W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:56 PM GMT

PDB ID	:	4B1U
Title	:	Structure of the Phactr1 RPEL domain and RPEL motif directed assemblies with G-actin reveal the molecular basis for actin binding cooperativity.
Authors	:	Mouilleron, S.; Wiezlak, M.; O'Reilly, N.; Treisman, R.; McDonald, N.Q.
Deposited on	:	2012-07-12
Resolution	:	2.00 Å(reported)

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

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 2.00 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.3%
Sidechain outliers		1.7%
RSRZ outliers		89.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
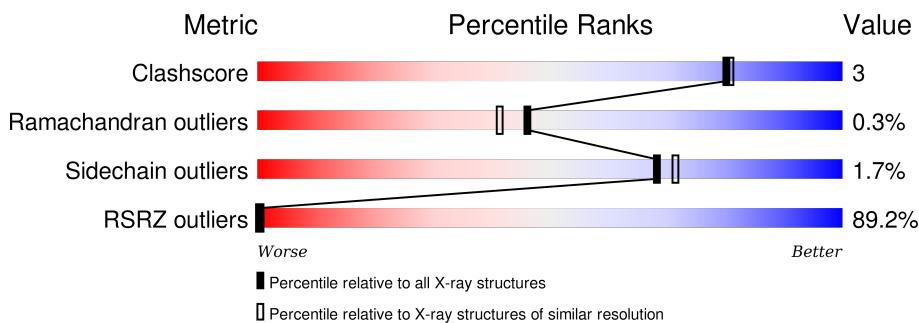
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 >=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	B	376	83% / 85% 8% 7%
2	M	32	84% / 75% 19% 6%
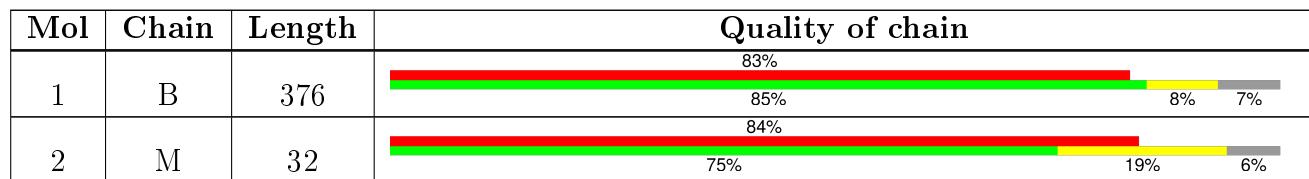
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	B	1378	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3149 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	B	349	Total	C	N	O	S	0	6	0
			2698	1720	445	513	20			

- Molecule 2 is a protein called PHOSPHATASE AND ACTIN REGULATOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	30	Total	C	N	O	S	0	1	0
			228	145	44	38	1			

