Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:24 am BST

PDB ID	:	4EAG
Title	:	Co-crystal structure of an chimeric AMPK core with ATP
Authors	:	Chen, L.; Wang, J.; Zhang, Y.-Y.; Yan, S.F.; Neumann, D.; Schlattner, U.; Wang, Z.-X.; Wu, J.-W.
Deposited on	:	2012-03-22
Resolution	:	2.70 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:

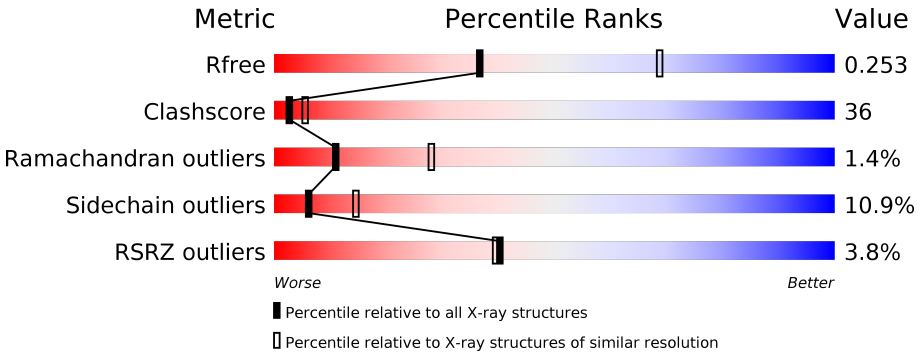
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	130	2% 25% 43% 8% 25%
2	B	85	13% 38% 27% • 32%
3	C	330	% 44% 36% 8% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TAM	C	403	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3755 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 EG:132E8.2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			813	525	144	138	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	GLY	-	EXPRESSION TAG	UNP O18645
A	454	PRO	-	EXPRESSION TAG	UNP O18645
A	455	HIS	-	EXPRESSION TAG	UNP O18645
A	456	MET	-	EXPRESSION TAG	UNP O18645
A	457	GLY	-	EXPRESSION TAG	UNP O18645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	58	Total	C	N	O	S	0	0	0
			468	311	77	77	3			

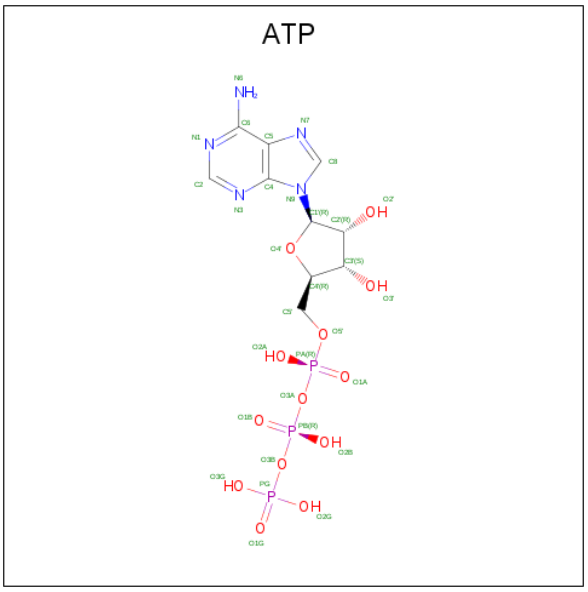
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	MET	-	EXPRESSION TAG	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

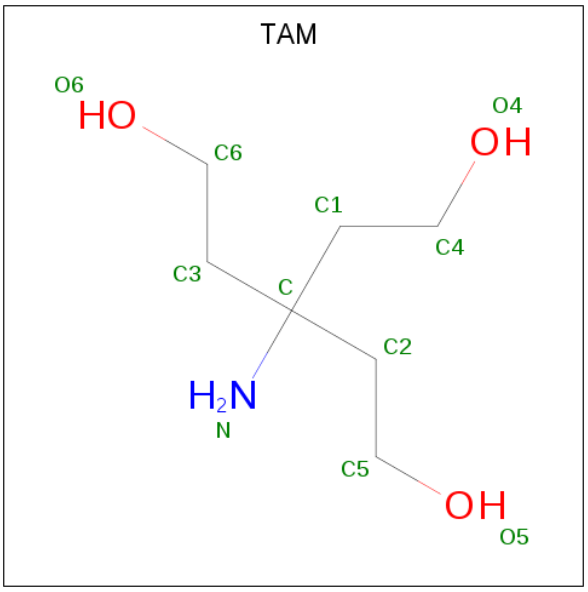
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	289	Total	C	N	O	S	0	0	0
			2320	1510	387	416	7			

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



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

- Molecule 5 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 6 is water.

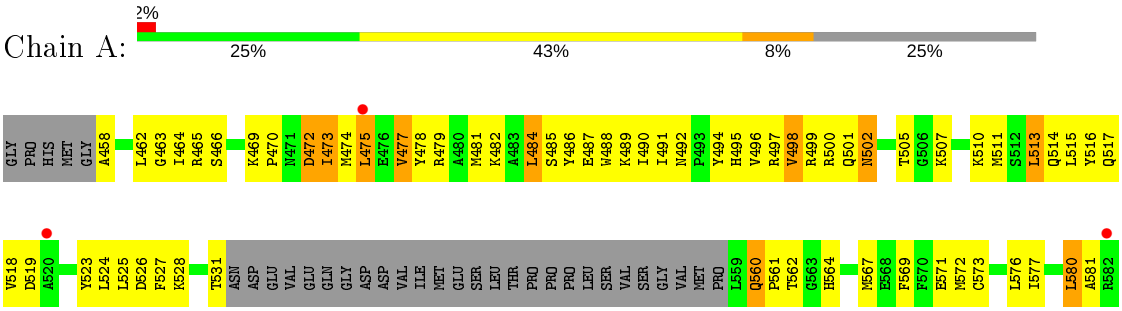
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	20	Total O 20 20	0	0
6	B	3	Total O 3 3	0	0
6	C	58	Total O 58 58	0	0

3 Residue-property plots (i)

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.

