A:54:ILE:HG21	1:A:118:GLN:HB2	1.97	0.45
1:A:169:GLN:HA	1:A:169:GLN:OE1	2.17	0.45
1:B:139:PHE:O	1:B:139:PHE:HD2	2.00	0.45
1:B:246:GLU:C	1:B:248:GLN:H	2.20	0.45
1:B:157:VAL:HG13	1:B:186:MET:CE	2.47	0.45
1:A:225:GLU:HA	1:A:239:LYS:HB2	1.99	0.44
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.55	0.44
1:B:165:LYS:HB2	1:B:165:LYS:HE2	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:369:ASP:CG	2:B:501:AMP:O3’	2.56	0.44
1:B:224:ARG:HH21	1:B:239:LYS:NZ	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:O	1:B:338:GLY:C	2.54	0.44
1:A:40:GLU:O	1:A:41:PRO:C	2.56	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:CB	1:A:208:ARG:CZ	2.96	0.43
1:A:52:HIS:NE2	1:A:77:ILE:HD13	2.33	0.43
1:A:405:LYS:N	1:A:405:LYS:HD2	2.32	0.43
1:A:50:VAL:HG21	1:A:121:VAL:HG11	2.00	0.43
1:B:43:LEU:HD21	1:B:140:LEU:HD11	2.00	0.43
1:B:157:VAL:HG13	1:B:186:MET:HE3	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
1:A:370:ILE:HA	1:A:370:ILE:HD12	1.52	0.43
1:A:409:GLU:O	1:A:413:ASN:ND2	2.52	0.43
1:B:215:TYR:N	1:B:215:TYR:HD1	2.17	0.43
1:B:236:PRO:CG	1:B:238:PHE:CE1	3.01	0.43
1:B:245:ASN:C	1:B:247:GLY:H	2.22	0.43
1:B:81:ASN:O	1:B:91:SER:HB3	2.18	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:A:160:MET:HB3	1:A:160:MET:HE2	1.94	0.42
1:B:205:PHE:HZ	1:B:214:LYS:HG3	1.84	0.42
1:A:161:HIS:O	1:A:162:ASN:C	2.59	0.42
1:B:64:VAL:HG23	1:B:65:MET:HG2	2.01	0.42
1:A:237:THR:HG22	1:A:237:THR:O	2.20	0.41
1:B:214:LYS:C	1:B:215:TYR:HD1	2.22	0.41
1:B:355:GLU:C	1:B:357:SER:H	2.24	0.41
1:B:181:PRO:HG2	1:B:370:ILE:HG12	2.02	0.41
1:A:139:PHE:CD1	1:A:139:PHE:C	2.94	0.41
1:A:202:ARG:HG3	1:A:203:ASN:N	2.35	0.41
1:A:54:ILE:HD13	1:A:54:ILE:HA	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:PRO:HD2	1:A:42:ILE:CD1	2.50	0.41
1:B:125:ALA:HA	1:B:126:PRO:HD3	1.96	0.41
1:B:343:ASP:HA	1:B:344:PRO:HD2	1.91	0.41
1:B:371:LEU:HA	1:B:371:LEU:HD12	1.88	0.41
1:B:411:MET:HA	1:B:414:ILE:HD11	2.03	0.41
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.51	0.41
1:B:268:VAL:CG1	1:B:404:SER:HA	2.50	0.41
1:A:169:GLN:O	1:A:172:VAL:HB	2.21	0.41
1:A:56:GLU:CD	1:B:48:TRP:HE1	2.24	0.41
1:A:399:ASN:ND2	1:A:399:ASN:N	2.64	0.40
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
1:B:224:ARG:NH1	1:B:240:ASP:OD1	2.52	0.40
1:B:80:ASP:OD1	1:B:92:ARG:CZ	2.69	0.40
1:A:398:VAL:HG13	1:A:399:ASN:O	2.20	0.40
1:B:45:VAL:HG12	1:B:189:LEU:HD23	2.04	0.40
1:A:406:ARG:O	1:A:407:PHE:C	2.60	0.40
1:A:65:MET:HE1	1:A:67:MET:HE1	2.03	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 ⓘ

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	308/393 (78%)	290 (94%)	16 (5%)	2 (1%)	25	47
1	B	287/393 (73%)	267 (93%)	16 (6%)	4 (1%)	11	22
All	All	595/786 (76%)	557 (94%)	32 (5%)	6 (1%)	15	32