- Molecule 3 is LATRUNCULIN B (three-letter code: LAB) (formula: $C_{20}H_{29}NO_5S$).
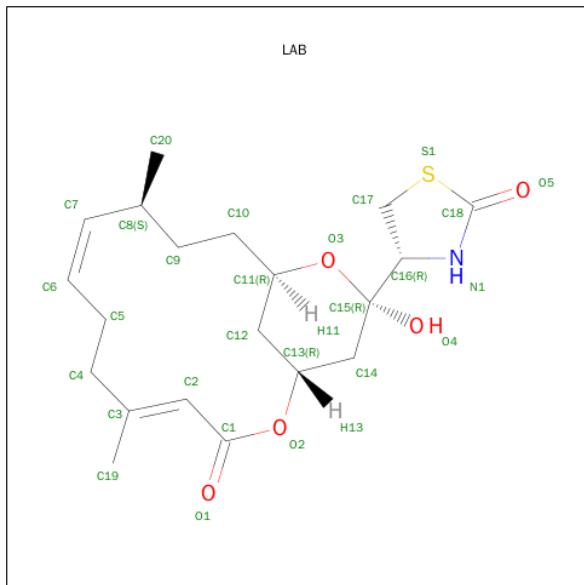
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
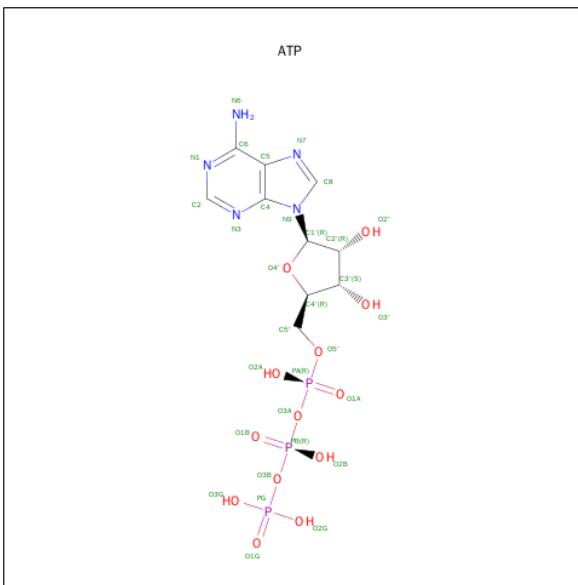
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).
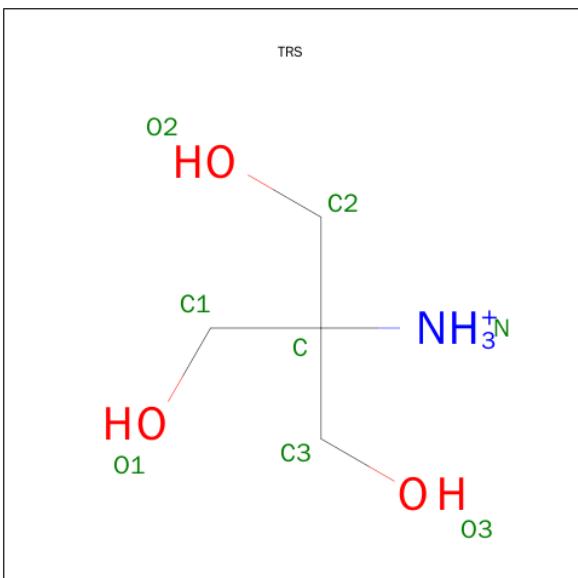
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total 1	Ca 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	148	Total 148	O 148	0	0
8	M	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

