



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:30 AM GMT

PDB ID : 3M6G  
Title : Crystal structure of actin in complex with lobophorolide  
Authors : Allingham, J.S.  
Deposited on : 2010-03-15  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

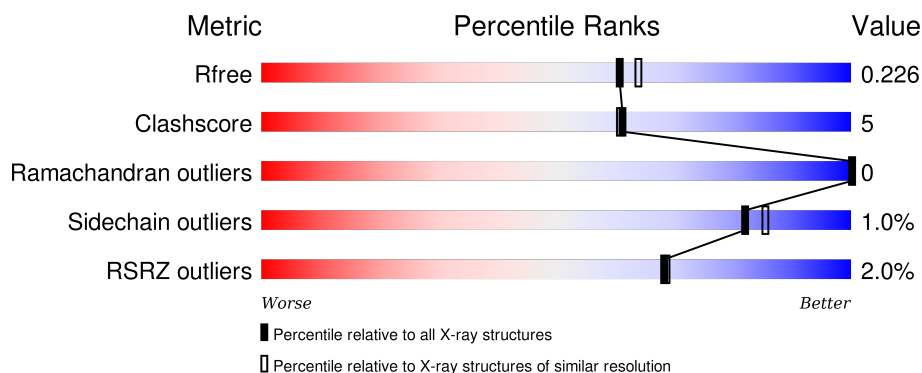
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	371	
1	B	371	

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	B	2390	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6494 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.

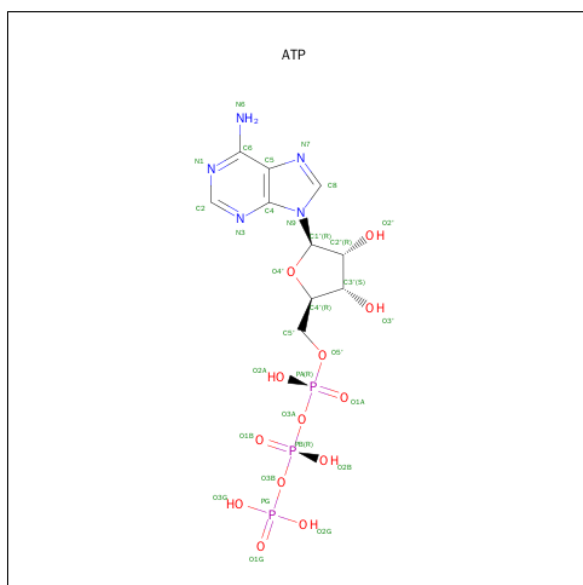
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	10	0
			2776	1771	451	533	21			
1	B	357	Total	C	N	O	S	0	16	0
			2849	1819	470	539	21			

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

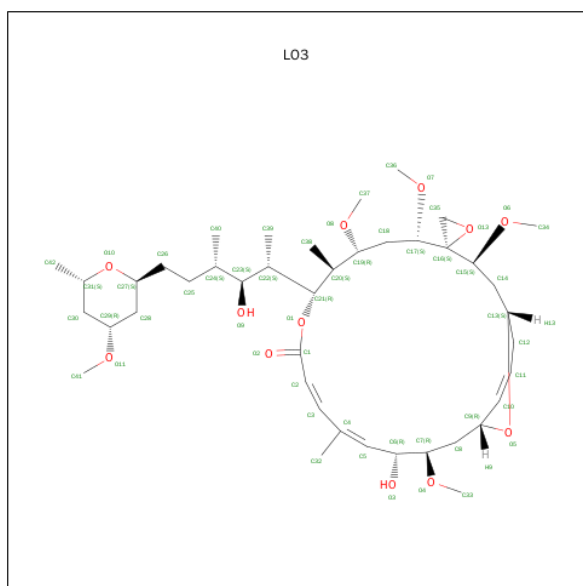
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- 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 (1S,3S,4S,5S,7R,8S,9R,12E,14E,16R,17R,19R)-16-HYDROXY-9-[(1S,2S,3S)-2-HYDROXY-5-[(2S,4R,6S)-4-METHOXY-6-METHYLTETRAHYDRO-2H-PYRAN-2-YL]-1,3-DIMETHYLPENTYL]-3,5,7,17-TETRAMETHOXY-8,14-DIMETHYL-11H-SPIRO[10,23-DIOXABICYCLO[17.3.1]TRICOSA-12,14,20-TRIENE-4,2'-OXIRAN]-11-ONE (three-letter code: LO3) (formula: C<sub>42</sub>H<sub>70</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			54	42	12		
4	B	1	Total	C	O	0	0
			54	42	12		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		