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 ⓘ

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%)	269 (92%)	25 (8%)	10	21
1	B	279/351 (80%)	260 (93%)	19 (7%)	16	32
All	All	573/702 (82%)	529 (92%)	44 (8%)	13	25

All (44) 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	248	GLN
1	A	303	GLU
1	A	304	ASP
1	A	341	GLU
1	A	370	ILE

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Mol	Chain	Res	Type
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	405	LYS
1	A	409	GLU
1	B	32	LYS
1	B	40	GLU
1	B	104	ARG
1	B	122	THR
1	B	138	ARG
1	B	154	SER
1	B	178	THR
1	B	204	VAL
1	B	225	GLU
1	B	231	LYS
1	B	234	ASP
1	B	240	ASP
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	207	HIS
1	A	399	ASN
1	A	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	501	-	22,25,25	0.97	0	25,38,38	1.59	6 (24%)
2	AMP	A	502	-	22,25,25	1.93	10 (45%)	25,38,38	1.36	2 (8%)
2	AMP	A	501	-	22,25,25	1.02	1 (4%)	25,38,38	1.53	4 (16%)
2	AMP	A	503	-	22,25,25	1.81	6 (27%)	25,38,38	1.51	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	501	-	-	5/6/26/26	0/3/3/3
2	AMP	A	502	-	-	3/6/26/26	0/3/3/3
2	AMP	A	501	-	-	3/6/26/26	0/3/3/3
2	AMP	A	503	-	-	4/6/26/26	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	C4-N3	-3.48	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	AMP	C2'-C1'	-3.23	1.48	1.53
2	A	502	AMP	P-O3P	-3.16	1.42	1.54
2	A	502	AMP	C2'-C1'	-3.11	1.49	1.53
2	A	503	AMP	P-O2P	-3.08	1.43	1.54
2	A	502	AMP	P-O2P	-2.97	1.43	1.54
2	A	503	AMP	C5-N7	-2.85	1.29	1.39
2	A	502	AMP	C4-N3	-2.79	1.31	1.35
2	A	502	AMP	O4'-C4'	-2.57	1.39	1.45
2	A	502	AMP	C5-N7	-2.56	1.30	1.39
2	A	503	AMP	P-O3P	-2.53	1.45	1.54
2	A	502	AMP	P-O1P	-2.35	1.43	1.50
2	A	502	AMP	C2'-C3'	-2.33	1.47	1.53
2	A	501	AMP	O4'-C1'	2.32	1.44	1.41
2	A	502	AMP	P-O5'	-2.14	1.53	1.60
2	A	503	AMP	P-O5'	-2.02	1.53	1.60
2	A	502	AMP	C3'-C4'	-2.01	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	AMP	N3-C2-N1	-3.94	122.52	128.68
2	A	503	AMP	O4'-C1'-C2'	-3.89	101.25	106.93
2	B	501	AMP	N3-C2-N1	-3.62	123.02	128.68
2	A	501	AMP	N3-C2-N1	-3.60	123.05	128.68
2	A	501	AMP	O3P-P-O5'	-3.06	98.58	106.73
2	B	501	AMP	O3P-P-O5'	-2.94	98.90	106.73
2	A	503	AMP	O3P-P-O1P	2.85	121.83	110.68
2	A	503	AMP	N3-C2-N1	-2.81	124.29	128.68
2	B	501	AMP	C4-C5-N7	-2.78	106.51	109.40
2	A	503	AMP	C4-C5-N7	-2.75	106.53	109.40
2	B	501	AMP	O3P-P-O2P	2.62	117.65	107.64
2	B	501	AMP	C3'-C2'-C1'	2.47	104.70	100.98
2	A	501	AMP	C4-C5-N7	-2.44	106.86	109.40
2	A	502	AMP	C4-C5-N7	-2.28	107.02	109.40
2	A	501	AMP	O3P-P-O2P	2.17	115.91	107.64
2	B	501	AMP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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

