



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 PM UTC

PDB ID : 2V9J / pdb_00002v9j
Title : Crystal structure of the regulatory fragment of mammalian AMPK in complexes with Mg.ATP-AMP
Authors : Xiao, B.; Heath, R.; Saiu, P.; Leiper, F.C.; Leone, P.; Jing, C.; Walker, P.A.; Haire, L.; Eccleston, J.F.; Davis, C.T.; Martin, S.R.; Carling, D.; Gamblin, S.J.
Deposited on : 2007-08-23
Resolution : 2.53 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

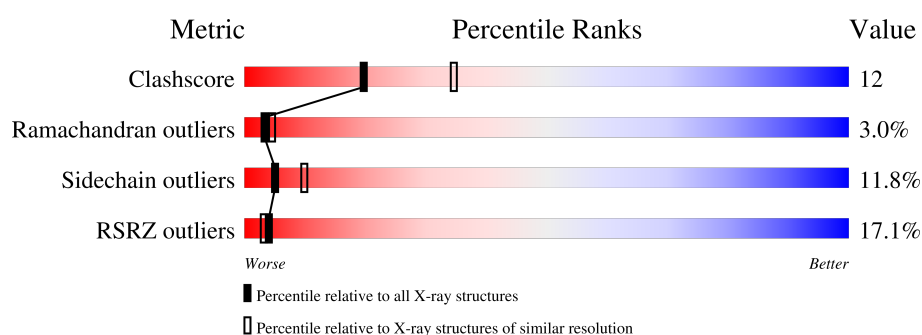
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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))
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	157	16% 38% 22% • • 35%
2	B	87	21% 60% 17% 5% • 16%
3	E	330	12% 68% 20% • • 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4114 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUB-UNIT ALPHA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			843	536	149	152	6			

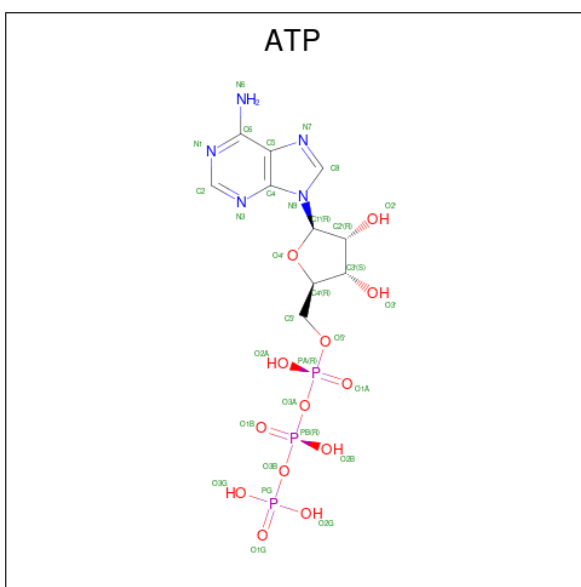
- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			601	392	103	103	3			

- Molecule 3 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1.

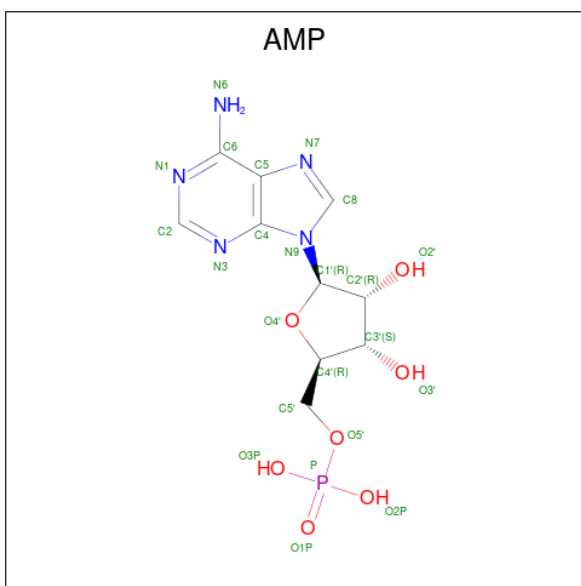
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	304	Total	C	N	O	S	0	0	0
			2441	1584	407	443	7			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total 2	Mg 2	0	0

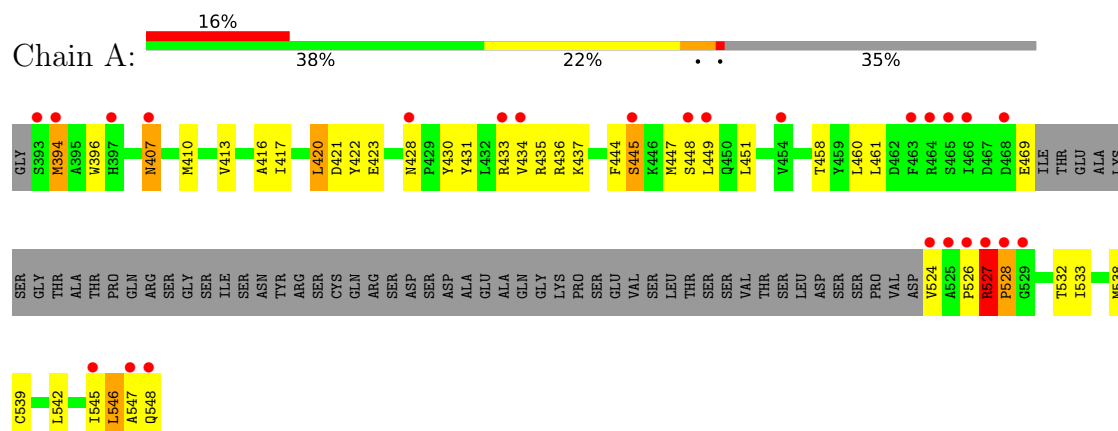
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total 35	O 35	0	0
7	B	27	Total 27	O 27	0	0
7	E	80	Total 80	O 80	0	0

