wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:13 AM GMT

PDB ID	:	3LC6
Title	:	The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli
Authors	:	Zheng, J.; Jia, Z.
Deposited on	:	2010-01-09
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

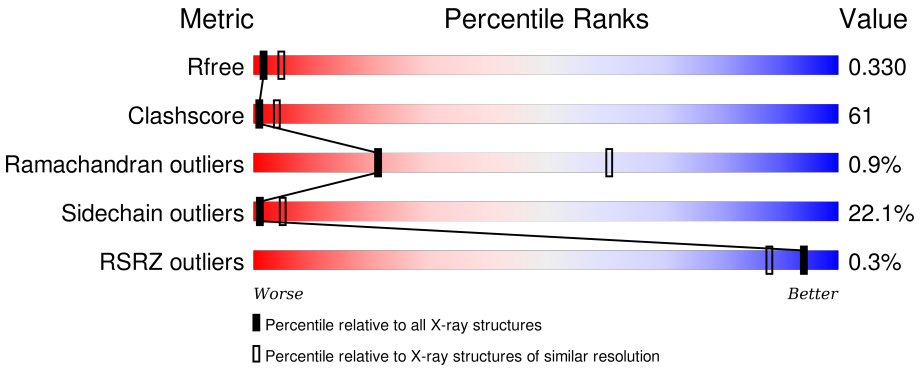
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	578	% 24% 56% 14% • 5%
1	B	578	27% 52% 14% 7%

2 Entry composition

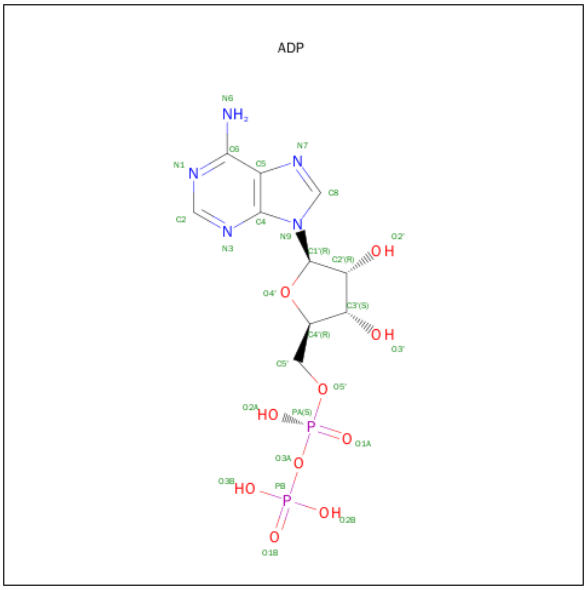
There are 5 unique types of molecules in this entry. The entry contains 9107 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4526	2906	800	799	21			
1	B	539	Total	C	N	O	S	0	0	0
			4454	2861	785	788	20			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

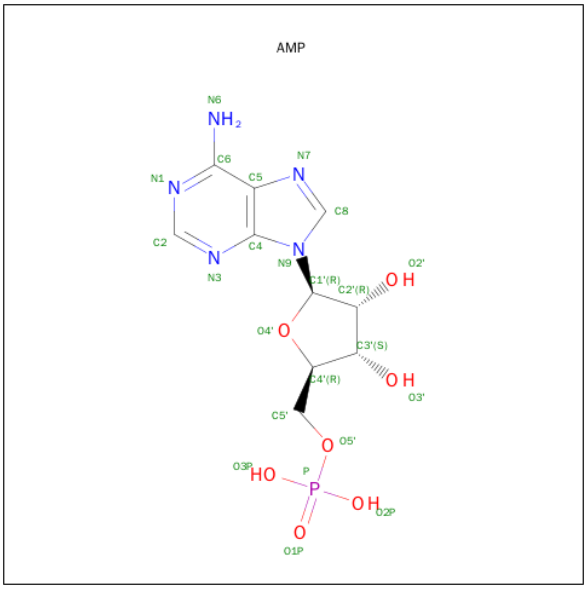


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 5 is water.