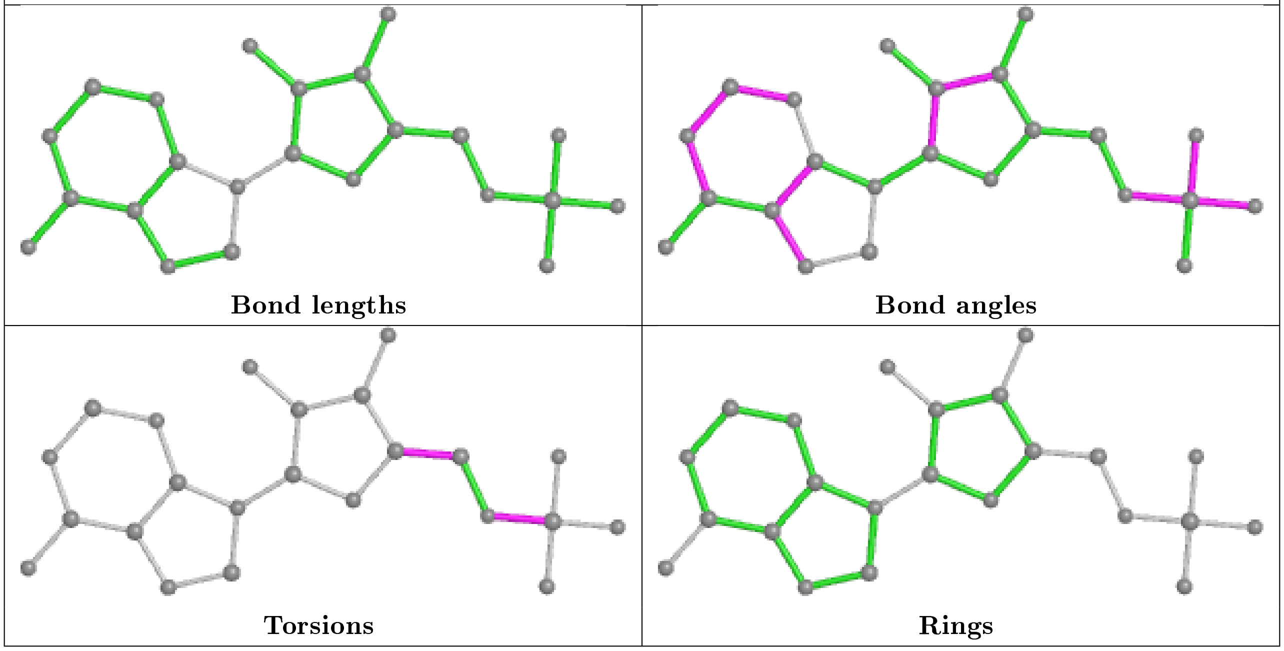
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	AMP	6	0
2	A	501	AMP	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AMP B 501