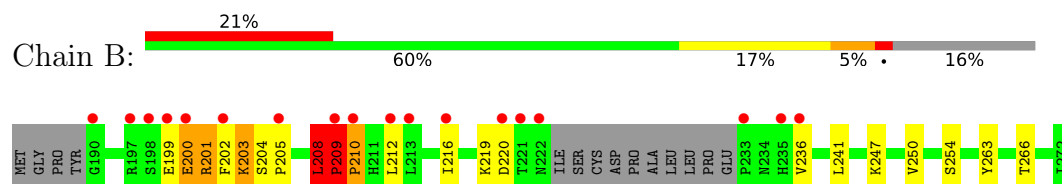
3 Residue-property plots [i](#)

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

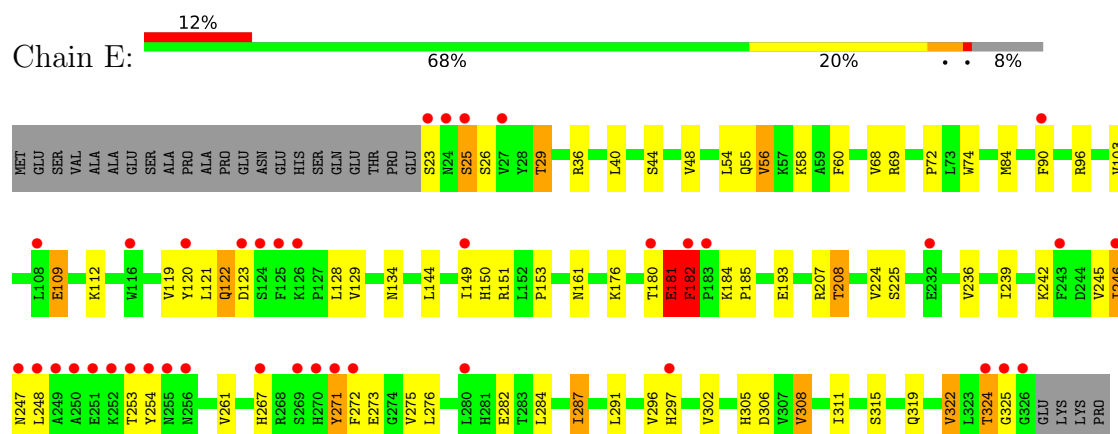
• Molecule 1: 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1



• Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-2



• Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.79Å 120.69Å 127.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.53 20.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.00-2.53) 96.1 (20.00-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.266 0.273 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4114	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: MG, AMP, ATP

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	0.64	0/861	0.88	1/1161 (0.1%)
2	B	0.66	0/616	0.91	1/832 (0.1%)
3	E	0.63	0/2493	0.91	2/3384 (0.1%)
All	All	0.63	0/3970	0.90	4/5377 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	E	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	181	GLU	N-CA-C	-6.83	96.25	110.80
2	B	209	PRO	N-CA-C	6.32	118.41	110.70
1	A	528	PRO	N-CA-C	6.12	120.82	111.15
3	E	182	PHE	N-CA-C	5.69	120.34	108.39