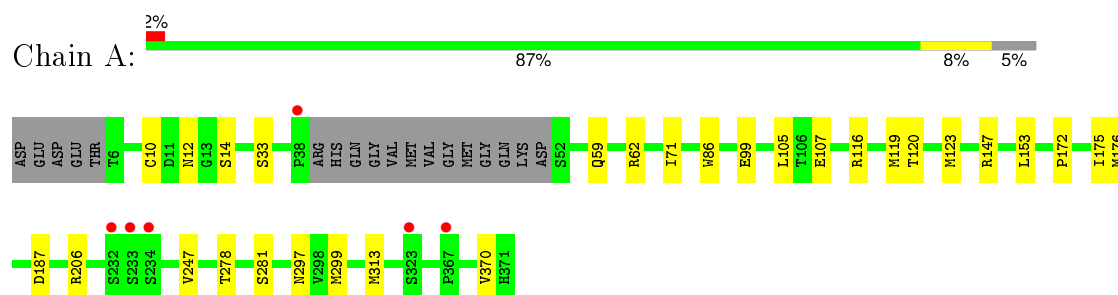
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	326	Total 326	O 326	0	0
6	B	367	Total 367	O 367	0	0

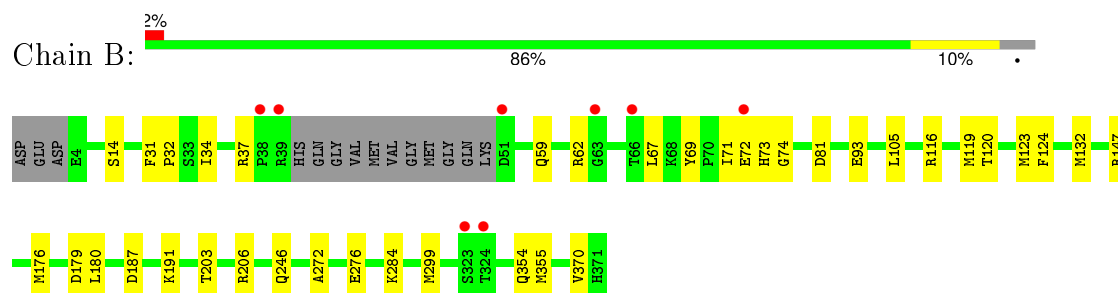
### 3 Residue-property plots [i](#)

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: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.93Å 86.42Å 100.87Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	45.00 – 2.00 39.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.00-2.00) 97.8 (39.70-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.183 , 0.227 0.183 , 0.226	Depositor DCC
$R_{free}$ test set	3084 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60826 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LO3, MG, CA, 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	0.52	0/2860	0.60	0/3885
1	B	0.54	0/2949	0.63	0/4003
All	All	0.53	0/5809	0.62	0/7888

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 [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	2776	0	2727	24	0
1	B	2849	0	2828	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	3	0
3	B	31	0	12	5	0
4	A	54	0	65	0	0
4	B	54	0	65	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	326	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	367	0	0	6	1
All	All	6494	0	5709	63	1

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 5.