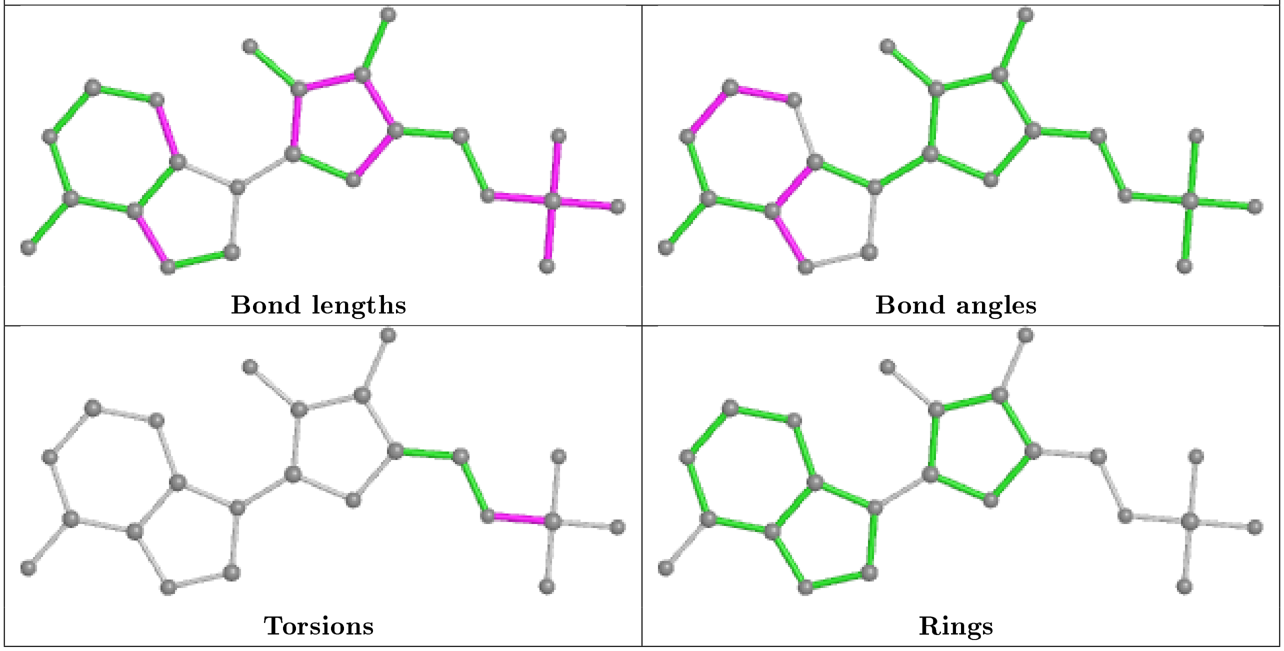
Bond lengths

Bond angles

Torsions

Rings

Ligand AMP A 502



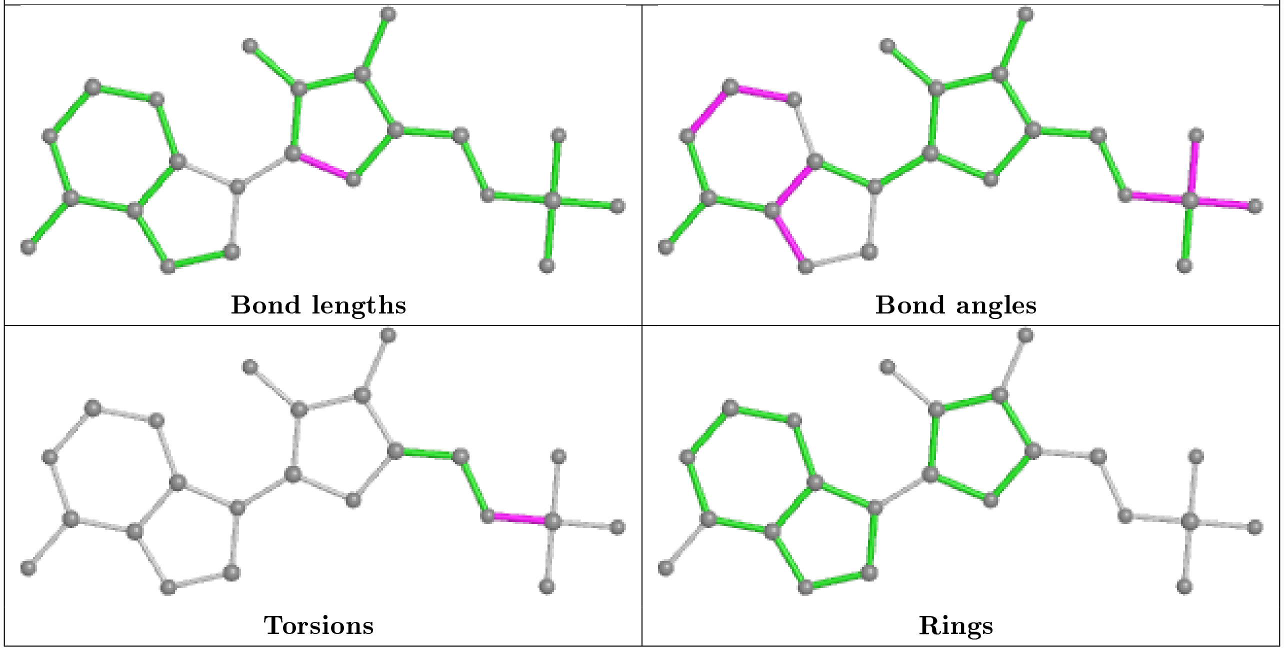
Bond lengths

Bond angles

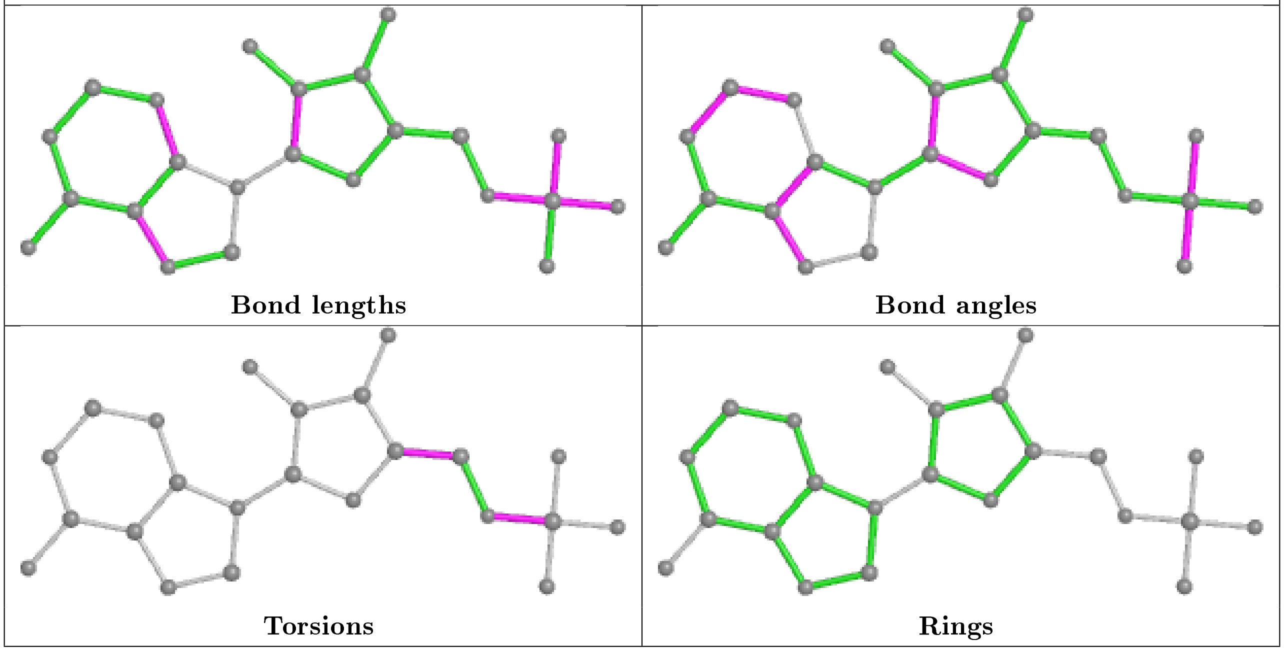
Torsions

Rings

Ligand AMP A 501



Ligand AMP A 503



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	318/393 (80%)	0.93	23 (7%)	15	11	25, 70, 122, 146	0
1	B	301/393 (76%)	1.11	48 (15%)	1	1	24, 74, 138, 178	0
All	All	619/786 (78%)	1.02	71 (11%)	4	3	24, 72, 133, 178	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	336	PHE	6.8
1	B	251	HIS	6.8
1	B	359	LYS	4.9
1	B	233	LYS	4.7
1	B	230	GLU	4.3
1	A	229	LYS	4.2
1	B	257	LYS	3.9
1	B	249	LYS	3.8
1	B	241	ASN	3.7
1	B	416	THR	3.7
1	A	301	ARG	3.6
1	B	274	LEU	3.6
1	A	138	ARG	3.5
1	A	241	ASN	3.5
1	B	235	LEU	3.5
1	A	402	GLN	3.5
1	A	398	VAL	3.4
1	B	415	LEU	3.4
1	B	214	LYS	3.4
1	A	137	THR	3.3
1	B	293	GLN	3.3
1	A	228	ASP	3.3