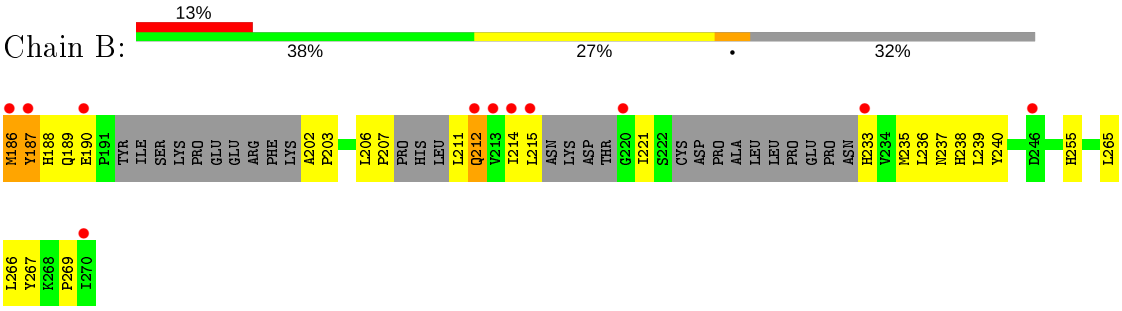
- Molecule 1: EG:132E8.2 protein

Chain A:



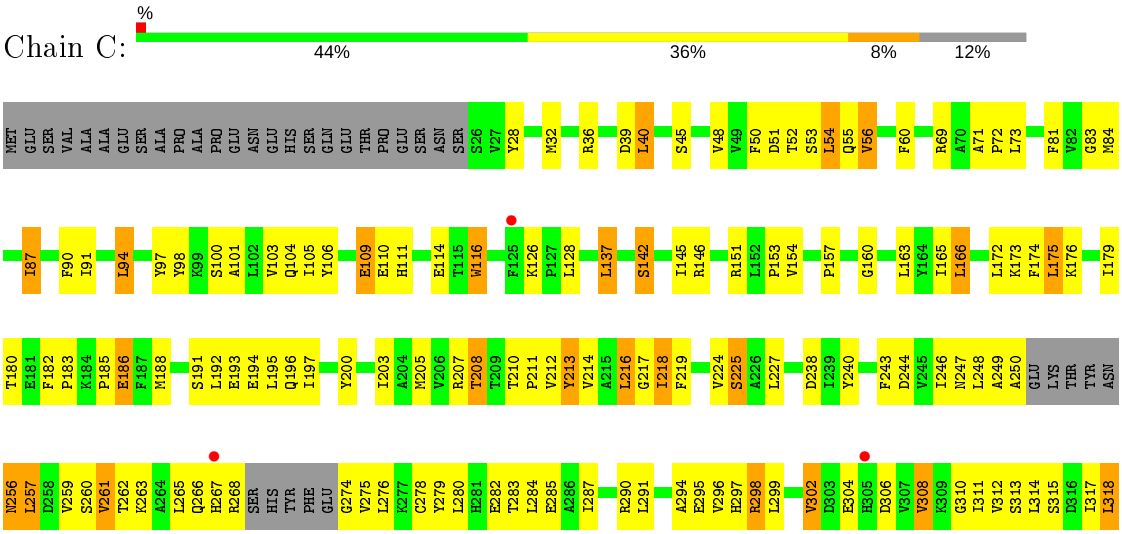
- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

Chain B:



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

Chain C:




Q319
A320
L323
T324
GLY
GLY
GLU
LYS
LYS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	108.67Å 151.28Å 109.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.70 29.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	77.6 (29.86-2.70) 77.7 (29.86-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.10 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.208 , 0.252 0.206 , 0.253	Depositor DCC
R_{free} test set	984 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3755	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAM, 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	0.47	0/831	0.64	0/1114
2	B	0.39	0/477	0.59	0/641
3	C	0.48	0/2366	0.66	0/3210
All	All	0.47	0/3674	0.64	0/4965

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	813	0	834	100	0
2	B	468	0	496	71	0
3	C	2320	0	2405	147	0
4	C	62	0	24	8	0
5	C	11	0	17	9	0
6	A	20	0	0	2	0
6	B	3	0	0	1	0
6	C	58	0	0	3	0
All	All	3755	0	3776	268	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 36.