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	E	182	PHE	Peptide

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	843	0	842	35	0
2	B	601	0	625	22	0
3	E	2441	0	2506	44	0
4	E	62	0	24	2	0
5	E	23	0	12	1	0
6	E	2	0	0	0	0
7	A	35	0	0	1	0
7	B	27	0	0	0	0
7	E	80	0	0	4	0
All	All	4114	0	4009	92	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 12.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HA	1:A:546:LEU:HD12	1.17	1.16
2:B:203:LYS:HD3	2:B:204:SER:H	1.03	1.16
1:A:527:ARG:HG3	1:A:528:PRO:HD3	1.52	0.91
2:B:203:LYS:HD3	2:B:204:SER:N	1.84	0.91
1:A:532:THR:H	3:E:161:ASN:HD21	1.23	0.87
1:A:526:PRO:HG3	3:E:128:LEU:HD23	1.56	0.85
1:A:413:VAL:HA	1:A:546:LEU:CD1	2.04	0.84
2:B:203:LYS:CD	2:B:204:SER:H	1.88	0.83
1:A:542:LEU:O	1:A:546:LEU:HD22	1.82	0.79
2:B:208:LEU:O	2:B:210:PRO:HD3	1.82	0.79
3:E:282:GLU:HB2	3:E:287:ILE:HD11	1.64	0.78
3:E:225:SER:HB3	4:E:1328:ATP:O3G	1.89	0.73
3:E:109:GLU:OE2	3:E:109:GLU:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:150:HIS:HE1	7:E:2080:HOH:O	1.75	0.68
1:A:416:ALA:HB2	1:A:546:LEU:HB3	1.75	0.67
1:A:447:MET:CE	1:A:542:LEU:HD12	2.23	0.67
3:E:150:HIS:CE1	7:E:2080:HOH:O	2.48	0.65
2:B:208:LEU:HB3	2:B:209:PRO:HD3	1.77	0.65
1:A:527:ARG:CG	1:A:528:PRO:HD3	2.26	0.64
3:E:55:GLN:HB2	3:E:58:LYS:HD2	1.81	0.61
2:B:219:LYS:HG3	2:B:220:ASP:N	2.16	0.61
3:E:324:THR:HA	7:E:2071:HOH:O	2.01	0.60
3:E:253:THR:O	3:E:254:TYR:HB2	2.02	0.59
3:E:144:LEU:HA	3:E:149:ILE:HG22	1.84	0.59
1:A:449:LEU:HD23	1:A:461:LEU:HD11	1.84	0.58
3:E:84:MET:HE3	3:E:153:PRO:HG3	1.85	0.58
2:B:200:GLU:HB3	2:B:203:LYS:HG3	1.86	0.57
1:A:396:TRP:HB2	2:B:216:ILE:HB	1.86	0.57
1:A:447:MET:HE2	1:A:538:MET:HB3	1.87	0.56
2:B:247:LYS:O	2:B:250:VAL:HG12	2.06	0.56
3:E:282:GLU:HB2	3:E:287:ILE:CD1	2.35	0.56
1:A:417:ILE:HG23	1:A:422:TYR:HB2	1.89	0.55
2:B:200:GLU:O	2:B:202:PHE:N	2.33	0.55
1:A:447:MET:HE3	1:A:542:LEU:HD12	1.88	0.54
1:A:532:THR:H	3:E:161:ASN:ND2	1.99	0.53
3:E:144:LEU:HD23	3:E:149:ILE:HG23	1.91	0.53
1:A:423:GLU:OE2	1:A:435:ARG:NH1	2.41	0.53
1:A:524:VAL:N	7:A:2028:HOH:O	2.41	0.53
2:B:200:GLU:C	2:B:202:PHE:H	2.17	0.53
1:A:447:MET:HE1	1:A:542:LEU:HD12	1.90	0.52
3:E:273:GLU:O	3:E:273:GLU:HG3	2.10	0.52
2:B:200:GLU:C	2:B:202:PHE:N	2.66	0.52
3:E:56:VAL:HG13	3:E:60:PHE:CE1	2.45	0.51
3:E:120:TYR:C	3:E:122:GLN:H	2.18	0.51
1:A:546:LEU:HD23	1:A:547:ALA:N	2.25	0.51
3:E:271:TYR:HD2	3:E:272:PHE:H	1.59	0.51
2:B:203:LYS:H	2:B:203:LYS:HD2	1.76	0.50
2:B:208:LEU:O	2:B:210:PRO:CD	2.59	0.49
3:E:69:ARG:HB3	3:E:151:ARG:NH1	2.28	0.49
3:E:56:VAL:HG13	3:E:60:PHE:HE1	1.76	0.49
3:E:36:ARG:HD3	3:E:134:ASN:HA	1.95	0.48
1:A:410:MET:HE2	1:A:410:MET:HA	1.95	0.48
2:B:200:GLU:HA	2:B:203:LYS:HB3	1.94	0.48
3:E:109:GLU:OE2	3:E:109:GLU:CA	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:181:GLU:O	3:E:181:GLU:HG2	2.14	0.47
3:E:319:GLN:NE2	7:E:2067:HOH:O	2.28	0.47
1:A:420:LEU:HD11	1:A:545:ILE:HG13	1.97	0.47
3:E:297:HIS:ND1	4:E:1327:ATP:O3G	2.37	0.46
1:A:437:LYS:HB2	1:A:444:PHE:CE2	2.51	0.46
3:E:180:THR:O	3:E:181:GLU:HB3	2.16	0.46
3:E:25:SER:O	3:E:29:THR:HB	2.16	0.45
3:E:225:SER:OG	5:E:1329:AMP:O2P	2.35	0.45
1:A:428:ASN:HB2	1:A:431:TYR:HB3	1.99	0.45
3:E:48:VAL:O	3:E:72:PRO:HD2	2.17	0.45
1:A:417:ILE:HG13	1:A:542:LEU:HD21	1.97	0.45
1:A:394:MET:HG2	2:B:219:LYS:HA	1.99	0.45
2:B:254:SER:HA	2:B:266:THR:O	2.17	0.44
1:A:539:CYS:SG	2:B:241:LEU:HD22	2.58	0.44
3:E:23:SER:HA	3:E:185:PRO:HB3	2.00	0.44
3:E:60:PHE:CE2	3:E:90:PHE:HB2	2.52	0.44
3:E:236:VAL:HB	3:E:308:VAL:HG12	2.00	0.44
1:A:447:MET:HE3	1:A:542:LEU:CD1	2.48	0.44
1:A:420:LEU:O	1:A:421:ASP:HB2	2.18	0.43
1:A:430:TYR:CE2	2:B:205:PRO:HG3	2.54	0.42
3:E:273:GLU:O	3:E:273:GLU:CG	2.67	0.42
1:A:445:SER:HB3	1:A:538:MET:CE	2.50	0.42
1:A:545:ILE:O	1:A:545:ILE:HG22	2.20	0.42
3:E:182:PHE:HB2	3:E:184:LYS:HB2	2.01	0.42
3:E:322:VAL:C	3:E:324:THR:H	2.28	0.42
3:E:176:LYS:O	3:E:180:THR:OG1	2.36	0.42
2:B:263:TYR:O	3:E:44:SER:HA	2.19	0.41
1:A:533:ILE:HG21	3:E:74:TRP:CD2	2.54	0.41
3:E:242:LYS:O	3:E:245:VAL:HB	2.21	0.41
3:E:120:TYR:C	3:E:122:GLN:N	2.79	0.41
3:E:305:HIS:O	3:E:306:ASP:HB2	2.20	0.41
1:A:407:ASN:OD1	1:A:407:ASN:N	2.49	0.41
2:B:236:VAL:O	2:B:236:VAL:HG22	2.21	0.41
3:E:246:ILE:H	3:E:246:ILE:HG13	1.71	0.41
1:A:410:MET:HE3	1:A:451:LEU:HD22	2.02	0.40
3:E:207:ARG:O	3:E:208:THR:C	2.63	0.40
2:B:200:GLU:HG2	2:B:203:LYS:HB3	2.03	0.40
1:A:546:LEU:HD23	1:A:546:LEU:C	2.47	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	98/157 (62%)	93 (95%)	4 (4%)	1 (1%)	12	23
2	B	69/87 (79%)	53 (77%)	11 (16%)	5 (7%)	1	1
3	E	302/330 (92%)	278 (92%)	16 (5%)	8 (3%)	4	6
All	All	469/574 (82%)	424 (90%)	31 (7%)	14 (3%)	3	4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	122	GLN
3	E	181	GLU
2	B	201	ARG
2	B	208	LEU
3	E	208	THR
3	E	325	GLY
2	B	209	PRO
3	E	25	SER
3	E	26	SER
3	E	121	LEU
3	E	324	THR
1	A	527	ARG
2	B	200	GLU
2	B	210	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	94/141 (67%)	80 (85%)	14 (15%)	3	5
2	B	69/81 (85%)	65 (94%)	4 (6%)	18	36
3	E	277/299 (93%)	243 (88%)	34 (12%)	4	9
All	All	440/521 (84%)	388 (88%)	52 (12%)	5	10