1	B	243	PHE	3.2
1	B	32	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	3.1
1	B	261	LEU	3.0
1	B	215	TYR	3.0
1	B	258	LYS	3.0
1	B	246	GLU	3.0
1	A	403	TYR	3.0
1	B	236	PRO	3.0
1	B	335	ARG	2.8
1	B	33	VAL	2.8
1	B	127	ILE	2.8
1	A	226	ALA	2.8
1	B	256	SER	2.7
1	B	401	GLU	2.7
1	B	229	LYS	2.7
1	B	238	PHE	2.7
1	B	138	ARG	2.6
1	B	228	ASP	2.6
1	B	211	VAL	2.6
1	B	231	LYS	2.6
1	A	346	VAL	2.6
1	A	238	PHE	2.6
1	A	404	SER	2.5
1	A	340	GLY	2.5
1	B	35	LEU	2.5
1	B	337	PHE	2.5
1	B	224	ARG	2.5
1	B	208	ARG	2.4
1	A	400	PRO	2.4
1	A	240	ASP	2.4
1	B	38	ALA	2.4
1	B	266	ARG	2.4
1	B	272	ALA	2.3
1	B	342	PHE	2.2
1	B	227	SER	2.2
1	B	414	ILE	2.2
1	B	240	ASP	2.1
1	B	346	VAL	2.1
1	B	34	LYS	2.1
1	A	405	LYS	2.0
1	A	236	PRO	2.0
1	A	225	GLU	2.0
1	A	190	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	33	VAL	2.0
1	A	268	VAL	2.0
1	B	213	ARG	2.0
1	B	218	LYS	2.0
1	A	170	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