All (268) 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:510:LYS:HE2	2:B:186:MET:HE2	1.29	1.14
1:A:561:PRO:HG2	3:C:160:GLY:HA2	1.32	1.11
2:B:186:MET:SD	2:B:186:MET:N	2.30	1.04
1:A:516:TYR:CD2	2:B:206:LEU:HB2	1.92	1.03
3:C:176:LYS:HA	3:C:179:ILE:HD12	1.45	0.97
1:A:511:MET:HE1	1:A:572:MET:HB3	1.46	0.96
1:A:516:TYR:HD2	2:B:206:LEU:HB2	1.25	0.96
1:A:499:ARG:HB2	2:B:186:MET:CG	1.98	0.93
3:C:151:ARG:HH12	5:C:403:TAM:H32	1.37	0.89
1:A:510:LYS:HE2	2:B:186:MET:CE	2.01	0.89
1:A:499:ARG:HB2	2:B:186:MET:HG3	1.54	0.88
1:A:510:LYS:CE	2:B:186:MET:HE2	2.03	0.88
3:C:315:SER:HB3	4:C:402:ATP:O1B	1.76	0.85
3:C:98:TYR:HA	3:C:103:VAL:HG23	1.59	0.84
1:A:560:GLN:HE22	3:C:81:PHE:H	1.24	0.81
3:C:290:ARG:O	3:C:294:ALA:HB3	1.81	0.80
3:C:98:TYR:HD1	3:C:103:VAL:HG21	1.48	0.77
3:C:211:PRO:HA	3:C:259:VAL:O	1.83	0.77
1:A:499:ARG:HB2	2:B:186:MET:HG2	1.66	0.77
1:A:489:LYS:HG3	2:B:186:MET:HA	1.67	0.77
3:C:195:LEU:HB3	3:C:197:ILE:HD12	1.64	0.76
1:A:510:LYS:CE	2:B:186:MET:CE	2.62	0.76
1:A:510:LYS:HD3	2:B:186:MET:HE3	1.66	0.75
1:A:499:ARG:CB	2:B:186:MET:CG	2.64	0.75
5:C:403:TAM:O5	5:C:403:TAM:H61	1.85	0.75
1:A:505:THR:HG22	1:A:507:LYS:H	1.52	0.73
1:A:510:LYS:CD	2:B:186:MET:CE	2.66	0.73
1:A:515:LEU:HD12	1:A:516:TYR:H	1.52	0.73
3:C:313:SER:HB3	4:C:402:ATP:O2B	1.89	0.73
3:C:259:VAL:HG12	3:C:260:SER:N	2.05	0.72
3:C:182:PHE:CD2	3:C:183:PRO:HD2	2.25	0.72
1:A:560:GLN:NE2	3:C:81:PHE:HB2	2.07	0.70
2:B:211:LEU:O	2:B:212:GLN:HB2	1.91	0.70
3:C:109:GLU:OE1	3:C:116:TRP:HZ3	1.75	0.69
1:A:497:ARG:HG2	2:B:186:MET:SD	2.32	0.69
1:A:499:ARG:CB	2:B:186:MET:HG3	2.21	0.69
3:C:111:HIS:HB2	3:C:116:TRP:CZ3	2.28	0.68
3:C:193:GLU:HB2	3:C:280:LEU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ARG:HG2	1:A:524:LEU:HD23	1.75	0.68
3:C:97:TYR:HE2	3:C:105:ILE:HG22	1.59	0.68
1:A:490:ILE:HA	1:A:496:VAL:HG23	1.77	0.67
1:A:497:ARG:CD	2:B:186:MET:SD	2.82	0.67
3:C:40:LEU:CD1	3:C:166:LEU:HD11	2.25	0.66
2:B:236:LEU:O	2:B:237:ASN:HB2	1.96	0.66
3:C:290:ARG:O	3:C:294:ALA:CB	2.42	0.66
1:A:510:LYS:HD3	2:B:186:MET:CE	2.26	0.66
1:A:494:TYR:HH	2:B:202:ALA:N	1.95	0.65
1:A:469:LYS:O	1:A:472:ASP:HB2	1.97	0.65
1:A:477:VAL:O	1:A:481:MET:HG3	1.95	0.65
1:A:486:TYR:CE2	1:A:500:ARG:HD2	2.32	0.65
1:A:470:PRO:HD3	1:A:523:TYR:CE2	2.31	0.65
1:A:516:TYR:CE2	2:B:206:LEU:HD13	2.32	0.64
1:A:567:MET:HE3	2:B:266:LEU:HD22	1.78	0.64
2:B:211:LEU:O	2:B:211:LEU:HD12	1.97	0.64
1:A:494:TYR:CE2	2:B:203:PRO:HG3	2.32	0.64
2:B:239:LEU:HD12	2:B:240:TYR:N	2.11	0.64
3:C:302:VAL:HG13	3:C:306:ASP:HA	1.79	0.64
1:A:499:ARG:CB	2:B:186:MET:HG2	2.27	0.63
2:B:214:ILE:C	2:B:215:LEU:HD22	2.19	0.63
1:A:497:ARG:HD3	2:B:186:MET:SD	2.39	0.62
3:C:172:LEU:HD13	3:C:318:LEU:HD13	1.81	0.62
1:A:561:PRO:HG2	3:C:160:GLY:CA	2.20	0.62
3:C:185:PRO:HD2	3:C:188:MET:HG3	1.81	0.62
3:C:263:LYS:HD2	3:C:266:GLN:HE22	1.65	0.61
2:B:187:TYR:HD2	2:B:188:HIS:N	1.98	0.61
1:A:510:LYS:CD	2:B:186:MET:HE2	2.30	0.61
1:A:560:GLN:HE21	3:C:81:PHE:HB2	1.64	0.61
2:B:214:ILE:HG22	2:B:215:LEU:N	2.16	0.61
3:C:240:TYR:CE2	3:C:244:ASP:HB3	2.37	0.60
3:C:109:GLU:HG2	3:C:110:GLU:N	2.17	0.59
1:A:573:CYS:O	1:A:577:ILE:HG13	2.02	0.59
1:A:510:LYS:CD	2:B:186:MET:HE3	2.32	0.59
3:C:176:LYS:HE2	3:C:180:THR:HG21	1.85	0.59
3:C:238:ASP:HA	3:C:275:VAL:HG21	1.83	0.59
3:C:97:TYR:HH	3:C:116:TRP:HH2	1.49	0.59
2:B:214:ILE:HG22	2:B:215:LEU:H	1.67	0.59
3:C:87:ILE:HD11	3:C:246:ILE:HG12	1.85	0.59
3:C:87:ILE:O	3:C:87:ILE:HD13	2.03	0.59
3:C:97:TYR:HE1	3:C:116:TRP:CZ2	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:GLU:HG3	3:C:116:TRP:HH2	1.68	0.58
3:C:279:TYR:CD1	3:C:279:TYR:N	2.72	0.58
1:A:462:LEU:HB2	2:B:240:TYR:CE2	2.39	0.57
3:C:224:VAL:HG21	4:C:402:ATP:C5	2.40	0.57
3:C:310:GLY:C	3:C:311:ILE:HD12	2.24	0.57
2:B:267:TYR:HB2	3:C:50:PHE:HD2	1.69	0.57
3:C:296:VAL:HG22	3:C:297:HIS:N	2.20	0.57
1:A:560:GLN:HE22	3:C:81:PHE:N	1.98	0.57
1:A:501:GLN:HG3	1:A:502:ASN:N	2.20	0.56
1:A:524:LEU:C	1:A:524:LEU:HD13	2.25	0.56
3:C:83:GLY:HA2	3:C:128:LEU:HD13	1.88	0.56
1:A:515:LEU:HD12	1:A:516:TYR:N	2.20	0.56
