wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:57 PM GMT

PDB ID	:	1RFQ
Title	:	Actin Crystal Dynamics: Structural Implications for F-actin Nucleation, Polymerization and Branching Mediated by the Anti-parallel Dimer
Authors	:	Reutzel, R.; Yoshioka, C.; Govindasamy, L.; Yarmola, E.G.; Agbandje-McKenna, M.; Bubb, M.R.; McKenna, R.
Deposited on	:	2003-11-10
Resolution	:	3.00 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:

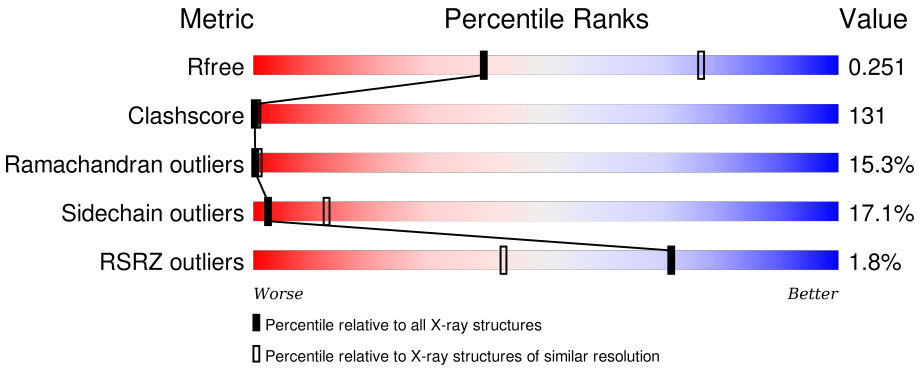
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	375	13% 58% 23%
1	B	375	3% 8% 59% 26%

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
2	MG	A	378	-	-	-	X
3	ATP	A	376	-	-	X	-
3	ATP	B	386	-	-	X	-
4	LAR	A	377	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5824 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.

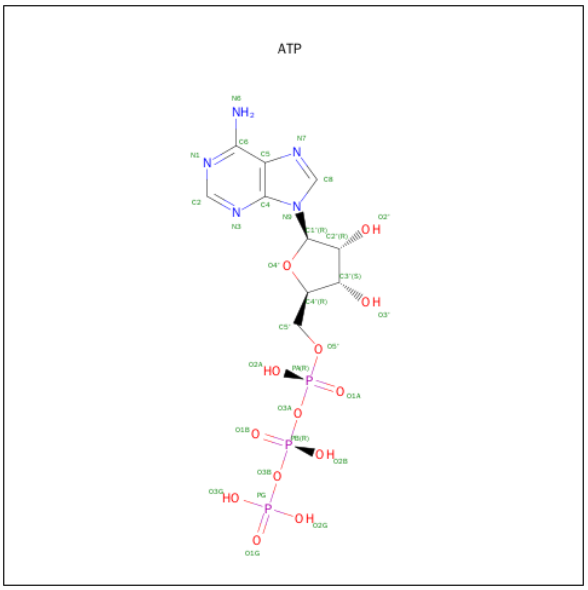
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2829	1794	476	540	19			
1	B	361	Total	C	N	O	S	0	0	0
			2829	1794	476	540	19			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

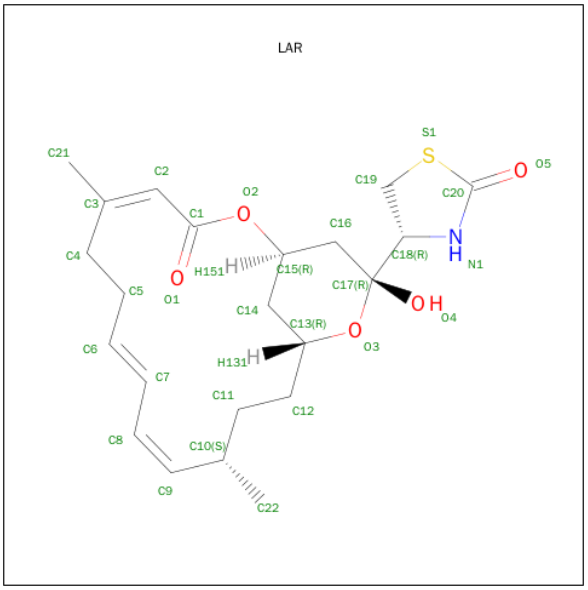
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 5 is water.