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
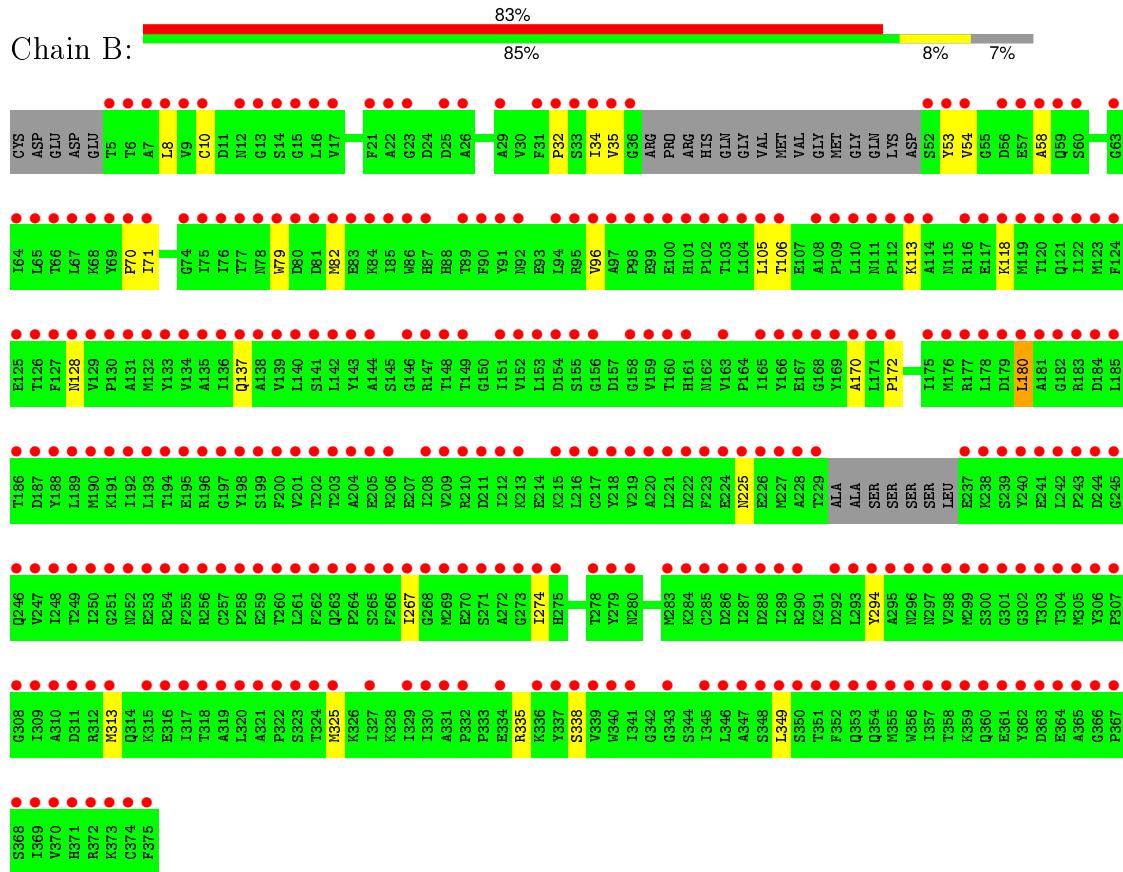
• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1
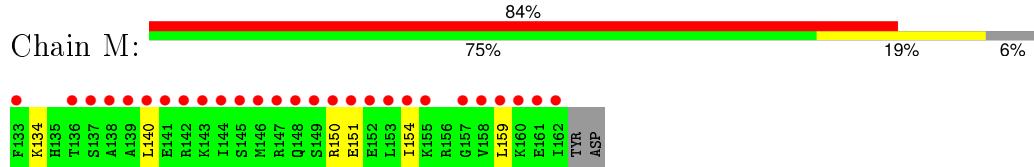
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.60Å 77.60Å 128.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.93 – 2.00 28.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.93-2.00) 98.1 (28.93-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.23 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.195 , 0.236 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 72.1	EDS
Estimated twinning fraction	0.245 for -h,-k,l	Xtriage
L-test for twinning [2]	$<|L|> = 0.29, <L^2> = 0.12$	Xtriage
Outliers	0 of 60467 reflections	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	3149	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, ATP, MG, CA, LAB

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	B	0.42	0/2772	0.54	0/3764
2	M	0.31	0/235	0.49	0/312
All	All	0.41	0/3007	0.54	0/4076

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	B	2698	0	2625	18	0
2	M	228	0	225	3	0
3	B	27	0	29	0	0
4	B	31	0	12	0	0
5	B	1	0	0	0	0
6	B	8	0	12	0	0
7	M	1	0	0	0	0
8	B	148	0	0	0	0
8	M	7	0	0	0	0
All	All	3149	0	2903	20	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 3.

All (20) 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:B:274:ILE:HG13	1:B:313:MET:HE1	1.88	0.56
1:B:10[B]:CYS:HB2	1:B:105:LEU:HD23	1.87	0.56
1:B:71:ILE:HG13	1:B:82:MET:HE3	1.89	0.54
1:B:35:VAL:HG22	1:B:54:VAL:HG22	1.89	0.53
1:B:180:LEU:HD22	1:B:267:ILE:HD11	1.92	0.52
1:B:71:ILE:HG13	1:B:82:MET:CE	2.40	0.51
1:B:10[A]:CYS:HB3	1:B:105:LEU:HD23	1.95	0.49
2:M:151:GLU:HA	2:M:154:ILE:HD12	1.93	0.49
2:M:150:ARG:O	2:M:154:ILE:HG13	2.13	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.13	0.48
1:B:79:TRP:CE2	1:B:118:LYS:HE3	2.48	0.48
1:B:294:TYR:CD2	1:B:325:MET:HG2	2.50	0.47
1:B:70:PRO:HB2	1:B:82:MET:CE	2.46	0.46
1:B:32:PRO:HB2	1:B:34:ILE:HG12	1.97	0.45
1:B:349:LEU:HD11	2:M:140:LEU:HD23	2.00	0.44
1:B:82:MET:HE2	1:B:82:MET:HB2	1.59	0.44
1:B:8:LEU:HD11	1:B:96:VAL:HG21	2.01	0.42
1:B:106:THR:HB	1:B:137:GLN:HG3	2.02	0.42
1:B:53:TYR:HB3	1:B:58:ALA:HA	2.03	0.41
1:B:335:ARG:HA	1:B:338[A]:SER:OG	2.20	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	B	349/376 (93%)	342 (98%)	7 (2%)	0	100	100
2	M	29/32 (91%)	28 (97%)	0	1 (3%)	5	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	378/408 (93%)	370 (98%)	7 (2%)	1 (0%)	46 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	134	LYS