All (63) 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:71[B]:ILE:HG22	1:A:71[B]:ILE:O	1.35	1.10
1:A:187:ASP:OD1	1:A:206:ARG:NH1	1.84	1.10
1:A:14[B]:SER:OG	3:A:1380:ATP:O1G	1.82	0.97
1:B:14[B]:SER:OG	3:B:2380:ATP:PG	2.25	0.95
1:A:71[B]:ILE:CG2	1:A:71[B]:ILE:O	2.11	0.94
1:B:71[B]:ILE:O	1:B:71[B]:ILE:HG22	1.67	0.93
1:B:73[B]:HIS:HE1	1:B:179[B]:ASP:OD1	1.57	0.86
1:B:14[B]:SER:OG	3:B:2380:ATP:O1G	1.94	0.84
1:A:14[B]:SER:HG	3:A:1380:ATP:PG	2.01	0.84
1:B:116:ARG:HA	1:B:119[B]:MET:HE2	1.62	0.82
1:A:14[B]:SER:OG	3:A:1380:ATP:PG	2.41	0.78
1:B:116:ARG:HA	1:B:119[B]:MET:CE	2.18	0.73
1:B:73[B]:HIS:CE1	1:B:179[B]:ASP:OD1	2.41	0.72
1:B:14[B]:SER:HA	1:B:71[B]:ILE:O	1.91	0.70
1:A:176:MET:HE3	1:A:281:SER:HA	1.76	0.68
1:A:12:ASN:ND2	1:A:86:TRP:HE1	1.93	0.66
1:B:73[B]:HIS:CE1	1:B:179[B]:ASP:CG	2.69	0.66
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.46	0.63
1:B:187:ASP:OD1	1:B:206:ARG:NH2	2.30	0.62
1:A:147:ARG:NH2	6:A:448:HOH:O	2.32	0.62
1:B:176:MET:HE2	1:B:284:LYS:HD2	1.81	0.62
1:B:71[B]:ILE:O	1:B:71[B]:ILE:CG2	2.41	0.61
1:B:73[B]:HIS:CE1	1:B:179[B]:ASP:OD2	2.55	0.60
1:B:37:ARG:NH2	1:B:81:ASP:OD1	2.30	0.59
1:B:59:GLN:O	1:B:62:ARG:HG3	2.03	0.58
1:A:278:THR:HG21	1:A:297[A]:ASN:HD21	1.68	0.58
1:B:120:THR:OG1	1:B:370:VAL:HG21	2.04	0.58
1:B:354:GLN:HG2	6:B:383:HOH:O	2.04	0.56
1:B:73[B]:HIS:HE1	1:B:179[B]:ASP:CG	2.08	0.56
1:B:105:LEU:HD11	1:B:123:MET:HG3	1.88	0.56
1:A:99[B]:GLU:OE1	6:A:674:HOH:O	2.18	0.56
1:B:14[B]:SER:OG	3:B:2380:ATP:O2G	2.23	0.54

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:MET:CE	1:B:284:LYS:HD2	2.37	0.54
1:B:14[B]:SER:HG	3:B:2380:ATP:PG	2.22	0.53
1:B:355:MET:CE	4:B:600:LO3:H41A	2.38	0.53
1:B:62:ARG:HG2	1:B:67:LEU:HD11	1.93	0.50
1:A:105:LEU:HD11	1:A:123:MET:HG3	1.92	0.50
1:A:116:ARG:HD3	6:A:630:HOH:O	2.12	0.49
1:A:107:GLU:OE1	1:A:116:ARG:HD2	2.13	0.49
1:A:176:MET:HE3	1:A:281:SER:CA	2.42	0.47
1:A:10[A]:CYS:HB3	1:A:105:LEU:HD23	1.96	0.47
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.96	0.47
1:A:120:THR:OG1	1:A:370:VAL:HG21	2.15	0.47
1:B:14[B]:SER:HA	1:B:71[B]:ILE:HG22	1.96	0.46
1:A:10[B]:CYS:HB2	1:A:105:LEU:HD23	1.98	0.46
1:B:272:ALA:HB1	1:B:276[B]:GLU:HB3	1.97	0.45
1:B:31:PHE:CE2	1:B:93:GLU:HG3	2.52	0.45
1:B:34[B]:ILE:HG22	1:B:69[B]:TYR:CD1	2.52	0.44
1:B:246:GLN:HB2	6:B:661:HOH:O	2.17	0.44
1:B:32:PRO:HB2	1:B:34[B]:ILE:HG12	2.00	0.44
1:B:191:LYS:HE3	6:B:651:HOH:O	2.18	0.44
1:A:153:LEU:HD22	1:A:313:MET:CE	2.48	0.44
1:B:72[B]:GLU:CB	6:B:395:HOH:O	2.67	0.42
1:B:116:ARG:HA	1:B:119[B]:MET:HE1	2.01	0.42
1:A:86:TRP:CH2	1:A:119[A]:MET:HG3	2.55	0.42
1:B:124:PHE:CZ	1:B:132[B]:MET:HG2	2.55	0.42
1:B:14[A]:SER:OG	1:B:74:GLY:N	2.53	0.42
1:B:72[A]:GLU:CB	6:B:665:HOH:O	2.68	0.42
1:B:147:ARG:NH2	6:B:491:HOH:O	2.48	0.42
1:A:14[B]:SER:HA	1:A:71[B]:ILE:HG22	2.02	0.41
1:A:59:GLN:O	1:A:62:ARG:HB2	2.20	0.41
1:B:14[B]:SER:OG	3:B:2380:ATP:O3B	2.38	0.40