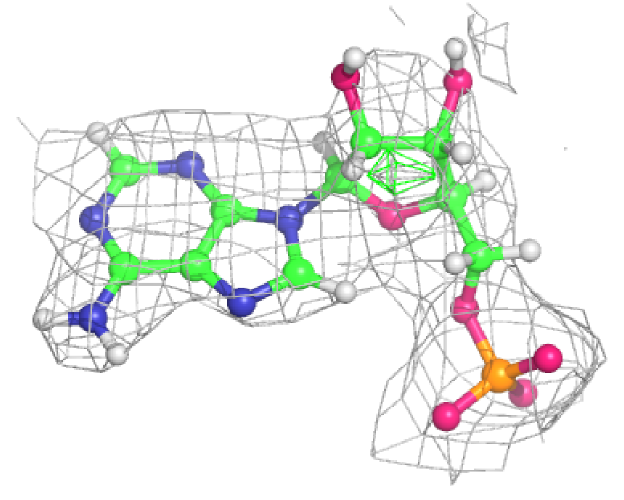
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled '$Q< 0.9$'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

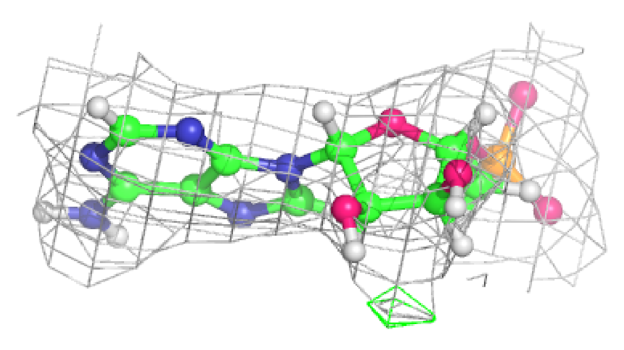
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	AMP	B	501	23/23	0.74	0.19	103,136,166,169	0
2	AMP	A	501	23/23	0.77	0.25	67,142,195,197	0
2	AMP	A	502	23/23	0.94	0.19	50,67,80,90	0
2	AMP	A	503	23/23	0.94	0.21	43,68,85,90	0

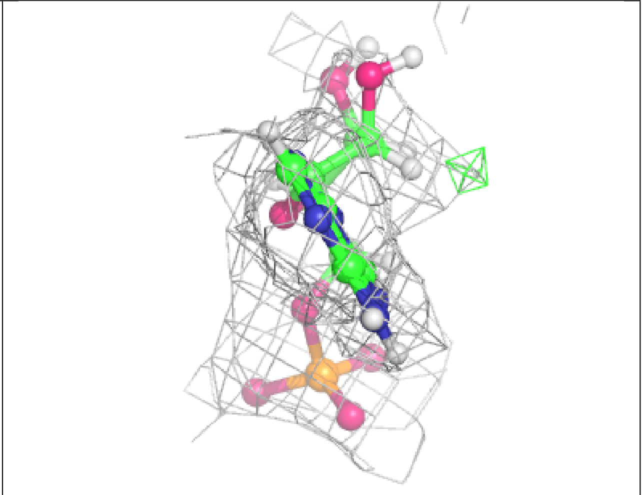
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