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	B	286/319 (90%)	282 (99%)	4 (1%)	74 77
2	M	21/29 (72%)	20 (95%)	1 (5%)	31 26
All	All	307/348 (88%)	302 (98%)	5 (2%)	68 73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	113	LYS
1	B	128	ASN
1	B	180	LEU
1	B	225	ASN
2	M	159	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	LAB	B	1376	-	27,29,29	2.39	10 (37%)	28,41,41	1.54	5 (17%)
4	ATP	B	1377	5	24,33,33	0.88	1 (4%)	31,52,52	1.91	7 (22%)
6	TRS	B	1379	-	7,7,7	1.14	1 (14%)	9,9,9	1.33	2 (22%)

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	LAB	B	1376	-	-	0/21/49/49	0/1/3/3
4	ATP	B	1377	5	-	0/18/38/38	0/3/3/3
6	TRS	B	1379	-	-	0/9/9/9	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1376	LAB	C17-S1	-4.29	1.73	1.81
3	B	1376	LAB	O2-C13	-3.02	1.38	1.46
6	B	1379	TRS	C-N	-2.81	1.46	1.50
3	B	1376	LAB	O3-C11	-2.76	1.37	1.44
3	B	1376	LAB	C17-C16	-2.13	1.49	1.53
3	B	1376	LAB	C7-C6	2.09	1.41	1.31
3	B	1376	LAB	O2-C1	2.41	1.39	1.34
4	B	1377	ATP	C5-C4	2.49	1.46	1.40
3	B	1376	LAB	C2-C1	2.49	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1376	LAB	C16-N1	2.79	1.49	1.46
3	B	1376	LAB	C2-C3	3.81	1.41	1.33
3	B	1376	LAB	C18-N1	7.73	1.48	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1377	ATP	N3-C2-N1	-7.19	123.39	128.89
3	B	1376	LAB	O2-C1-O1	-3.39	118.02	123.30
4	B	1377	ATP	PA-O3A-PB	-3.38	123.23	132.73
4	B	1377	ATP	C2'-C1'-N9	-3.00	109.71	114.29
6	B	1379	TRS	O2-C2-C	-2.96	105.20	111.18
4	B	1377	ATP	C4-C5-N7	-2.60	107.09	109.48
3	B	1376	LAB	C16-N1-C18	-2.19	110.17	113.04
4	B	1377	ATP	O3A-PA-O5'	-2.15	97.24	102.94
3	B	1376	LAB	O4-C15-O3	-2.14	106.50	109.94
6	B	1379	TRS	O1-C1-C	-2.05	107.04	111.18
4	B	1377	ATP	O3G-PG-O2G	2.03	115.12	107.38
4	B	1377	ATP	C2-N1-C6	2.07	122.47	118.77
3	B	1376	LAB	O2-C1-C2	3.43	119.98	111.51
3	B	1376	LAB	C17-C16-N1	3.63	109.88	100.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	349/376 (92%)	4.39	311 (89%)	0	0	15, 32, 58, 73	0
2	M	30/32 (93%)	5.38	27 (90%)	0	0	36, 48, 62, 74	1 (3%)
All	All	379/408 (92%)	4.47	338 (89%)	0	0	15, 34, 59, 74	1 (0%)