All (1) 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)
6:B:666:HOH:O	6:B:676:HOH:O[1_455]	2.09	0.11

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/371 (97%)	350 (98%)	9 (2%)	0	100	100
1	B	369/371 (100%)	362 (98%)	7 (2%)	0	100	100
All	All	728/742 (98%)	712 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/314 (95%)	296 (99%)	3 (1%)	82	85
1	B	308/314 (98%)	305 (99%)	3 (1%)	82	85
All	All	607/628 (97%)	601 (99%)	6 (1%)	82	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	247	VAL
1	A	299	MET
1	B	180	LEU
1	B	203	THR
1	B	299	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	88	HIS
1	A	92	ASN
1	A	225	ASN
1	B	92	ASN
1	B	121	GLN
1	B	173	HIS
1	B	225	ASN

### 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 10 ligands modelled in this entry, 6 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	1380	2	24,33,33	0.91	2 (8%)	31,52,52	1.81	5 (16%)
4	LO3	A	600	-	57,57,57	3.15	25 (43%)	57,80,80	3.69	29 (50%)
3	ATP	B	2380	2	24,33,33	0.84	1 (4%)	31,52,52	1.70	3 (9%)
4	LO3	B	600	-	57,57,57	3.27	27 (47%)	57,80,80	3.71	27 (47%)

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	1380	2	-	0/18/38/38	0/3/3/3
4	LO3	A	600	-	-	0/76/102/102	0/1/4/4
3	ATP	B	2380	2	-	0/18/38/38	0/3/3/3
4	LO3	B	600	-	-	0/76/102/102	0/1/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	LO3	C7-C6	-6.00	1.41	1.52
4	B	600	LO3	C7-C6	-5.91	1.42	1.52
4	A	600	LO3	C8-C9	-5.82	1.39	1.53
4	B	600	LO3	C8-C9	-5.34	1.40	1.53
4	B	600	LO3	C26-C25	-5.19	1.37	1.53
4	A	600	LO3	C26-C25	-5.11	1.37	1.53
4	A	600	LO3	C8-C7	-4.83	1.43	1.52
4	B	600	LO3	C8-C7	-4.23	1.44	1.52
4	A	600	LO3	C2-C1	-4.05	1.38	1.48
4	B	600	LO3	C2-C1	-4.02	1.38	1.48
4	A	600	LO3	O3-C6	-4.00	1.35	1.43
4	B	600	LO3	O3-C6	-3.90	1.35	1.43
4	B	600	LO3	C28-C29	-3.52	1.42	1.52
4	A	600	LO3	C28-C29	-3.51	1.42	1.52
4	B	600	LO3	C30-C29	-3.48	1.42	1.52
4	A	600	LO3	C30-C29	-3.39	1.42	1.52
4	B	600	LO3	C18-C17	-3.38	1.44	1.52
4	A	600	LO3	C14-C13	-3.22	1.43	1.52
4	B	600	LO3	C14-C13	-3.21	1.43	1.52
4	A	600	LO3	C18-C17	-3.14	1.44	1.52
4	A	600	LO3	O10-C27	-3.13	1.38	1.44
4	B	600	LO3	O10-C27	-2.81	1.39	1.44
4	B	600	LO3	C16-C17	-2.71	1.46	1.53
4	A	600	LO3	C6-C5	-2.60	1.45	1.50
4	A	600	LO3	C39-C22	-2.42	1.48	1.53
4	B	600	LO3	C6-C5	-2.39	1.45	1.50
4	A	600	LO3	C16-C17	-2.38	1.47	1.53
4	B	600	LO3	C39-C22	-2.28	1.48	1.53
4	A	600	LO3	C3-C2	-2.25	1.26	1.33
4	B	600	LO3	C3-C2	-2.14	1.26	1.33
4	A	600	LO3	C3-C4	-2.13	1.41	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	LO3	C3-C4	-2.12	1.41	1.45
4	A	600	LO3	O1-C21	-2.01	1.41	1.44
4	B	600	LO3	O4-C33	-2.00	1.34	1.42
4	B	600	LO3	C26-C27	2.07	1.59	1.51
4	B	600	LO3	O13-C16	2.09	1.48	1.45
4	B	600	LO3	O6-C34	2.09	1.50	1.42
4	B	600	LO3	C38-C20	2.23	1.58	1.53
4	B	600	LO3	O11-C29	2.23	1.49	1.43
3	A	1380	ATP	C2-N3	2.27	1.36	1.32
3	B	2380	ATP	C5-C4	2.34	1.45	1.40
4	A	600	LO3	C26-C27	2.37	1.60	1.51
3	A	1380	ATP	C5-C4	2.81	1.46	1.40
4	A	600	LO3	O11-C29	2.89	1.50	1.43
4	A	600	LO3	O13-C16	2.93	1.50	1.45
4	B	600	LO3	C16-C15	3.58	1.61	1.53
4	A	600	LO3	C40-C24	3.81	1.62	1.53
4	A	600	LO3	C16-C15	3.87	1.62	1.53
4	B	600	LO3	C40-C24	3.92	1.63	1.53
4	B	600	LO3	O5-C13	4.42	1.52	1.44
4	A	600	LO3	O5-C13	5.54	1.54	1.44
4	A	600	LO3	C35-C16	8.56	1.60	1.46
4	B	600	LO3	C35-C16	9.22	1.61	1.46
4	A	600	LO3	O13-C35	11.36	1.74	1.44
4	B	600	LO3	O13-C35	13.87	1.81	1.44