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	394	MET
1	A	407	ASN
1	A	420	LEU
1	A	433	ARG
1	A	434	VAL
1	A	436	ARG
1	A	445	SER
1	A	448	SER
1	A	458	THR
1	A	460	LEU
1	A	469	GLU
1	A	527	ARG
1	A	546	LEU
1	A	548	GLN
2	B	199	GLU
2	B	201	ARG
2	B	203	LYS
2	B	212	LEU
3	E	29	THR
3	E	40	LEU
3	E	54	LEU
3	E	56	VAL
3	E	68	VAL
3	E	96	ARG
3	E	103	VAL
3	E	109	GLU
3	E	112	LYS
3	E	119	VAL
3	E	123	ASP
3	E	129	VAL
3	E	181	GLU
3	E	182	PHE
3	E	193	GLU
3	E	224	VAL

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Mol	Chain	Res	Type
3	E	239	ILE
3	E	246	ILE
3	E	247	ASN
3	E	248	LEU
3	E	261	VAL
3	E	267	HIS
3	E	271	TYR
3	E	275	VAL
3	E	276	LEU
3	E	284	LEU
3	E	287	ILE
3	E	291	LEU
3	E	296	VAL
3	E	302	VAL
3	E	308	VAL
3	E	311	ILE
3	E	315	SER
3	E	322	VAL

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

Mol	Chain	Res	Type
2	B	214	GLN
3	E	66	ASN
3	E	134	ASN
3	E	147	ASN
3	E	161	ASN
3	E	168	HIS
3	E	202	ASN
3	E	255	ASN
3	E	266	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	E	1328	6	32,33,33	1.64	9 (28%)	48,52,52	1.97	12 (25%)
5	AMP	E	1329	-	25,25,25	1.52	4 (16%)	37,38,38	1.91	10 (27%)
4	ATP	E	1327	6	32,33,33	1.61	6 (18%)	48,52,52	1.78	10 (20%)

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
4	ATP	E	1328	6	-	3/22/38/38	0/3/3/3
5	AMP	E	1329	-	-	3/10/26/26	0/3/3/3
4	ATP	E	1327	6	-	2/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1329	AMP	C5-C4	4.90	1.47	1.39
4	E	1327	ATP	C5-C4	4.90	1.47	1.39
4	E	1328	ATP	C5-C4	4.51	1.47	1.39
4	E	1327	ATP	PG-O1G	3.90	1.62	1.50
4	E	1328	ATP	PG-O1G	3.79	1.62	1.50
4	E	1328	ATP	PA-O3A	2.85	1.62	1.59
5	E	1329	AMP	C5-C6	2.84	1.48	1.41
4	E	1327	ATP	C5-C6	2.69	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1328	ATP	C5-C6	2.69	1.48	1.41
4	E	1327	ATP	PB-O1B	2.56	1.59	1.50
5	E	1329	AMP	C8-N7	2.54	1.36	1.31
5	E	1329	AMP	C5-N7	-2.47	1.34	1.39
4	E	1328	ATP	PB-O1B	2.45	1.59	1.50
4	E	1327	ATP	C5-N7	-2.41	1.34	1.39
4	E	1328	ATP	C4-N9	-2.20	1.33	1.37
4	E	1328	ATP	PB-O3B	2.19	1.61	1.59
4	E	1328	ATP	C8-N7	2.12	1.35	1.31
4	E	1327	ATP	C8-N7	2.11	1.35	1.31
4	E	1328	ATP	C5-N7	-2.10	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1328	ATP	C5-C4-N3	-5.55	119.08	126.72
5	E	1329	AMP	C5-C4-N3	-5.37	119.33	126.72
4	E	1327	ATP	C5-C4-N3	-5.01	119.82	126.72
4	E	1328	ATP	N3-C4-N9	4.49	134.81	127.17
4	E	1327	ATP	N3-C2-N1	-4.35	122.00	128.58
4	E	1327	ATP	N3-C4-N9	4.12	134.18	127.17
4	E	1327	ATP	C2-N3-C4	3.84	121.21	111.83
4	E	1328	ATP	C2-N3-C4	3.80	121.12	111.83
5	E	1329	AMP	C4-C5-N7	-3.78	106.26	110.58
5	E	1329	AMP	C2-N3-C4	3.75	120.99	111.83
4	E	1328	ATP	O2B-PB-O3A	3.74	117.38	107.27
5	E	1329	AMP	N3-C4-N9	3.67	133.41	127.17
4	E	1328	ATP	C4-C5-N7	-3.49	106.59	110.58
5	E	1329	AMP	N3-C2-N1	-3.48	123.31	128.58
4	E	1328	ATP	N3-C2-N1	-3.40	123.44	128.58
4	E	1328	ATP	O3G-PG-O2G	3.28	120.09	107.80
4	E	1328	ATP	C4-N9-C8	3.27	109.18	105.74
4	E	1327	ATP	C4-C5-N7	-3.05	107.10	110.58
4	E	1327	ATP	O3G-PG-O2G	2.89	118.64	107.80
4	E	1327	ATP	C2-N1-C6	2.79	123.32	118.73
5	E	1329	AMP	C6-C5-N7	2.78	137.45	132.09
4	E	1328	ATP	C5-N7-C8	2.72	107.73	103.45
4	E	1327	ATP	C6-C5-N7	2.51	136.93	132.09
4	E	1328	ATP	N9-C8-N7	-2.50	110.38	113.94
5	E	1329	AMP	O3P-P-O1P	2.49	120.53	110.83
4	E	1327	ATP	C4-N9-C8	2.44	108.30	105.74
4	E	1328	ATP	C6-C5-N7	2.43	136.77	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1329	AMP	C5-N7-C8	2.39	107.21	103.45
4	E	1327	ATP	C5-N7-C8	2.33	107.11	103.45
4	E	1328	ATP	O2A-PA-O3A	2.31	113.51	107.27
5	E	1329	AMP	O3P-P-O5'	-2.11	101.17	106.67
5	E	1329	AMP	C2-N1-C6	2.09	122.16	118.73