3:C:97:TYR:OH	3:C:109:GLU:HG3	2.06	0.56
3:C:213:TYR:HB3	3:C:257:LEU:O	2.06	0.55
2:B:235:MET:HB3	2:B:238:HIS:HD2	1.71	0.55
1:A:516:TYR:HD2	2:B:206:LEU:CB	2.08	0.55
3:C:259:VAL:CG1	3:C:260:SER:N	2.69	0.55
3:C:52:THR:O	3:C:114:GLU:HB2	2.07	0.55
3:C:40:LEU:HD11	3:C:166:LEU:HD11	1.87	0.55
1:A:473:ILE:O	1:A:477:VAL:HG13	2.07	0.55
1:A:489:LYS:HG3	2:B:187:TYR:H	1.71	0.55
3:C:248:LEU:O	3:C:250:ALA:N	2.38	0.54
1:A:497:ARG:CG	2:B:186:MET:SD	2.96	0.54
1:A:458:ALA:O	2:B:215:LEU:HD13	2.08	0.54
1:A:516:TYR:CD2	2:B:206:LEU:CB	2.80	0.54
3:C:109:GLU:CD	3:C:116:TRP:HZ3	2.12	0.53
3:C:109:GLU:CD	3:C:116:TRP:CZ3	2.82	0.53
3:C:259:VAL:HG12	3:C:263:LYS:HB3	1.90	0.53
3:C:48:VAL:O	3:C:72:PRO:HD2	2.09	0.53
3:C:297:HIS:HE1	5:C:403:TAM:H51	1.73	0.53
1:A:498:VAL:HG11	1:A:513:LEU:HD22	1.92	0.52
1:A:477:VAL:HG23	1:A:481:MET:HE2	1.90	0.52
1:A:489:LYS:HG3	2:B:186:MET:CA	2.39	0.52
3:C:259:VAL:HG12	3:C:260:SER:H	1.75	0.52
3:C:296:VAL:HG22	3:C:297:HIS:H	1.75	0.51
3:C:224:VAL:HG21	4:C:402:ATP:C6	2.45	0.51
3:C:313:SER:OG	4:C:402:ATP:H2'	2.10	0.51
3:C:280:LEU:H	3:C:280:LEU:HD12	1.75	0.51
1:A:561:PRO:HG3	3:C:157:PRO:HA	1.91	0.51
3:C:72:PRO:HA	3:C:84:MET:HE2	1.92	0.51
3:C:72:PRO:HG3	3:C:165:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:VAL:CG1	3:C:263:LYS:HB3	2.41	0.51
3:C:263:LYS:HD2	3:C:266:GLN:NE2	2.25	0.51
3:C:60:PHE:HE2	3:C:246:ILE:HD12	1.76	0.51
2:B:237:ASN:ND2	2:B:255:HIS:CD2	2.79	0.51
3:C:314:LEU:HB2	4:C:402:ATP:O2G	2.10	0.51
2:B:202:ALA:N	6:B:303:HOH:O	2.43	0.50
1:A:510:LYS:HG2	2:B:186:MET:HE2	1.93	0.50
3:C:256:ASN:OD1	3:C:256:ASN:N	2.43	0.50
3:C:94:LEU:HD23	3:C:106:TYR:CG	2.47	0.50
3:C:224:VAL:HG22	3:C:225:SER:N	2.26	0.50
1:A:489:LYS:HD2	2:B:186:MET:N	2.26	0.50
1:A:514:GLN:HG2	1:A:516:TYR:CE1	2.47	0.50
1:A:580:LEU:O	1:A:581:ALA:C	2.51	0.49
1:A:470:PRO:HG3	1:A:523:TYR:CZ	2.46	0.49
1:A:497:ARG:NH2	6:A:607:HOH:O	2.45	0.49
1:A:514:GLN:HG2	1:A:516:TYR:HE1	1.77	0.49
2:B:265:LEU:HD12	2:B:265:LEU:N	2.27	0.49
3:C:28:TYR:O	3:C:32:MET:HG2	2.12	0.49
3:C:98:TYR:CA	3:C:103:VAL:HG23	2.37	0.49
1:A:462:LEU:HD12	1:A:463:GLY:N	2.28	0.49
1:A:491:ILE:O	1:A:492:ASN:HB3	2.13	0.49
2:B:187:TYR:HE2	2:B:188:HIS:HD2	1.60	0.49
2:B:214:ILE:O	2:B:215:LEU:HD22	2.12	0.49
3:C:188:MET:O	3:C:285:GLU:HB2	2.13	0.48
3:C:109:GLU:O	3:C:110:GLU:HG3	2.13	0.48
3:C:294:ALA:O	3:C:295:GLU:HB2	2.14	0.48
3:C:55:GLN:O	3:C:56:VAL:C	2.52	0.48
3:C:243:PHE:O	3:C:247:ASN:ND2	2.46	0.48
1:A:495:HIS:HA	1:A:513:LEU:O	2.13	0.48
1:A:524:LEU:HD13	1:A:525:LEU:N	2.28	0.48
2:B:235:MET:HB3	2:B:238:HIS:CD2	2.49	0.48
3:C:291:LEU:HD13	3:C:299:LEU:HG	1.94	0.48
3:C:51:ASP:O	3:C:54:LEU:HB2	2.14	0.48
3:C:224:VAL:CG2	4:C:402:ATP:C5	2.97	0.48
1:A:466:SER:HB3	1:A:473:ILE:HD11	1.95	0.47
3:C:208:THR:O	3:C:262:THR:OG1	2.22	0.47
3:C:60:PHE:HB2	3:C:90:PHE:CE2	2.49	0.47
2:B:239:LEU:HD12	2:B:240:TYR:H	1.79	0.47
3:C:94:LEU:HA	3:C:106:TYR:CD1	2.49	0.47
3:C:274:GLY:N	6:C:520:HOH:O	2.47	0.47
1:A:470:PRO:HD3	1:A:523:TYR:HE2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:ILE:N	2:B:221:ILE:HD12	2.30	0.47
1:A:464:ILE:O	1:A:524:LEU:HD22	2.15	0.47
2:B:187:TYR:C	2:B:187:TYR:CD2	2.88	0.47
3:C:109:GLU:HG2	3:C:110:GLU:H	1.79	0.47
3:C:142:SER:HB2	3:C:146:ARG:NH2	2.30	0.47
1:A:473:ILE:HG22	1:A:474:MET:N	2.29	0.47
3:C:166:LEU:HD12	3:C:166:LEU:HA	1.66	0.47
3:C:211:PRO:O	3:C:214:VAL:N	2.38	0.47
3:C:280:LEU:HD12	3:C:280:LEU:N	2.29	0.47
3:C:297:HIS:CE1	5:C:403:TAM:H51	2.48	0.47
3:C:320:ALA:O	3:C:324:THR:HB	2.16	0.46
1:A:517:GLN:HG2	1:A:519:ASP:O	2.15	0.46
3:C:83:GLY:HA2	3:C:128:LEU:CD1	2.45	0.46
3:C:173:LYS:HB3	3:C:173:LYS:HE2	1.70	0.46
3:C:195:LEU:O	3:C:196:GLN:HB2	2.15	0.46
1:A:478:TYR:HD1	1:A:488:TRP:CE2	2.33	0.46
3:C:97:TYR:OH	3:C:116:TRP:HH2	1.97	0.46
3:C:191:SER:OG	3:C:194:GLU:HG3	2.15	0.46
3:C:259:VAL:CG1	3:C:260:SER:H	2.29	0.46
5:C:403:TAM:H22	6:C:521:HOH:O	2.16	0.46
3:C:104:GLN:H	3:C:104:GLN:CD	2.18	0.46
3:C:97:TYR:HE1	3:C:116:TRP:HZ2	1.63	0.46
1:A:475:LEU:HD22	1:A:479:ARG:HG3	1.98	0.46
3:C:172:LEU:HD13	3:C:318:LEU:CD1	2.45	0.46