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2380	ATP	N3-C2-N1	-7.47	123.17	128.89
3	A	1380	ATP	N3-C2-N1	-7.46	123.18	128.89
4	B	600	LO3	O13-C35-C16	-7.05	50.99	59.73
4	A	600	LO3	O13-C35-C16	-5.41	53.02	59.73
4	A	600	LO3	O3-C6-C5	-5.08	99.27	110.41
4	B	600	LO3	C32-C4-C3	-5.01	109.76	118.10
4	A	600	LO3	C32-C4-C3	-4.82	110.08	118.10
4	B	600	LO3	O3-C6-C5	-4.22	101.15	110.41
4	A	600	LO3	C31-C30-C29	-3.73	104.66	111.38
4	B	600	LO3	C32-C4-C5	-3.49	111.49	122.60
4	B	600	LO3	C35-O13-C16	-3.36	57.60	60.66
4	B	600	LO3	C31-C30-C29	-3.21	105.59	111.38
4	A	600	LO3	C32-C4-C5	-3.19	112.46	122.60
4	A	600	LO3	C38-C20-C19	-2.98	106.94	111.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	LO3	O10-C27-C26	-2.77	99.30	107.80
3	A	1380	ATP	C4-C5-N7	-2.75	106.95	109.48
4	B	600	LO3	C38-C20-C19	-2.31	107.98	111.55
3	A	1380	ATP	C2'-C1'-N9	-2.25	110.85	114.29
4	A	600	LO3	C35-O13-C16	-2.25	58.61	60.66
4	B	600	LO3	C39-C22-C21	-2.14	107.38	111.38
4	A	600	LO3	C42-C31-C30	-2.08	109.91	113.38
3	B	2380	ATP	C2'-C1'-N9	-2.03	111.19	114.29
3	A	1380	ATP	O2B-PB-O3B	2.01	114.21	105.09
4	A	600	LO3	C36-O7-C17	2.04	119.55	113.63
4	B	600	LO3	O11-C29-C28	2.15	116.45	109.59
4	B	600	LO3	C36-O7-C17	2.19	119.97	113.63
3	B	2380	ATP	O3G-PG-O2G	2.25	115.95	107.38
4	B	600	LO3	C18-C17-C16	2.25	119.67	115.46
4	B	600	LO3	C38-C20-C21	2.27	115.63	111.38
4	B	600	LO3	C40-C24-C23	2.28	115.86	111.42
4	A	600	LO3	O5-C9-C8	2.32	119.71	109.44
4	B	600	LO3	C23-C22-C21	2.36	115.41	110.82
4	B	600	LO3	O1-C1-O2	2.37	126.98	123.30
3	A	1380	ATP	O3G-PG-O2G	2.37	116.41	107.38
4	B	600	LO3	C19-C18-C17	2.47	121.02	115.02
4	A	600	LO3	C26-C25-C24	2.51	120.87	115.07
4	B	600	LO3	C25-C26-C27	2.54	119.33	114.04
4	B	600	LO3	C26-C25-C24	2.56	121.00	115.07
4	A	600	LO3	C38-C20-C21	2.61	116.27	111.38
4	B	600	LO3	O5-C9-C8	2.64	121.10	109.44
4	A	600	LO3	O11-C29-C28	2.71	118.23	109.59
4	A	600	LO3	O1-C1-O2	2.85	127.72	123.30
4	A	600	LO3	C23-C22-C21	2.95	116.57	110.82
4	A	600	LO3	O10-C31-C30	3.01	113.89	109.09
4	A	600	LO3	C18-C17-C16	3.11	121.28	115.46
4	A	600	LO3	C19-C18-C17	3.30	123.03	115.02