There are no chirality outliers.

All (8) torsion outliers are listed below:

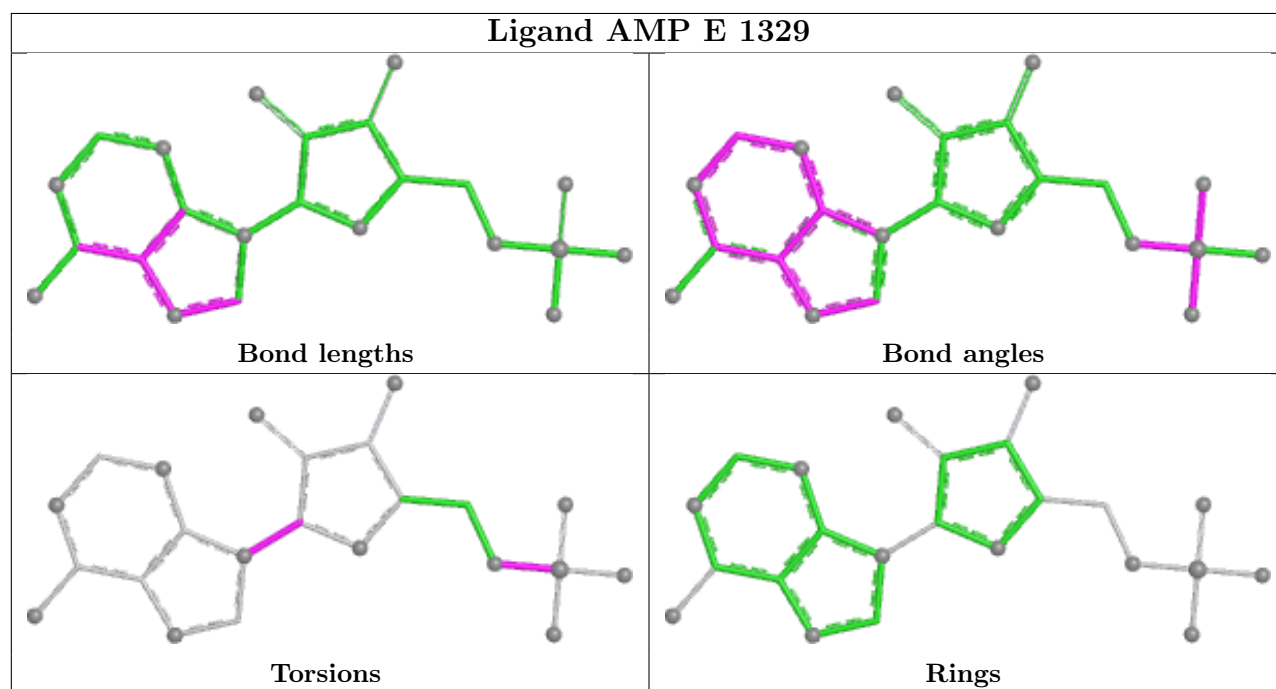
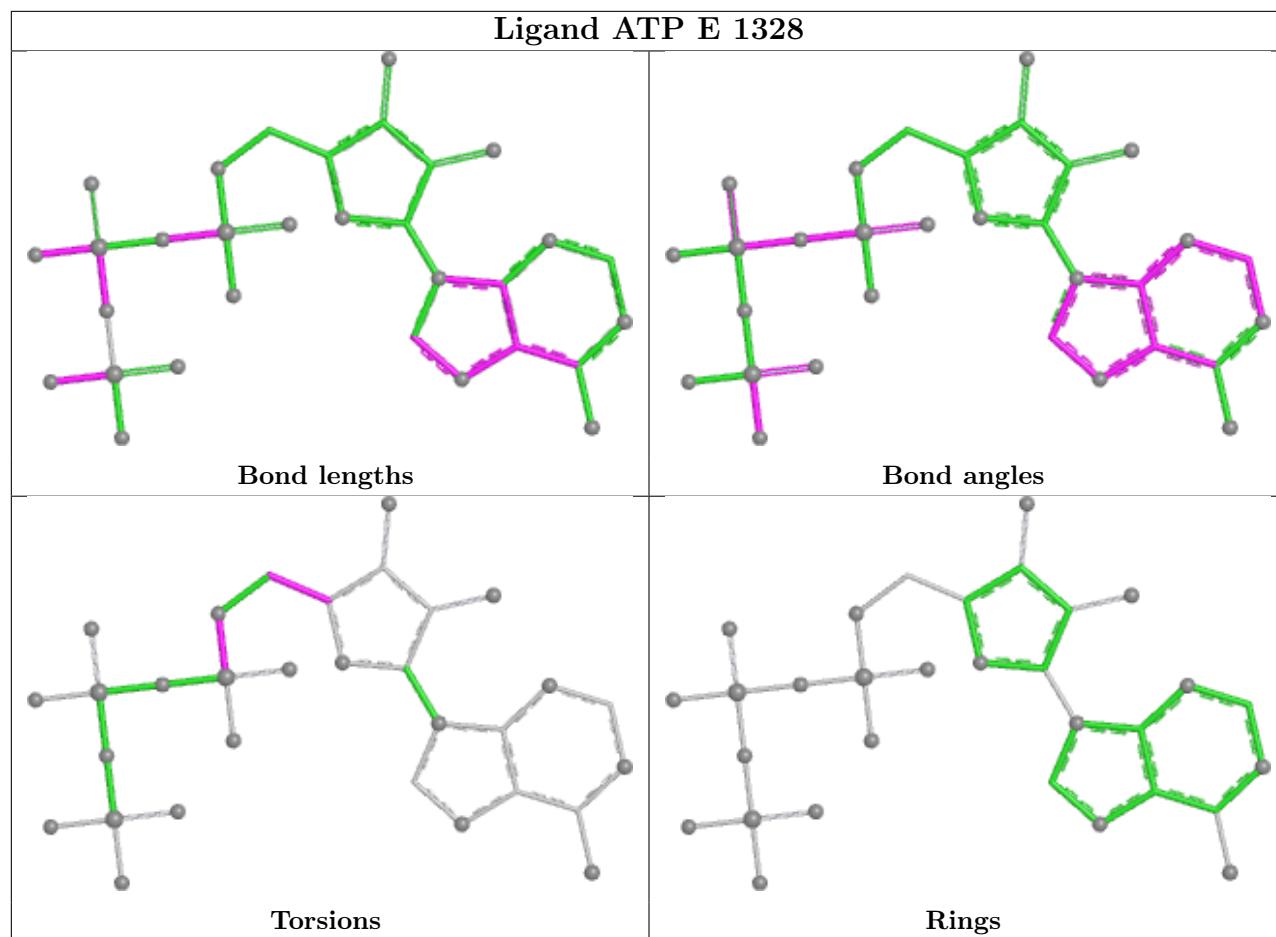
Mol	Chain	Res	Type	Atoms
4	E	1328	ATP	O4'-C4'-C5'-O5'
5	E	1329	AMP	C5'-O5'-P-O1P
5	E	1329	AMP	C5'-O5'-P-O2P
4	E	1328	ATP	C3'-C4'-C5'-O5'
4	E	1327	ATP	C5'-O5'-PA-O1A
4	E	1327	ATP	C5'-O5'-PA-O3A
4	E	1328	ATP	C5'-O5'-PA-O1A
5	E	1329	AMP	C2'-C1'-N9-C8