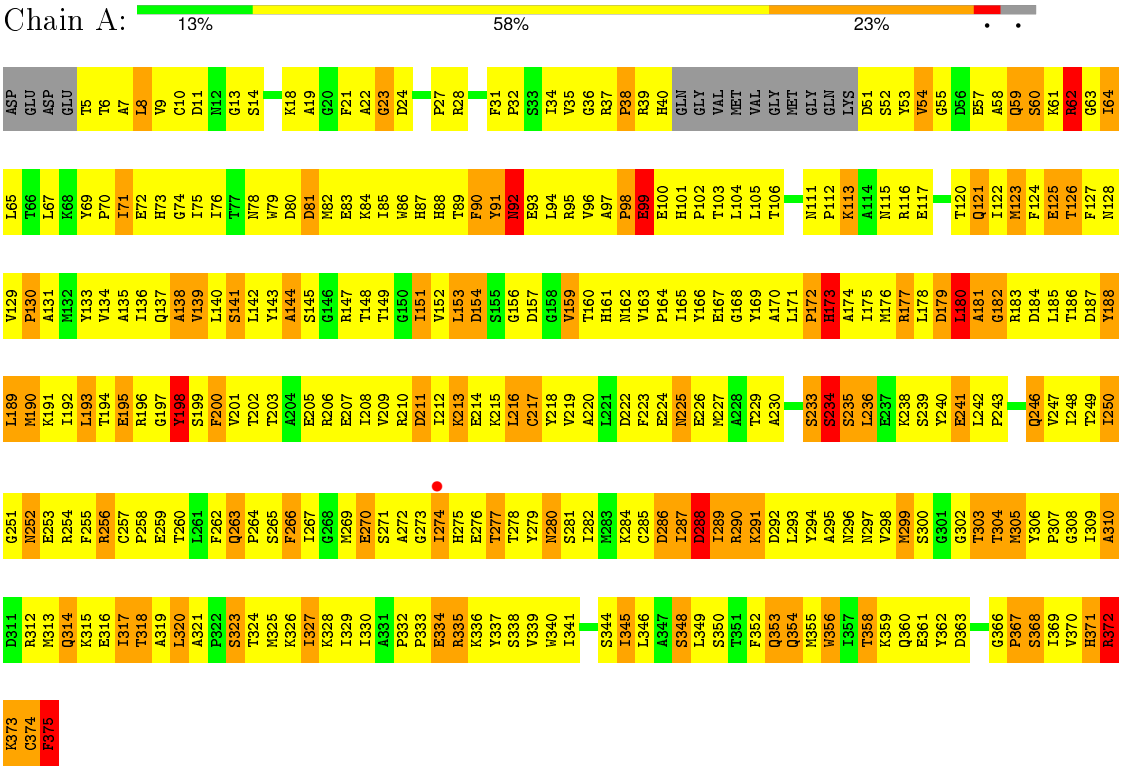
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	22	Total	O	0	0
			22	22		

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.

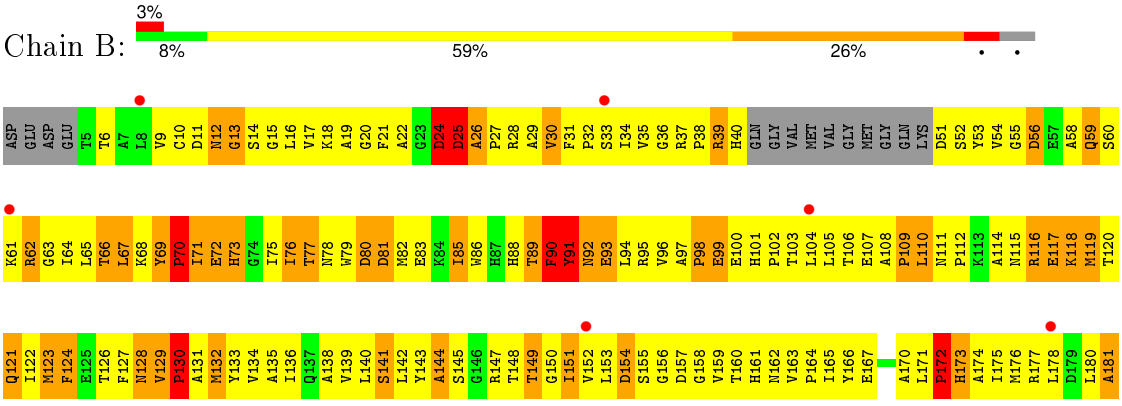
- Molecule 1: Actin, alpha skeletal muscle