All (338) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	GLY	17.6
1	B	65	LEU	17.4
1	B	229	THR	17.3
2	M	162	ILE	14.9
1	B	66	THR	14.0
1	B	325	MET	13.6
1	B	324	THR	13.4
1	B	77	THR	11.7
1	B	52	SER	11.3
1	B	169	TYR	11.1
1	B	125	GLU	10.7
1	B	212	ILE	10.7
2	M	161	GLU	10.4
1	B	53	TYR	10.2
1	B	265	SER	9.8
1	B	194	THR	9.7
1	B	94	LEU	9.6
1	B	95	ARG	9.4
1	B	192	ILE	9.3
1	B	363	ASP	9.1
1	B	67	LEU	9.0
1	B	274	ILE	8.8
1	B	225	ASN	8.8
1	B	64	ILE	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	370	VAL	8.6
1	B	60	SER	8.5
1	B	75	ILE	8.5
1	B	348[A]	SER	8.4
1	B	179	ASP	8.4
1	B	209	VAL	8.3
1	B	10[A]	CYS	8.3
1	B	270	GLU	8.1
1	B	180	LEU	8.1
1	B	127	PHE	8.0
1	B	323	SER	7.9
1	B	350	SER	7.8
1	B	78	ASN	7.8
1	B	108	ALA	7.5
1	B	365	ALA	7.5
2	M	144	ILE	7.5
2	M	133	PHE	7.5
1	B	354	GLN	7.4
2	M	138	ALA	7.3
1	B	122	ILE	7.3
2	M	159	LEU	7.2
1	B	100	GLU	7.2
1	B	56	ASP	7.1
1	B	368	SER	7.1
2	M	137	SER	7.1
1	B	114	ALA	7.0
1	B	369	ILE	7.0
2	M	152	GLU	6.9
1	B	262	PHE	6.8
1	B	267	ILE	6.8
1	B	6	THR	6.7
1	B	166	TYR	6.7
1	B	374	CYS	6.7
1	B	86	TRP	6.6
1	B	5	THR	6.6
1	B	76	ILE	6.6
1	B	351	THR	6.6
1	B	242	LEU	6.6
2	M	148	GLN	6.5
2	M	155	LYS	6.5
1	B	247	VAL	6.4
1	B	364	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
2	M	160	LYS	6.4
1	B	358	THR	6.3
1	B	375	PHE	6.2
1	B	167	GLU	6.2
1	B	202	THR	6.2
1	B	250	ILE	6.2
2	M	146	MET	6.2
1	B	35	VAL	6.2
1	B	321	ALA	6.1
1	B	273	GLY	6.0
1	B	319	ALA	6.0
1	B	208	ILE	6.0
1	B	297	ASN	5.9
1	B	249	THR	5.9
1	B	289	ILE	5.8
1	B	239	SER	5.8
1	B	349	LEU	5.7
1	B	14[A]	SER	5.7
1	B	311	ASP	5.7
1	B	170	ALA	5.7
1	B	352	PHE	5.6
1	B	85	ILE	5.6
1	B	357	ILE	5.6
1	B	327	ILE	5.6
1	B	199[A]	SER	5.6
1	B	204	ALA	5.6
2	M	153	LEU	5.5
1	B	320	LEU	5.5
1	B	269	MET	5.5
1	B	322	PRO	5.4
1	B	280	ASN	5.4
1	B	148	THR	5.4
1	B	196	ARG	5.4
1	B	91	TYR	5.4
2	M	151	GLU	5.4
1	B	118	LYS	5.4
1	B	124	PHE	5.3
1	B	341	ILE	5.3
1	B	221	LEU	5.3
1	B	113	LYS	5.3
1	B	25	ASP	5.3
1	B	330	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	288	ASP	5.2
1	B	104	LEU	5.1
1	B	99	GLU	5.1
2	M	136	THR	5.1
1	B	171	LEU	5.1
1	B	36	GLY	5.0
1	B	96	VAL	5.0
1	B	258	PRO	5.0
1	B	355	MET	5.0
1	B	373	LYS	5.0
1	B	159	VAL	5.0