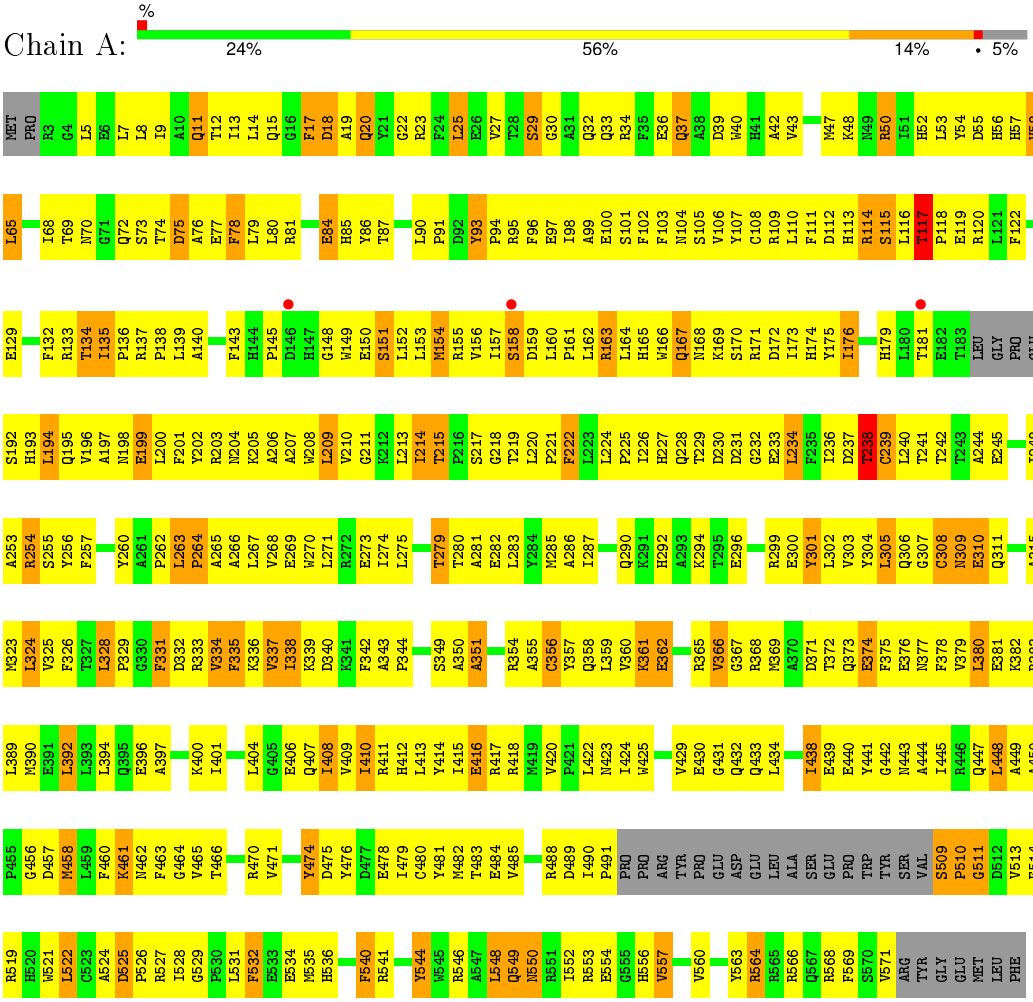
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	31	Total O 31 31	0	0
5	B	45	Total O 45 45	0	0

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 errors 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.