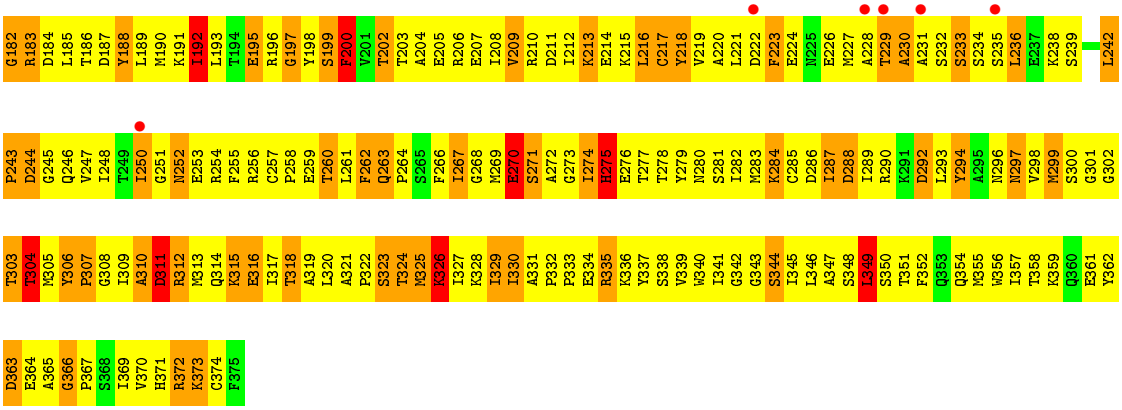
Chain A:



- Molecule 1: Actin, alpha skeletal muscle

Chain B:




G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 M227 A228 T229 A230 A231 S232 S233 S234 S235 L236 E237 K238 S239 L242
P243 D244 G245 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 E270 S271 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 N297 V298 M299 S300 G301 G302
T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360 E361 Y362
D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 K373 C374 F375

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	101.50Å 101.50Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 46.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 98.6 (46.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.261 0.205 , 0.251	Depositor DCC
R_{free} test set	2858 reflections (15.83%)	DCC
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 125.7	EDS
Estimated twinning fraction	0.089 for -h,-l,-k 0.088 for -h,l,k 0.094 for l,-k,h 0.096 for -l,-k,-h 0.368 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 21063 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5824	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, ATP, LAR

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	0.63	2/2891 (0.1%)	1.03	20/3919 (0.5%)
1	B	0.64	2/2891 (0.1%)	1.02	18/3919 (0.5%)
All	All	0.63	4/5782 (0.1%)	1.02	38/7838 (0.5%)

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	0	4
1	B	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	SER	N-CA	16.41	1.79	1.46
1	B	200	PHE	N-CA	11.99	1.70	1.46
1	B	25	ASP	C-N	-6.15	1.20	1.34
1	A	374	CYS	CB-SG	-5.57	1.72	1.81

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	200	PHE	CB-CG-CD1	12.53	129.57	120.80
1	B	200	PHE	CB-CG-CD2	-11.75	112.57	120.80
1	A	272	ALA	C-N-CA	-10.81	99.61	122.30
1	A	200	PHE	CB-CG-CD2	9.51	127.46	120.80
1	A	270	GLU	N-CA-CB	9.40	127.52	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	TYR	Sidechain
1	A	234	SER	Mainchain,Peptide
1	A	372	ARG	Mainchain
1	B	91	TYR	Mainchain

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	2829	0	2794	703	0
1	B	2829	0	2793	838	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	9	0
3	B	31	0	12	10	0
4	A	29	0	31	2	0
4	B	29	0	31	10	0
5	A	22	0	0	6	0
5	B	22	0	0	6	0
All	All	5824	0	5673	1501	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 131.