1	B	218	TYR	5.0
1	B	105	LEU	4.9
1	B	295	ALA	4.9
1	B	279	TYR	4.9
1	B	31	PHE	4.8
1	B	222	ASP	4.8
1	B	59	GLN	4.8
1	B	143	TYR	4.8
2	M	141	GLU	4.8
1	B	188	TYR	4.8
1	B	200	PHE	4.8
1	B	80	ASP	4.8
1	B	203	THR	4.7
1	B	156	GLY	4.7
1	B	309	ILE	4.7
1	B	278	THR	4.7
1	B	110	LEU	4.7
1	B	21	PHE	4.7
1	B	79	TRP	4.7
2	M	154	ILE	4.6
1	B	331	ALA	4.6
1	B	139	VAL	4.6
1	B	183	ARG	4.6
1	B	140	LEU	4.6
2	M	139	ALA	4.6
1	B	34	ILE	4.6
1	B	129	VAL	4.6
1	B	303	THR	4.5
1	B	177	ARG	4.5
1	B	257	CYS	4.5
1	B	197	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	M	145	SER	4.5
1	B	266	PHE	4.5
1	B	224	GLU	4.5
1	B	238	LYS	4.4
1	B	252	ASN	4.4
2	M	143	LYS	4.4
1	B	69	TYR	4.4
1	B	216	LEU	4.4
1	B	251	GLY	4.4
2	M	158	VAL	4.4
1	B	189	LEU	4.4
1	B	126	THR	4.3
1	B	195	GLU	4.3
1	B	371	HIS	4.3
1	B	175	ILE	4.3
1	B	306	TYR	4.2
2	M	157	GLY	4.2
1	B	264	PRO	4.2
1	B	261	LEU	4.2
1	B	217	CYS	4.2
1	B	128	ASN	4.2
1	B	153	LEU	4.2
1	B	147	ARG	4.1
1	B	136	ILE	4.1
1	B	97	ALA	4.1
1	B	246	GLN	4.1
1	B	92	ASN	4.1
1	B	206	ARG	4.1
1	B	26	ALA	4.1
1	B	135	ALA	4.1
1	B	121	GLN	4.0
1	B	346	LEU	4.0
1	B	133	TYR	4.0
1	B	310	ALA	4.0
1	B	259	GLU	4.0
1	B	316	GLU	3.9
1	B	223	PHE	3.9
1	B	275	HIS	3.9
1	B	340	TRP	3.9
1	B	58	ALA	3.9
1	B	151	ILE	3.9
1	B	255	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	356	TRP	3.9
1	B	347	ALA	3.9
1	B	83	GLU	3.9
1	B	198	TYR	3.9
1	B	294	TYR	3.9
1	B	7	ALA	3.9
1	B	120	THR	3.9
1	B	71	ILE	3.8
1	B	220	ALA	3.8
1	B	293	LEU	3.8
1	B	81	ASP	3.8
1	B	168	GLY	3.8
1	B	117	GLU	3.8
1	B	329	ILE	3.7
1	B	8	LEU	3.7
1	B	256	ARG	3.7
1	B	132	MET	3.7
2	M	149	SER	3.7
1	B	337	TYR	3.7
1	B	109	PRO	3.6
1	B	142	LEU	3.6
1	B	248	ILE	3.6
1	B	33	SER	3.6
1	B	9	VAL	3.6
1	B	298	VAL	3.6
1	B	90	PHE	3.6
1	B	12	ASN	3.6
1	B	360	GLN	3.5
1	B	16	LEU	3.5
1	B	186	THR	3.5
1	B	290	ARG	3.5
1	B	63	GLY	3.5
1	B	299	MET	3.5
1	B	84	LYS	3.5
1	B	263	GLN	3.5
1	B	315	LYS	3.4
1	B	339	VAL	3.4
1	B	228	ALA	3.4
1	B	318	THR	3.4
1	B	119	MET	3.4
1	B	372	ARG	3.3
2	M	147	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	353	GLN	3.3
1	B	227	MET	3.3
1	B	243	PRO	3.3
1	B	253	GLU	3.3
1	B	23	GLY	3.2
1	B	160	THR	3.2
1	B	284	LYS	3.2
1	B	272	ALA	3.2
1	B	367	PRO	3.2