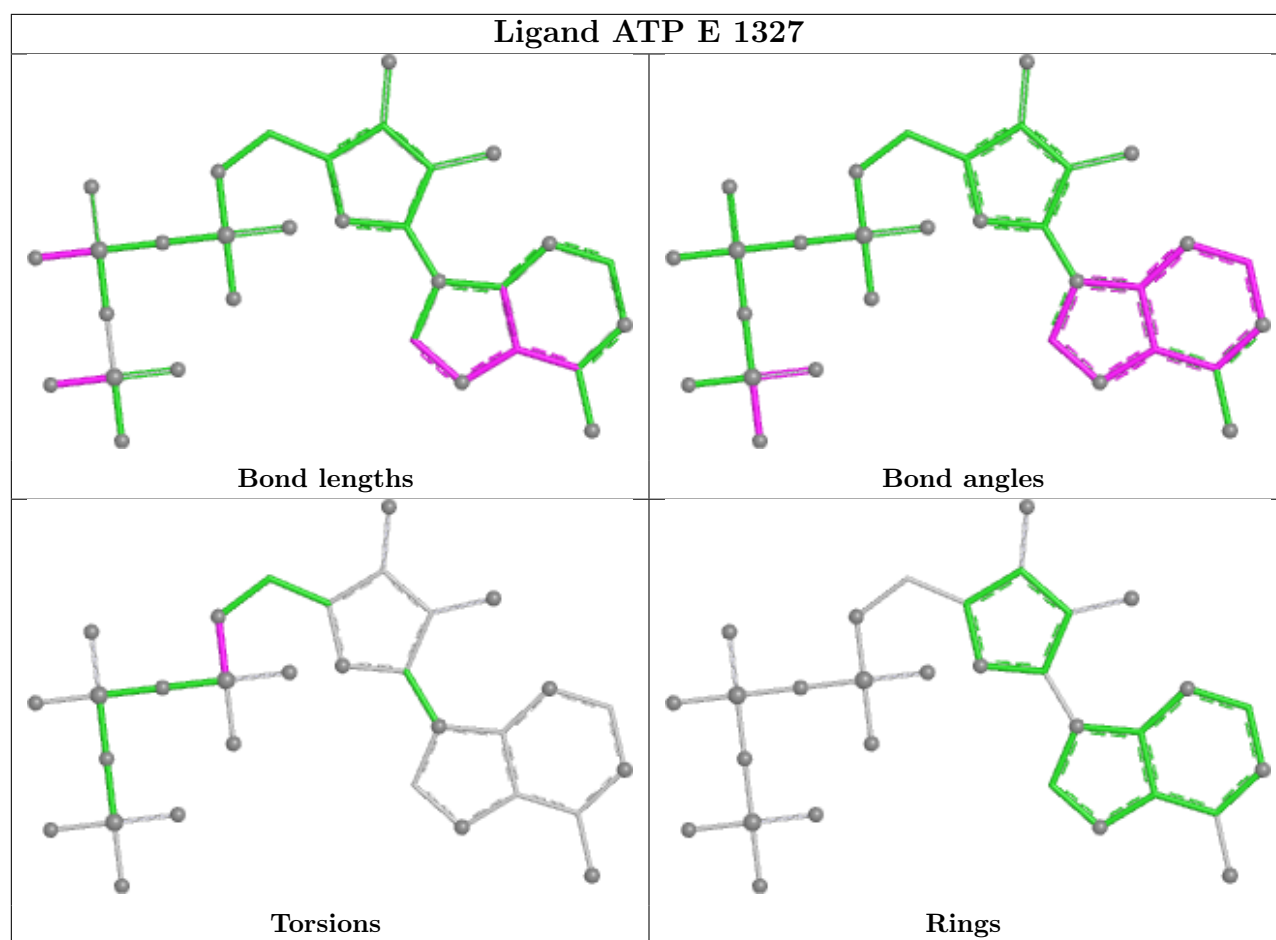
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1328	ATP	1	0
5	E	1329	AMP	1	0
4	E	1327	ATP	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	102/157 (64%)	1.41	25 (24%)	2 1	48, 58, 65, 75	0
2	B	73/87 (83%)	1.59	18 (24%)	2 1	41, 58, 86, 93	0
3	E	304/330 (92%)	1.03	39 (12%)	7 6	33, 51, 72, 77	0
All	All	479/574 (83%)	1.20	82 (17%)	4 3	33, 54, 76, 93	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	250	ALA	6.7
3	E	24	ASN	6.0
2	B	221	THR	6.0
3	E	326	GLY	5.6
2	B	209	PRO	4.8
3	E	249	ALA	4.7
3	E	253	THR	4.7
3	E	270	HIS	4.7
3	E	182	PHE	4.7
3	E	254	TYR	4.6
2	B	235	HIS	4.5
3	E	108	LEU	4.3
1	A	524	VAL	4.3
3	E	180	THR	4.2
1	A	468	ASP	4.0
1	A	393	SER	4.0
3	E	124	SER	3.9
2	B	220	ASP	3.8
3	E	23	SER	3.8
2	B	197	ARG	3.7
1	A	394	MET	3.6
3	E	123	ASP	3.6
3	E	271	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	233	PRO	3.5
1	A	454	VAL	3.4
3	E	272	PHE	3.3
3	E	120	TYR	3.3
3	E	267	HIS	3.2
1	A	525	ALA	3.1
3	E	125	PHE	3.1
3	E	27	VAL	3.1
3	E	252	LYS	3.1
3	E	116	TRP	3.0
3	E	149	ILE	2.9
1	A	528	PRO	2.9
2	B	202	PHE	2.9
1	A	428	ASN	2.9
3	E	256	ASN	2.9
3	E	324	THR	2.8
3	E	325	GLY	2.8
3	E	246	ILE	2.8
1	A	527	ARG	2.8
3	E	243	PHE	2.8
2	B	205	PRO	2.7
3	E	255	ASN	2.7
1	A	434	VAL	2.7
2	B	210	PRO	2.7
2	B	212	LEU	2.6
1	A	526	PRO	2.6
3	E	90	PHE	2.6
1	A	465	SER	2.6
2	B	236	VAL	2.5
1	A	547	ALA	2.5
3	E	232	GLU	2.5
2	B	199	GLU	2.4
1	A	407	ASN	2.4
3	E	248	LEU	2.3
2	B	190	GLY	2.3
1	A	448	SER	2.3
1	A	463	PHE	2.3
3	E	183	PRO	2.3
2	B	222	ASN	2.2
1	A	397	HIS	2.2
2	B	198	SER	2.2
3	E	269	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	529	GLY	2.2
3	E	251	GLU	2.2
1	A	464	ARG	2.2
3	E	297	HIS	2.2
1	A	449	LEU	2.2
1	A	433	ARG	2.2
3	E	126	LYS	2.2
3	E	280	LEU	2.2
3	E	247	ASN	2.1
1	A	545	ILE	2.1
1	A	548	GLN	2.1
2	B	213	LEU	2.1
2	B	216	ILE	2.1
3	E	25	SER	2.1
2	B	200	GLU	2.0
1	A	466	ILE	2.0
1	A	445	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