The worst 5 of 1501 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:373:LYS:NZ	1:B:373:LYS:CA	1.67	1.54
1:B:200:PHE:N	1:B:200:PHE:CA	1.70	1.52
1:A:235:SER:CA	1:A:235:SER:N	1.79	1.44
1:B:103:THR:O	1:B:356:TRP:CZ3	1.71	1.44
1:B:21:PHE:CB	1:B:24:ASP:OD2	1.65	1.43

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	357/375 (95%)	223 (62%)	84 (24%)	50 (14%)	0 1
1	B	357/375 (95%)	210 (59%)	88 (25%)	59 (16%)	0 1
All	All	714/750 (95%)	433 (61%)	172 (24%)	109 (15%)	0 1

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
1	A	92	ASN
1	A	99	GLU
1	A	138	ALA
1	A	139	VAL

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	307/318 (96%)	261 (85%)	46 (15%)	3 17
1	B	307/318 (96%)	248 (81%)	59 (19%)	2 10
All	All	614/636 (96%)	509 (83%)	105 (17%)	2 12

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	ARG

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Mol	Chain	Res	Type
1	B	99	GLU
1	B	311	ASP
1	B	56	ASP
1	B	72	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	B	59	GLN
1	B	354	GLN
1	A	371	HIS
1	B	73	HIS

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\|>2$
3	ATP	A	376	2	24,33,33	2.24	8 (33%)	31,52,52	2.98	11 (35%)
4	LAR	A	377	-	29,31,31	1.46	4 (13%)	29,43,43	1.98	5 (17%)
3	ATP	B	386	2	24,33,33	2.17	9 (37%)	31,52,52	3.14	10 (32%)
4	LAR	B	387	-	29,31,31	1.43	5 (17%)	29,43,43	1.98	5 (17%)

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
3	ATP	A	376	2	-	0/18/38/38	0/3/3/3
4	LAR	A	377	-	-	0/23/51/51	0/1/3/3
3	ATP	B	386	2	-	0/18/38/38	0/3/3/3
4	LAR	B	387	-	-	0/23/51/51	0/1/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	386	ATP	O5'-C5'	-4.54	1.26	1.44
3	A	376	ATP	O5'-C5'	-4.41	1.26	1.44
4	A	377	LAR	C20-N1	-3.01	1.32	1.36
3	A	376	ATP	PB-O1B	-2.85	1.40	1.51
4	B	387	LAR	C20-N1	-2.70	1.32	1.36

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	386	ATP	O5'-PA-O1A	-7.44	80.74	109.62
3	A	376	ATP	O5'-PA-O1A	-7.32	81.21	109.62
3	B	386	ATP	C5'-C4'-C3'	-4.60	96.93	115.21
3	A	376	ATP	O3A-PA-O5'	-4.04	92.23	102.94
3	B	386	ATP	C4'-O4'-C1'	-3.92	105.41	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	376	ATP	9	0
4	A	377	LAR	2	0
3	B	386	ATP	10	0
4	B	387	LAR	10	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	361/375 (96%)	0.07	1 (0%) 94 84	38, 57, 75, 82	0
1	B	361/375 (96%)	0.25	12 (3%) 50 22	42, 68, 83, 96	0
All	All	722/750 (96%)	0.16	13 (1%) 71 43	38, 63, 80, 96	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	3.6
1	B	33	SER	3.1
1	B	228	ALA	3.0
1	B	104	LEU	2.9
1	B	178	LEU	2.9

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
4	LAR	A	377	29/29	0.92	0.38	2.55	61,67,74,75	0
2	MG	A	378	1/1	0.93	0.26	2.41	36,36,36,36	0
4	LAR	B	387	29/29	0.89	0.31	1.14	66,71,78,78	0
2	MG	B	388	1/1	0.84	0.25	0.65	42,42,42,42	0
3	ATP	A	376	31/31	0.95	0.22	-0.31	37,50,55,56	0
3	ATP	B	386	31/31	0.93	0.19	-0.51	53,57,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.