1	B	193	LEU	3.2
1	B	312	ARG	3.2
1	B	172	PRO	3.2
1	B	68	LYS	3.2
1	B	101	HIS	3.2
1	B	296	ASN	3.1
1	B	317	ILE	3.1
1	B	149	THR	3.1
1	B	240	TYR	3.1
1	B	134	VAL	3.1
1	B	361	GLU	3.1
1	B	181	ALA	3.1
1	B	190	MET	3.1
1	B	313	MET	3.1
1	B	155	SER	3.1
1	B	22	ALA	3.0
1	B	82	MET	3.0
1	B	163	VAL	3.0
1	B	287	ILE	3.0
1	B	345	ILE	3.0
1	B	362	TYR	3.0
1	B	182	GLY	2.9
1	B	138	ALA	2.9
1	B	213	LYS	2.9
1	B	241	GLU	2.9
1	B	111	ASN	2.9
1	B	54	VAL	2.9
1	B	226	GLU	2.9
1	B	123	MET	2.9
1	B	178	LEU	2.9
1	B	137	GLN	2.8
1	B	215	LYS	2.8
1	B	185	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	308	GLY	2.8
1	B	244	ASP	2.8
1	B	201	VAL	2.8
1	B	165	ILE	2.8
1	B	336[A]	LYS	2.7
1	B	219	VAL	2.7
1	B	103	THR	2.7
1	B	32	PRO	2.7
1	B	191	LYS	2.7
1	B	70	PRO	2.7
1	B	15	GLY	2.7
1	B	141	SER	2.7
1	B	338[A]	SER	2.7
1	B	245	GLY	2.7
1	B	154	ASP	2.6
1	B	307	PRO	2.6
1	B	57	GLU	2.6
1	B	300	SER	2.6
1	B	359	LYS	2.6
1	B	254	ARG	2.6
2	M	142	ARG	2.6
1	B	211	ASP	2.6
1	B	260	THR	2.6
1	B	302	GLY	2.6
1	B	301	GLY	2.5
1	B	13	GLY	2.5
1	B	29	ALA	2.5
1	B	98	PRO	2.5
1	B	87	HIS	2.5
1	B	343	GLY	2.4
1	B	112	PRO	2.4
1	B	89	THR	2.4
1	B	334	GLU	2.4
1	B	285	CYS	2.4
1	B	131	ALA	2.4
1	B	130	PRO	2.4
1	B	210	ARG	2.4
1	B	106	THR	2.4
1	B	205	GLU	2.4
1	B	332	PRO	2.3
1	B	292	ASP	2.3
1	B	116	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	150	ARG	2.3
1	B	237	GLU	2.3
1	B	304	THR	2.3
1	B	184	ASP	2.3
1	B	102	PRO	2.2
1	B	144	ALA	2.2
1	B	176	MET	2.2
1	B	286	ASP	2.2
1	B	187	ASP	2.2
1	B	271	SER	2.1
2	M	140	LEU	2.1
1	B	146	GLY	2.1
1	B	158	GLY	2.1
1	B	17	VAL	2.1
1	B	161	HIS	2.1
1	B	74	GLY	2.1
1	B	283	MET	2.1
1	B	366	GLY	2.0
1	B	152	VAL	2.0
1	B	305	MET	2.0

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

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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MG	B	1378	1/1	0.74	0.64	6.35	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	LAB	B	1376	27/27	0.66	0.32	-0.01	20,27,34,36	0
4	ATP	B	1377	31/31	0.81	0.22	-1.39	13,17,22,24	1
7	CA	M	1163	1/1	0.92	0.13	-1.96	20,20,20,20	0
6	TRS	B	1379	8/8	0.61	0.56	-	21,45,56,60	0

6.5 Other polymers (i)

There are no such residues in this entry.