3:C:315:SER:CB	4:C:402:ATP:O1B	2.55	0.46
2:B:206:LEU:HD11	2:B:211:LEU:CD1	2.46	0.45
1:A:474:MET:O	1:A:478:TYR:CD2	2.70	0.45
1:A:474:MET:CE	1:A:515:LEU:HB2	2.46	0.45
3:C:109:GLU:HG3	3:C:116:TRP:CH2	2.50	0.45
3:C:203:ILE:HG22	3:C:205:MET:HG3	1.99	0.45
3:C:60:PHE:CE2	3:C:246:ILE:HD12	2.52	0.45
3:C:69:ARG:N	3:C:69:ARG:HD2	2.32	0.45
3:C:210:THR:HG23	3:C:211:PRO:HD2	1.98	0.45
1:A:494:TYR:HB2	6:A:619:HOH:O	2.16	0.44
2:B:267:TYR:HB2	3:C:50:PHE:CD2	2.52	0.44
3:C:299:LEU:HB2	3:C:312:VAL:HG13	1.99	0.44
3:C:240:TYR:HD2	3:C:265:LEU:HD21	1.81	0.44
3:C:296:VAL:HG22	3:C:298:ARG:H	1.83	0.44
2:B:269:PRO:HG2	3:C:53:SER:OG	2.17	0.44
3:C:278:CYS:HB2	3:C:282:GLU:OE2	2.18	0.44
1:A:499:ARG:CZ	2:B:186:MET:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:GLU:HG3	3:C:186:GLU:H	1.49	0.44
3:C:205:MET:SD	3:C:308:VAL:HG21	2.58	0.44
1:A:507:LYS:NZ	1:A:562:THR:O	2.47	0.44
2:B:206:LEU:HD12	2:B:207:PRO:HD2	2.00	0.43
1:A:477:VAL:CG2	1:A:478:TYR:N	2.81	0.43
1:A:489:LYS:CG	2:B:186:MET:HA	2.43	0.43
3:C:154:VAL:O	3:C:163:LEU:N	2.44	0.43
1:A:499:ARG:HB3	2:B:186:MET:CG	2.46	0.43
3:C:109:GLU:CG	3:C:110:GLU:N	2.82	0.43
1:A:462:LEU:HD12	1:A:463:GLY:H	1.82	0.43
1:A:516:TYR:CE2	2:B:206:LEU:CD1	3.01	0.43
3:C:87:ILE:HG13	3:C:243:PHE:CD2	2.54	0.43
3:C:151:ARG:NH1	5:C:403:TAM:H32	2.19	0.43
3:C:175:LEU:HD22	3:C:179:ILE:HG13	2.00	0.43
3:C:145:ILE:HD12	3:C:323:LEU:CD2	2.49	0.43
3:C:40:LEU:HB3	3:C:174:PHE:CD2	2.53	0.43
3:C:294:ALA:O	3:C:295:GLU:CB	2.66	0.43
1:A:474:MET:HB3	1:A:478:TYR:HE2	1.83	0.43
1:A:470:PRO:O	1:A:474:MET:HG2	2.19	0.42
3:C:185:PRO:HD2	3:C:188:MET:CG	2.46	0.42
3:C:71:ALA:HA	3:C:72:PRO:HD3	1.85	0.42
3:C:91:ILE:HD13	3:C:246:ILE:HG23	2.01	0.42
1:A:528:LYS:HG3	2:B:238:HIS:CE1	2.54	0.42
3:C:266:GLN:HE21	3:C:266:GLN:HB2	1.63	0.42
3:C:69:ARG:HD3	5:C:403:TAM:C6	2.50	0.42
3:C:195:LEU:CB	3:C:197:ILE:HD12	2.43	0.42
3:C:91:ILE:HA	3:C:91:ILE:HD13	1.88	0.42
3:C:216:LEU:O	3:C:217:GLY:C	2.56	0.42
1:A:505:THR:HG22	1:A:507:LYS:HG3	2.02	0.42
1:A:482:LYS:HD2	2:B:189:GLN:OE1	2.19	0.42
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.81	0.42
1:A:510:LYS:CG	2:B:186:MET:HE2	2.49	0.42
3:C:100:SER:O	3:C:101:ALA:HB3	2.20	0.42
3:C:310:GLY:O	3:C:311:ILE:HD12	2.20	0.42
1:A:527:PHE:HB2	2:B:239:LEU:HB3	2.02	0.42
3:C:265:LEU:HD22	3:C:268:ARG:CZ	2.50	0.41
1:A:487:GLU:OE2	1:A:499:ARG:NH2	2.53	0.41
1:A:484:LEU:HD21	1:A:576:LEU:HA	2.02	0.41
3:C:200:TYR:CD2	3:C:310:GLY:HA3	2.55	0.41
1:A:564:HIS:HB3	6:C:552:HOH:O	2.21	0.41
3:C:256:ASN:O	3:C:257:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:PHE:CE1	1:A:573:CYS:SG	3.14	0.41
3:C:313:SER:O	3:C:317:ILE:HG12	2.20	0.41
1:A:495:HIS:CD2	1:A:514:GLN:OE1	2.74	0.41
3:C:137:LEU:HD12	3:C:137:LEU:HA	1.48	0.41
3:C:207:ARG:O	3:C:208:THR:C	2.59	0.41
3:C:218:ILE:HD11	3:C:227:LEU:CD1	2.51	0.41
3:C:176:LYS:HE2	3:C:180:THR:CG2	2.48	0.41
3:C:260:SER:O	3:C:261:VAL:C	2.59	0.41
1:A:525:LEU:HD12	1:A:526:ASP:H	1.86	0.41
1:A:567:MET:O	1:A:571:GLU:HG3	2.20	0.41
3:C:191:SER:HA	3:C:283:THR:HA	2.01	0.41
3:C:192:LEU:HD21	3:C:287:ILE:HG13	2.03	0.41
5:C:403:TAM:N	5:C:403:TAM:O5	2.38	0.41
2:B:188:HIS:HE1	2:B:190:GLU:O	2.04	0.40
2:B:214:ILE:CG2	2:B:215:LEU:N	2.84	0.40
1:A:567:MET:HE1	2:B:266:LEU:HD13	2.03	0.40
3:C:84:MET:HE3	3:C:153:PRO:HG3	2.03	0.40
3:C:36:ARG:N	3:C:39:ASP:OD2	2.52	0.40
3:C:52:THR:HG22	3:C:73:LEU:HB3	2.02	0.40
2:B:187:TYR:CD2	2:B:188:HIS:N	2.84	0.40
3:C:163:LEU:N	3:C:163:LEU:HD23	2.37	0.40
3:C:279:TYR:CE2	3:C:302:VAL:HG12	2.57	0.40
1:A:510:LYS:HG2	2:B:186:MET:CE	2.51	0.40
3:C:211:PRO:O	3:C:212:VAL:C	2.59	0.40
5:C:403:TAM:H41	5:C:403:TAM:H21	1.64	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	94/130 (72%)	80 (85%)	13 (14%)	1 (1%)	14 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	48/85 (56%)	43 (90%)	4 (8%)	1 (2%)	7 18
3	C	283/330 (86%)	255 (90%)	24 (8%)	4 (1%)	11 28
All	All	425/545 (78%)	378 (89%)	41 (10%)	6 (1%)	11 28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	212	GLN
3	C	249	ALA
3	C	267	HIS
3	C	56	VAL
3	C	208	THR
1	A	473	ILE