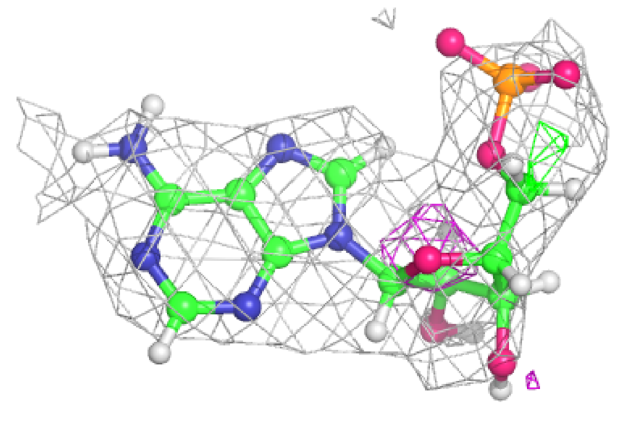


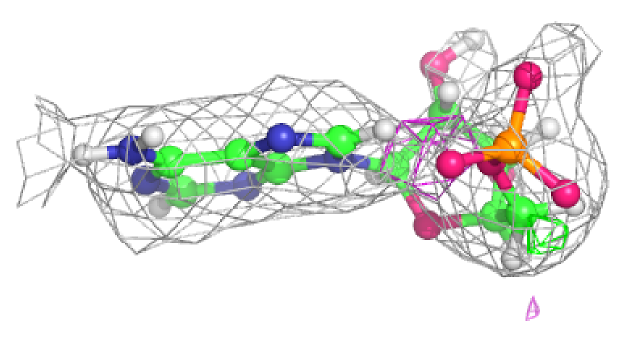


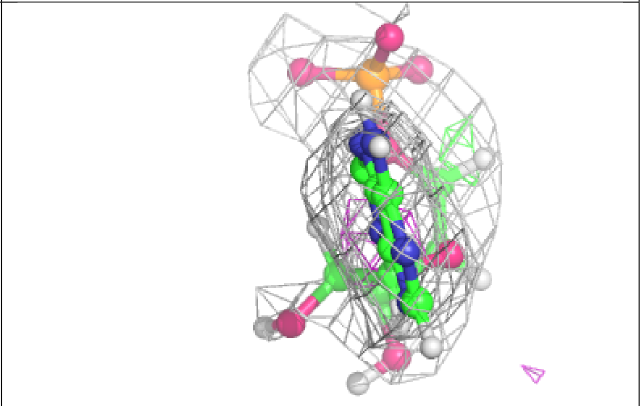


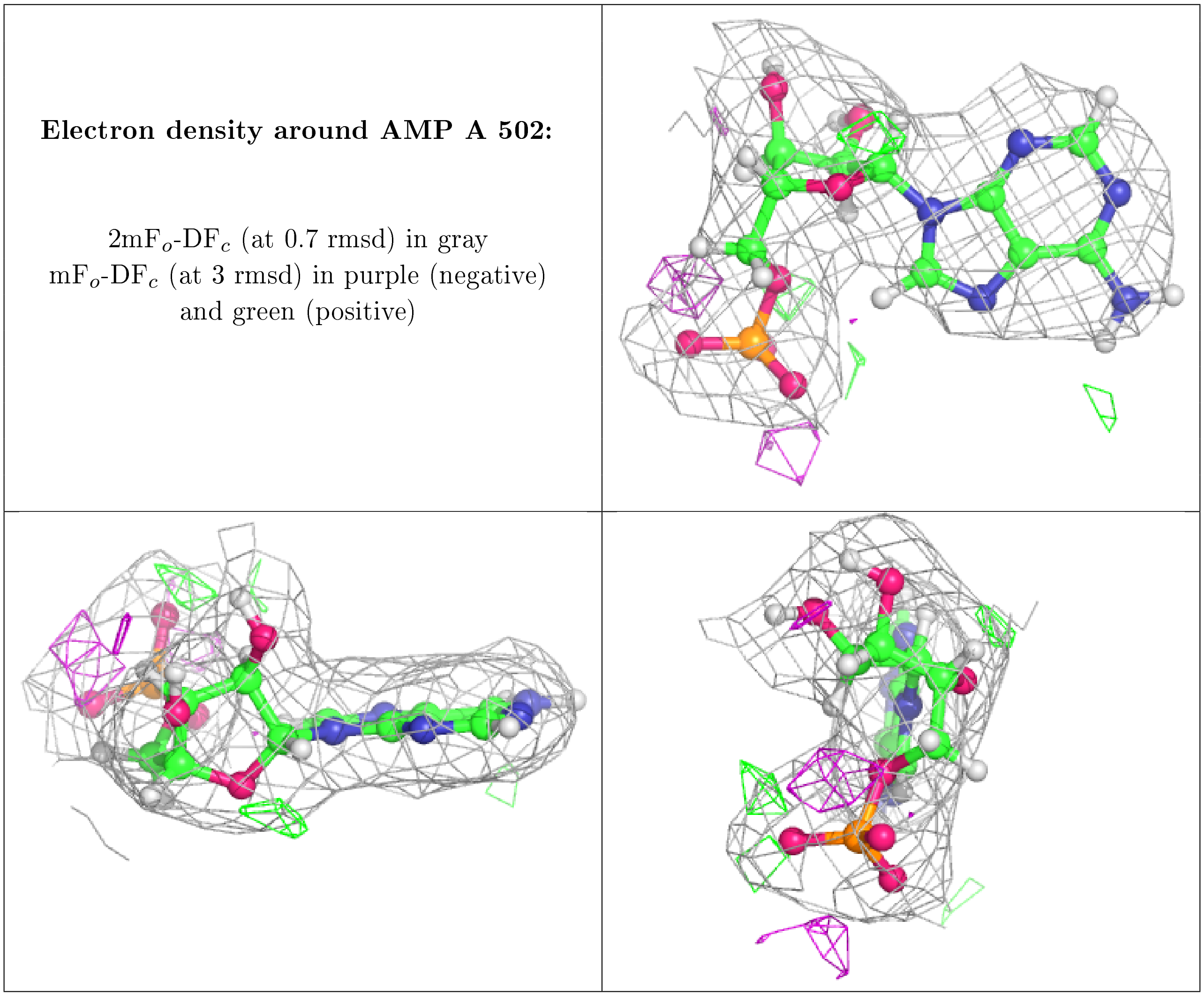
Electron density around AMP A 501:

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







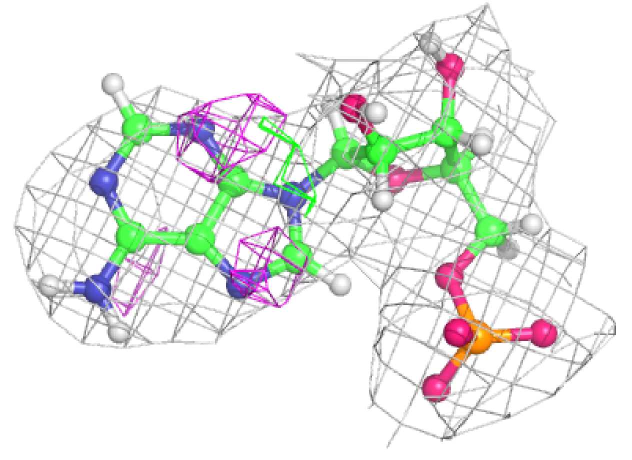


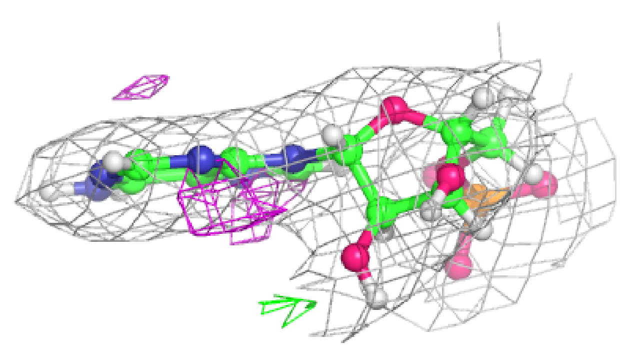
Electron density around AMP A 502:

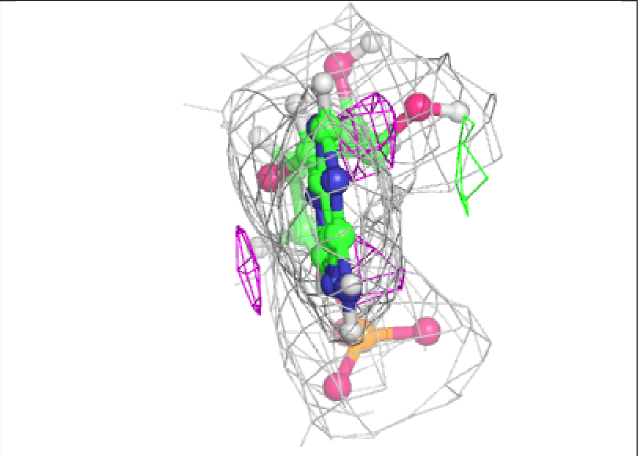
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AMP A 503:

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.