4	A	600	LO3	C40-C24-C23	3.42	118.09	111.42
4	A	600	LO3	C25-C26-C27	3.46	121.26	114.04
4	A	600	LO3	C31-O10-C27	3.72	121.14	113.62
4	A	600	LO3	C33-O4-C7	4.15	125.35	114.09
4	B	600	LO3	C31-O10-C27	4.27	122.26	113.62
4	B	600	LO3	C33-O4-C7	4.48	126.26	114.09
4	A	600	LO3	C30-C29-C28	4.60	121.35	112.00
4	B	600	LO3	O3-C6-C7	5.07	121.20	108.32
4	A	600	LO3	O3-C6-C7	5.33	121.87	108.32
4	B	600	LO3	C30-C29-C28	5.49	123.16	112.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	LO3	C37-O8-C19	5.70	129.57	114.09
4	B	600	LO3	C41-O11-C29	5.74	128.85	113.83
4	A	600	LO3	C41-O11-C29	6.40	130.59	113.83
4	A	600	LO3	C37-O8-C19	7.12	133.42	114.09
4	A	600	LO3	O13-C16-C35	8.65	68.37	59.62
4	B	600	LO3	O13-C16-C35	11.65	71.42	59.62
4	B	600	LO3	C2-C3-C4	16.06	150.70	126.22
4	A	600	LO3	C2-C3-C4	16.47	151.32	126.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1380	ATP	3	0
3	B	2380	ATP	5	0
4	B	600	LO3	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	353/371 (95%)	-0.27	6 (1%) 73 73	9, 21, 43, 57	0
1	B	357/371 (96%)	-0.16	8 (2%) 65 66	8, 18, 37, 48	0
All	All	710/742 (95%)	-0.21	14 (1%) 68 69	8, 20, 40, 57	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	PRO	4.7
1	B	66[A]	THR	3.7
1	B	324	THR	3.4
1	B	72[A]	GLU	2.8
1	A	38	PRO	2.7
1	B	39	ARG	2.7
1	A	234	SER	2.7
1	B	63	GLY	2.5
1	A	232	SER	2.4
1	B	51	ASP	2.4
1	B	323	SER	2.4
1	A	233	SER	2.2
1	A	323	SER	2.2
1	A	367	PRO	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 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. 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	B	2390	1/1	1.00	0.19	4.77	2,2,2,2	0
4	LO3	A	600	54/54	0.97	0.09	0.01	8,13,26,30	0
5	CA	B	372	1/1	0.98	0.13	-0.01	41,41,41,41	0
3	ATP	A	1380	31/31	0.98	0.09	-0.33	12,17,18,19	4
4	LO3	B	600	54/54	0.96	0.09	-0.41	5,13,20,22	0
3	ATP	B	2380	31/31	0.98	0.10	-0.55	7,14,17,17	4
5	CA	A	373	1/1	0.93	0.07	-	44,44,44,44	0
5	CA	B	373	1/1	0.90	0.07	-	64,64,64,64	0
5	CA	A	372	1/1	0.96	0.04	-	53,53,53,53	0
2	MG	A	1390	1/1	0.99	0.16	-	4,4,4,4	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.