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	88/116 (76%)	76 (86%)	12 (14%)	3 8
2	B	53/79 (67%)	50 (94%)	3 (6%)	20 44
3	C	264/299 (88%)	235 (89%)	29 (11%)	6 14
All	All	405/494 (82%)	361 (89%)	44 (11%)	6 14

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	ASP
1	A	475	LEU
1	A	477	VAL
1	A	484	LEU
1	A	485	SER
1	A	498	VAL
1	A	502	ASN
1	A	513	LEU

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Mol	Chain	Res	Type
1	A	518	VAL
1	A	531	THR
1	A	560	GLN
1	A	580	LEU
2	B	186	MET
2	B	187	TYR
2	B	233	HIS
3	C	40	LEU
3	C	45	SER
3	C	54	LEU
3	C	87	ILE
3	C	94	LEU
3	C	109	GLU
3	C	116	TRP
3	C	126	LYS
3	C	137	LEU
3	C	142	SER
3	C	166	LEU
3	C	175	LEU
3	C	186	GLU
3	C	213	TYR
3	C	216	LEU
3	C	218	ILE
3	C	219	PHE
3	C	225	SER
3	C	256	ASN
3	C	257	LEU
3	C	261	VAL
3	C	276	LEU
3	C	284	LEU
3	C	298	ARG
3	C	302	VAL
3	C	304	GLU
3	C	308	VAL
3	C	318	LEU
3	C	323	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	HIS
1	A	495	HIS

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Mol	Chain	Res	Type
1	A	502	ASN
1	A	560	GLN
1	A	564	HIS
2	B	212	GLN
2	B	237	ASN
2	B	238	HIS
2	B	255	HIS
3	C	111	HIS
3	C	161	ASN
3	C	202	ASN
3	C	247	ASN
3	C	256	ASN
3	C	266	GLN
3	C	297	HIS

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

3 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	$\#\|Z\|>2$
4	ATP	C	401	-	26,33,33	0.95	1 (3%)	31,52,52	1.48	5 (16%)
5	TAM	C	403	-	7,10,10	0.36	0	9,12,12	0.83	0
4	ATP	C	402	-	26,33,33	1.03	2 (7%)	31,52,52	1.63	8 (25%)

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	C	401	-	-	2/18/38/38	0/3/3/3
5	TAM	C	403	-	-	8/12/12/12	-
4	ATP	C	402	-	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	ATP	C5-C4	2.77	1.48	1.40
4	C	401	ATP	C5-C4	2.60	1.47	1.40
4	C	402	ATP	O4'-C1'	2.25	1.44	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	ATP	PB-O3B-PG	-4.04	118.95	132.83
4	C	401	ATP	PB-O3B-PG	-3.43	121.06	132.83
4	C	401	ATP	C4-C5-N7	-3.29	105.97	109.40
4	C	402	ATP	C4-C5-N7	-3.27	105.99	109.40
4	C	402	ATP	N3-C2-N1	-2.86	124.21	128.68
4	C	402	ATP	C2-N1-C6	2.47	122.97	118.75
4	C	401	ATP	PA-O3A-PB	-2.39	124.62	132.83
4	C	401	ATP	O3G-PG-O2G	2.27	116.33	107.64
4	C	402	ATP	C5-C6-N6	2.27	123.81	120.35
4	C	401	ATP	N3-C2-N1	-2.19	125.26	128.68
4	C	402	ATP	PA-O3A-PB	-2.18	125.35	132.83
4	C	402	ATP	C3'-C2'-C1'	2.12	104.16	100.98
4	C	402	ATP	O3G-PG-O2G	2.10	115.66	107.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	TAM	C2-C-C1-C4
5	C	403	TAM	C3-C-C1-C4
5	C	403	TAM	N-C-C1-C4
5	C	403	TAM	C1-C-C2-C5
5	C	403	TAM	C3-C-C2-C5
5	C	403	TAM	N-C-C2-C5
5	C	403	TAM	N-C-C3-C6
5	C	403	TAM	C2-C-C3-C6
4	C	402	ATP	PG-O3B-PB-O2B
4	C	402	ATP	PA-O3A-PB-O1B
4	C	401	ATP	PB-O3B-PG-O2G
4	C	401	ATP	PB-O3B-PG-O3G
4	C	402	ATP	PG-O3B-PB-O1B
4	C	402	ATP	PA-O3A-PB-O2B

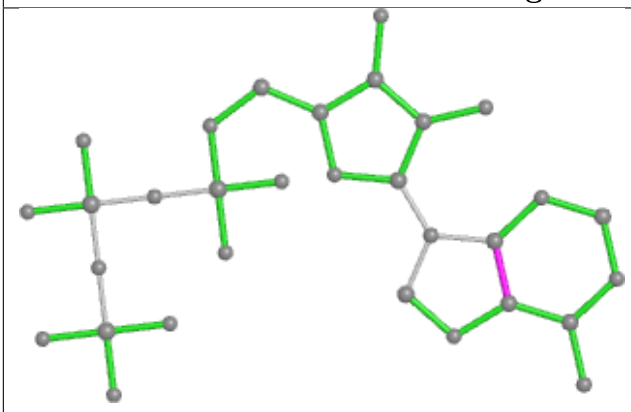
There are no ring outliers.