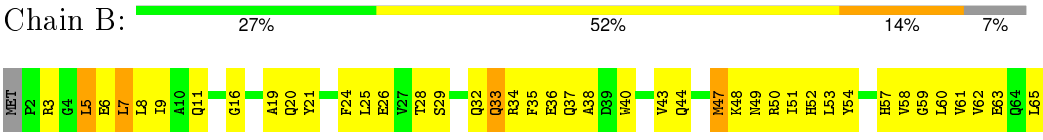
- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase

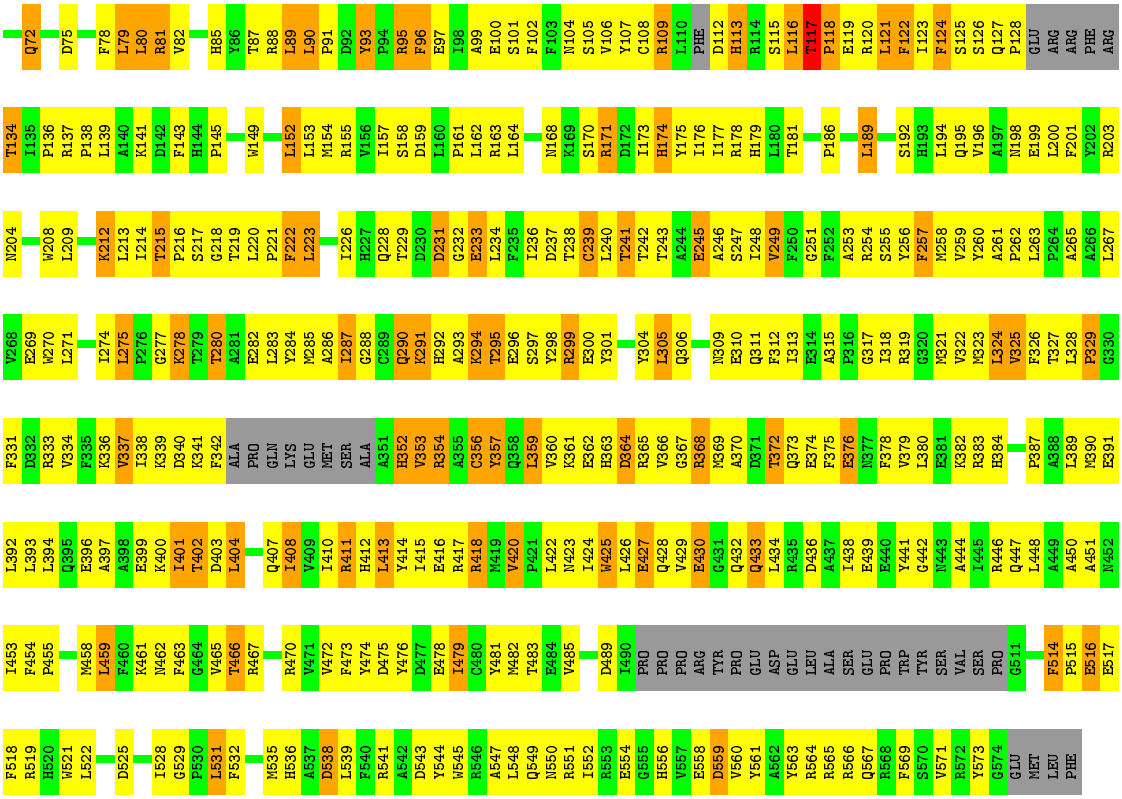
Chain A:



- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase

Chain B:




Q72 D75 F78 L79 L80 R81 V82 H85 Y86 T87 R88 L89 L90 P91 D92 Y93 P94 R95 F96 E97 I98 A99 E100 S101 F102 F103 N104 S105 V106 Y107 C108 R109 L110 PHE D112 H113 R114 S115 L116 T117 P118 E119 R120 L121 F122 I123 F124 S125 S126 Q127 P128 GLU ARG ARG PHE ARG
T134 I135 P136 R137 P138 L139 A140 K141 D142 F143 H144 P145 W149 L152 L153 M154 R155 V156 I157 S158 D159 L160 P161 L162 R163 L164 N168 K169 S170 R171 D172 I173 H174 Y175 I176 I177 R178 H179 L180 T181 P186 L189 S192 H193 L194 Q195 V196 A197 N198 E199 L200 F201 Y202 R203
N204 W208 L209 K212 L213 I214 T215 P216 S217 G218 T219 L220 P221 F222 L223 I226 H227 Q228 T229 D230 D231 G232 E233 L234 F235 I236 D237 T238 G239 L240 T241 T242 T243 A244 E245 A246 S247 I248 V249 F250 G251 F252 A253 R254 S255 Y256 F257 M258 V259 Y260 A261 P262 L263 P264 A265 A266 L267
V268 E269 W270 I271 I274 L275 P276 G277 K278 T279 T280 A281 E282 L283 Y284 M285 A286 I287 G288 C289 Q290 K291 H292 A293 K294 T295 E296 S297 Y298 R299 E300 Y301 Y304 L305 Q306 M309 E310 Q311 F312 I313 E314 A315 P316 G317 I318 R319 G320 M321 V322 M323 L324 V325 F326 T327 L328 P329 G330
F331 D332 R333 V334 F335 K336 V337 I338 K339 D340 K341 F342 ALA PRO GLN LYS GLU MET SER ALA A351 H352 V353 R354 A355 C356 Y357 Q358 L359 V360 K361 E362 H363 D364 R365 V366 G367 R368 M369 A370 D371 T372 Q373 E374 F375 E376 N377 F378 V379 L380 E381 K382 R383 H384 P387 A388 L389 M390 E391
L392 L393 L394 Q395 E396 A397 A398 E399 K400 I401 T402 D403 L404 Q407 I408 V409 I410 R411 H412 L413 Y414 I415 E416 R417 R418 Y419 V420 P421 L422 N423 I424 W425 L426 E427 Q428 V429 E430 G431 Q432 Q433 L434 R435 D436 A437 I438 E439 E440 Y441 G442 W443 A444 I445 R446 Q447 L448 A449 A450 A451 N452
I453 F454 P455 M458 L459 F460 K461 N462 F463 G464 V465 T466 R467 R470 V471 V472 F473 Y474 D475 Y476 D477 E478 I479 C480 Y481 M482 T483 E484 V485 D489 I490 PRO PRO PRO ARG TYR PRO GLU ASP GLU LEU ALA SER GLU PRO TRP TYR SER VAL SER PRO G511 F514 P515 E516 E517
F518 R519 H520 W521 L522 D525 I528 G529 P530 L531 F532 M535 H536 A537 D538 L539 F540 R541 A542 D543 Y544 W545 R546 A547 L548 Q549 N550 R551 I552 R553 E554 G555 H556 V557 E558 D559 V560 Y561 A562 Y563 R564 R565 R566 Q567 R568 F569 S570 V571 R572 Y573 G574 GLU MET LEU PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.14Å 133.76Å 187.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	83.1 (10.00-3.10) 83.7 (10.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	16.46 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.287 , 0.332 0.292 , 0.330	Depositor DCC
R_{free} test set	1191 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 82.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 24325 reflections	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	9107	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, MG, ADP

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	0.62	2/4643 (0.0%)	0.80	7/6283 (0.1%)
1	B	0.57	1/4567 (0.0%)	0.77	1/6179 (0.0%)
All	All	0.60	3/9210 (0.0%)	0.79	8/12462 (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
1	A	1	5
1	B	0	2
All	All	1	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	CYS	CB-SG	-6.93	1.70	1.82
1	A	511	GLY	N-CA	6.30	1.55	1.46
1	A	356	CYS	CB-SG	-5.39	1.73	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	PRO	N-CA-C	-8.62	89.69	112.10
1	A	239	CYS	N-CA-C	7.35	130.85	111.00
1	A	509	SER	N-CA-CB	-6.98	100.02	110.50
1	A	238	THR	N-CA-C	6.78	129.31	111.00
1	B	240	LEU	CA-CB-CG	6.74	130.80	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	239	CYS	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	THR	Peptide
1	A	128	PRO	Peptide
1	A	230	ASP	Peptide
1	A	350	ALA	Peptide
1	A	510	PRO	Peptide