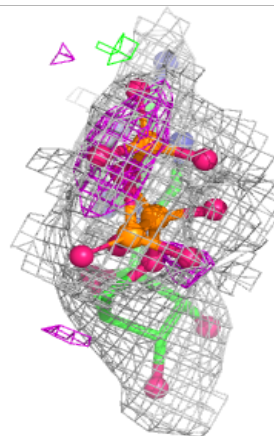
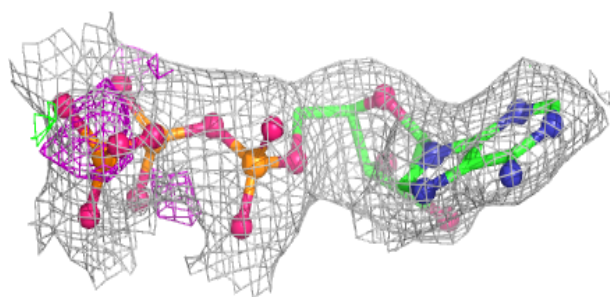
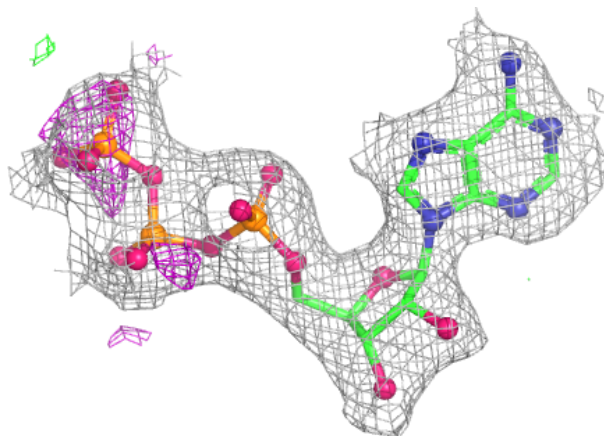
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	E	1331	1/1	0.77	0.29	60,60,60,60	0
6	MG	E	1330	1/1	0.81	0.09	58,58,58,58	0
4	ATP	E	1327	31/31	0.89	0.11	49,51,61,62	0
4	ATP	E	1328	31/31	0.89	0.10	21,31,62,63	0
5	AMP	E	1329	23/23	0.94	0.08	35,36,41,43	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.