2 monomers are involved in 17 short contacts:

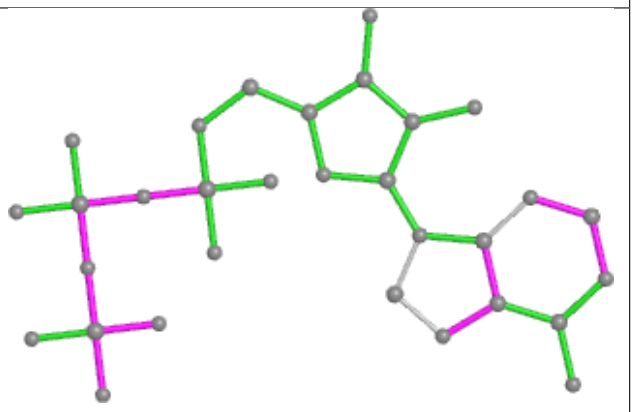
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	TAM	9	0
4	C	402	ATP	8	0

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.

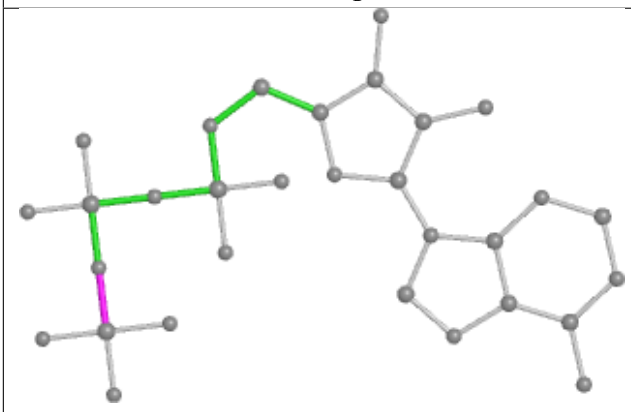
Ligand ATP C 401



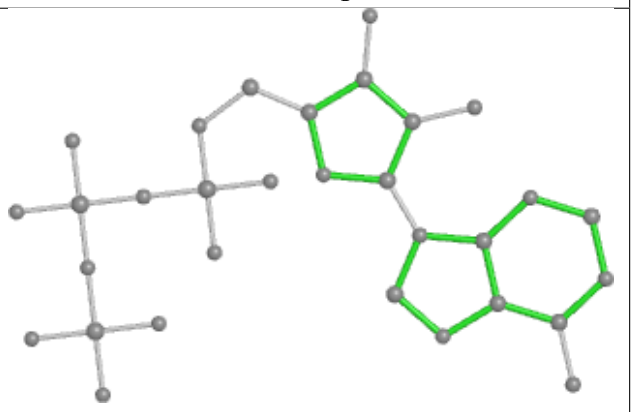
Bond lengths



Bond angles

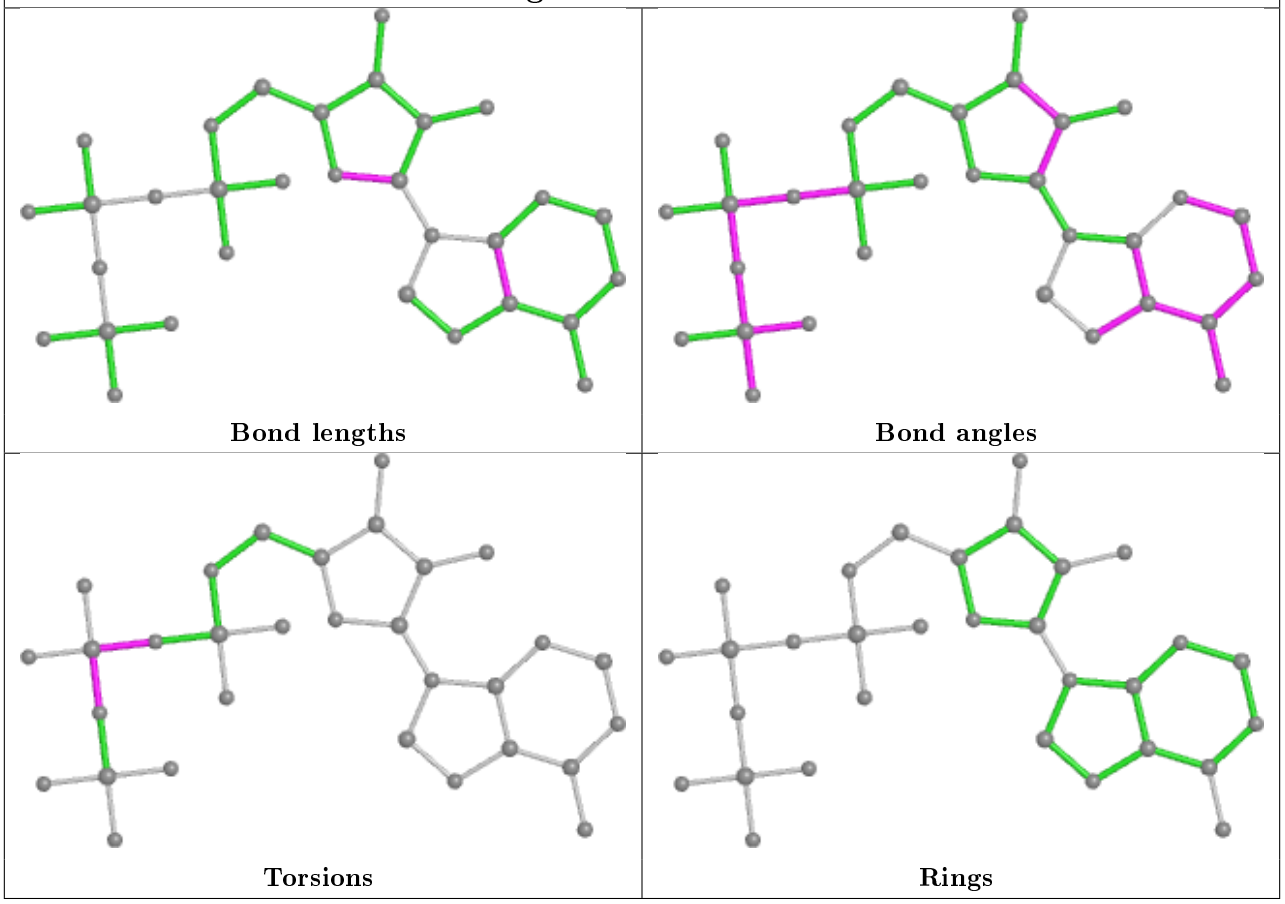


Torsions



Rings

Ligand ATP C 402



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, 95^{th} 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	98/130 (75%)	-0.16	3 (3%) 49 49	22, 53, 99, 108	0
2	B	58/85 (68%)	0.44	11 (18%) 1 0	19, 52, 109, 116	0
3	C	289/330 (87%)	-0.51	3 (1%) 82 83	5, 32, 70, 147	0
All	All	445/545 (81%)	-0.31	17 (3%) 40 39	5, 39, 89, 147	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	125	PHE	4.3
2	B	214	ILE	4.3
2	B	220	GLY	4.1
3	C	267	HIS	3.7
1	A	582	ARG	3.6
2	B	212	GLN	3.1
2	B	270	ILE	2.9
2	B	190	GLU	2.7
2	B	215	LEU	2.7
2	B	233	HIS	2.6
2	B	187	TYR	2.5
1	A	520	ALA	2.5
1	A	475	LEU	2.4
3	C	305	HIS	2.3
2	B	213	VAL	2.3
2	B	246	ASP	2.0
2	B	186	MET	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 carbohydrates in this entry.