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	4526	0	4449	592	7
1	B	4454	0	4376	518	7
2	A	27	0	12	5	0
3	A	1	0	0	0	0
4	B	23	0	12	2	0
5	A	31	0	0	12	0
5	B	45	0	0	11	0
All	All	9107	0	8849	1095	7

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 61.

The worst 5 of 1095 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:279:THR:OG1	1:A:282:GLU:HG3	1.16	1.29
1:A:200:LEU:HD23	1:A:201:PHE:N	1.48	1.29
1:A:128:PRO:HB2	1:A:129:GLU:CA	1.56	1.29
1:B:550:ASN:O	1:B:554:GLU:HG3	1.31	1.29
1:A:23:ARG:O	1:A:27:VAL:HG23	1.37	1.25

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ASN:ND2	1:B:427:GLU:CD[2_455]	1.48	0.72
1:A:423:ASN:CG	1:B:427:GLU:OE2[2_455]	1.55	0.65
1:A:423:ASN:ND2	1:B:427:GLU:OE1[2_455]	1.74	0.46
1:A:423:ASN:ND2	1:B:427:GLU:OE2[2_455]	1.98	0.22
1:A:423:ASN:CG	1:B:427:GLU:CD[2_455]	2.01	0.19

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	541/578 (94%)	470 (87%)	65 (12%)	6 (1%)	17	55
1	B	529/578 (92%)	457 (86%)	68 (13%)	4 (1%)	24	63
All	All	1070/1156 (93%)	927 (87%)	133 (12%)	10 (1%)	21	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	GLY
1	A	366	VAL
1	A	511	GLY
1	B	118	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	480/508 (94%)	382 (80%)	98 (20%)	1 6
1	B	472/508 (93%)	360 (76%)	112 (24%)	1 3
All	All	952/1016 (94%)	742 (78%)	210 (22%)	1 5

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	554	GLU
1	B	112	ASP
1	B	433	GLN
1	A	564	ARG
1	B	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	32	GLN
1	B	363	HIS
1	A	536	HIS
1	B	64	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ADP	A	1762	3	22,29,29	0.86	1 (4%)	27,45,45	2.79	5 (18%)
4	AMP	B	1604	-	20,25,25	1.05	1 (5%)	22,38,38	2.37	6 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1762	3	-	0/12/32/32	0/3/3/3
4	AMP	B	1604	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1762	ADP	C5-C4	2.57	1.46	1.40
4	B	1604	AMP	C5-C4	3.07	1.47	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1762	ADP	N3-C2-N1	-8.70	122.23	128.89
2	A	1762	ADP	C2'-C1'-N9	-8.67	101.05	114.29
4	B	1604	AMP	N3-C2-N1	-8.11	122.69	128.89
2	A	1762	ADP	PA-O3A-PB	-4.26	118.39	132.67
4	B	1604	AMP	C4-C5-N7	-3.91	105.88	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1762	ADP	5	0
4	B	1604	AMP	2	0

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	547/578 (94%)	-0.23	3 (0%) 91 83	2, 15, 29, 37	0
1	B	539/578 (93%)	-0.16	0 100 100	4, 18, 28, 34	0
All	All	1086/1156 (93%)	-0.19	3 (0%) 94 88	2, 17, 29, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	THR	3.4
1	A	158	SER	2.3
1	A	146	ASP	2.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	A	1762	27/27	0.95	0.15	-0.90	6,10,11,12	0
4	AMP	B	1604	23/23	0.93	0.17	-1.26	23,25,31,34	0
3	MG	A	579	1/1	0.98	0.20	-	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.