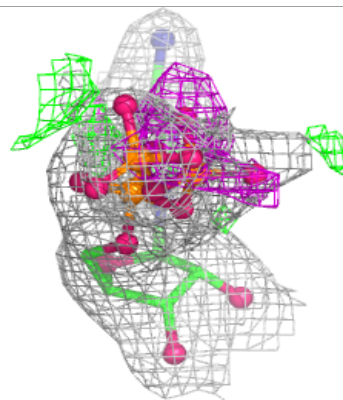
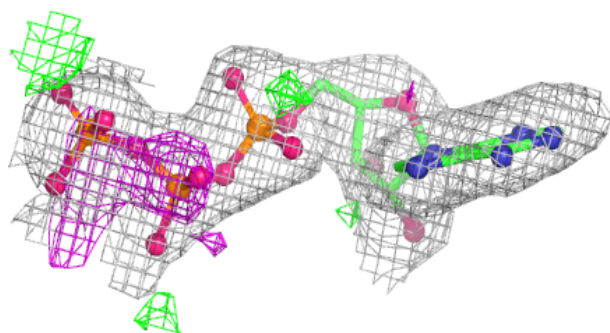
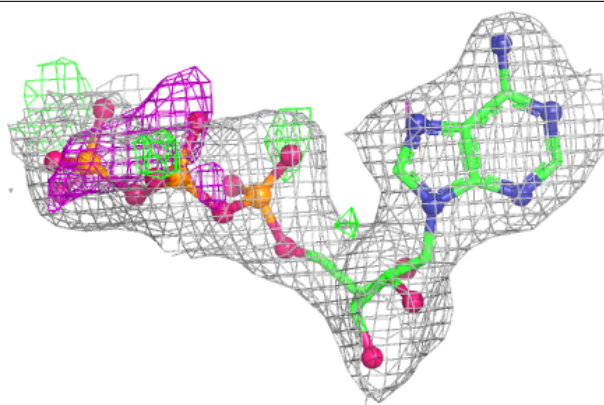
Electron density around ATP E 1327:

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



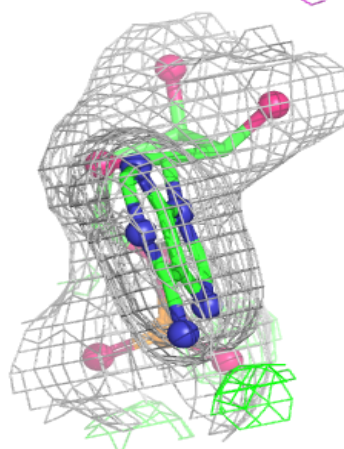
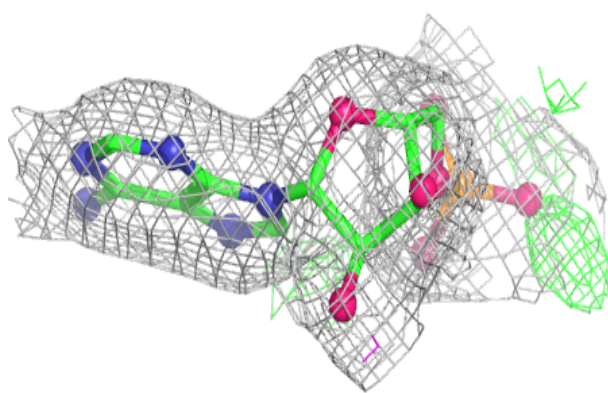
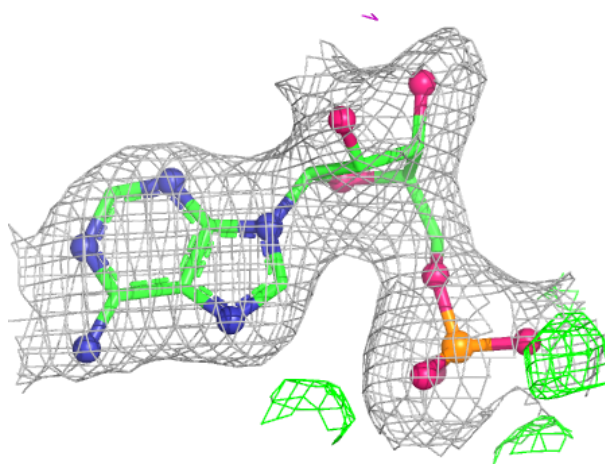
Electron density around ATP E 1328:

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



Electron density around AMP E 1329:

$2mF_o-DF_c$ (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.