6.4 Ligands (i)

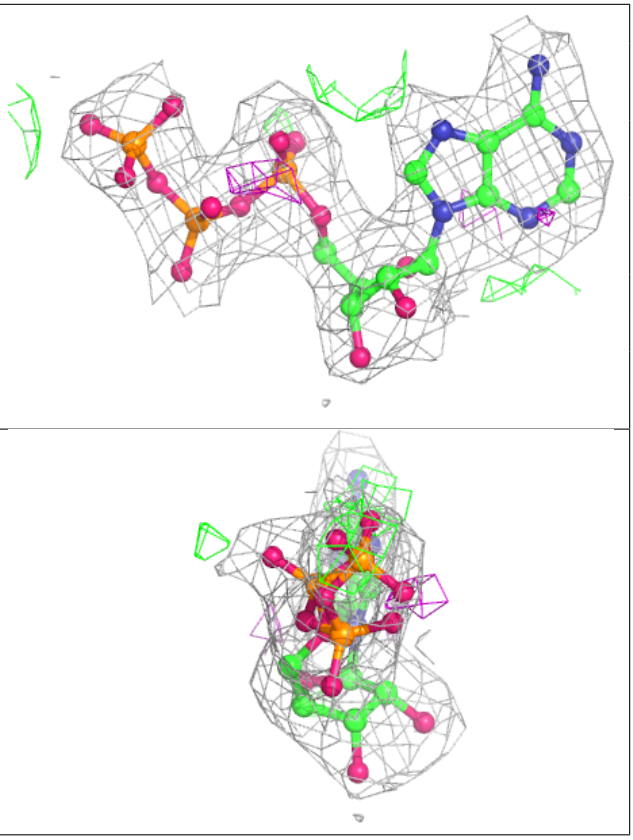
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	TAM	C	403	11/11	0.92	0.24	28,46,73,75	0
4	ATP	C	402	31/31	0.98	0.11	8,28,68,95	0
4	ATP	C	401	31/31	0.99	0.13	0,19,51,74	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.

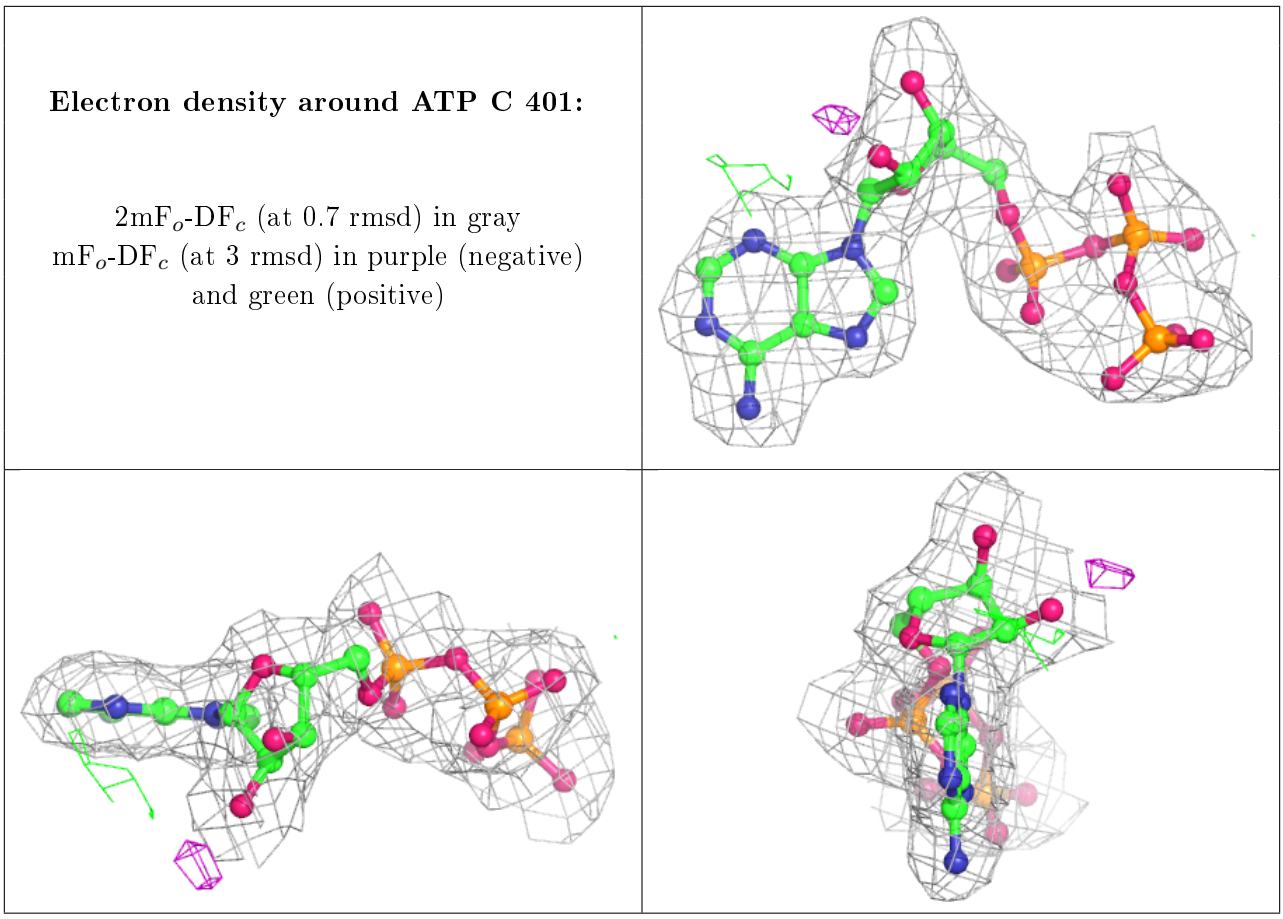
Electron density around ATP C 402:

$2mF_o$-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 C 401:

$2mF_o$-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.