Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:44 pm BST

PDB ID	:	2V52
Title	:	Structure of MAL-RPEL2 complexed to G-actin
Authors	:	Mouilleron, S.; Guettler, S.; Langer, C.A.; Treisman, R.; McDonald, N.Q.
Deposited on	:	2008-10-01
Resolution	:	1.45 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:

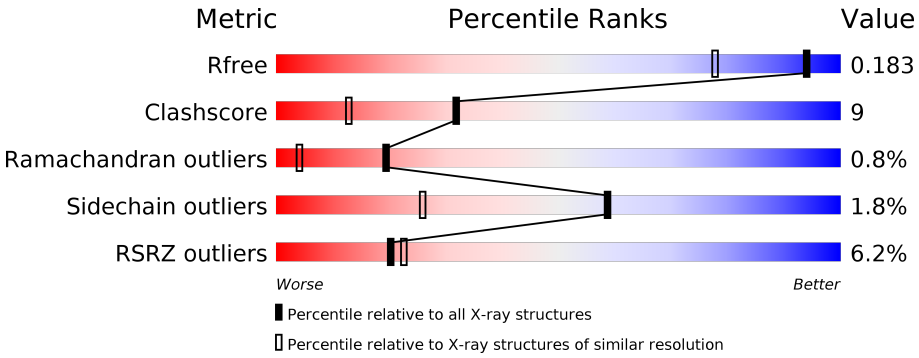
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	B	377	6% 77% 16% • • 5%
2	M	32	6% 69% 16% 9% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3738 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.

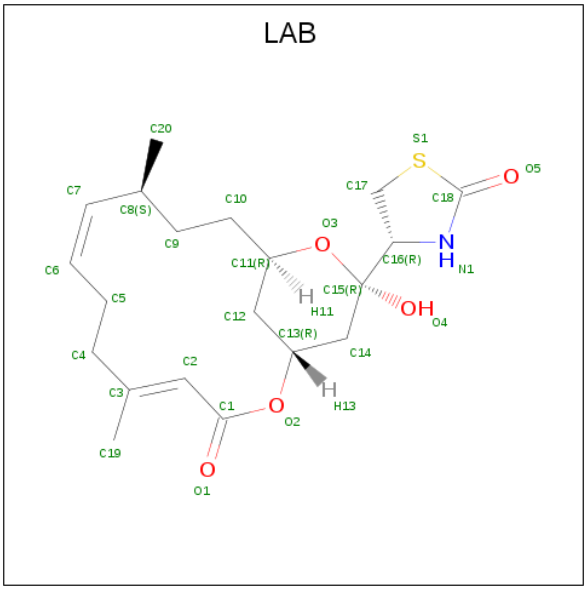
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	360	Total	C	N	O	S	0	35	0
			3003	1921	486	572	24			

- Molecule 2 is a protein called MKL/MYOCARDIN-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	30	Total	C	N	O	S	0	7	0
			305	189	69	46	1			

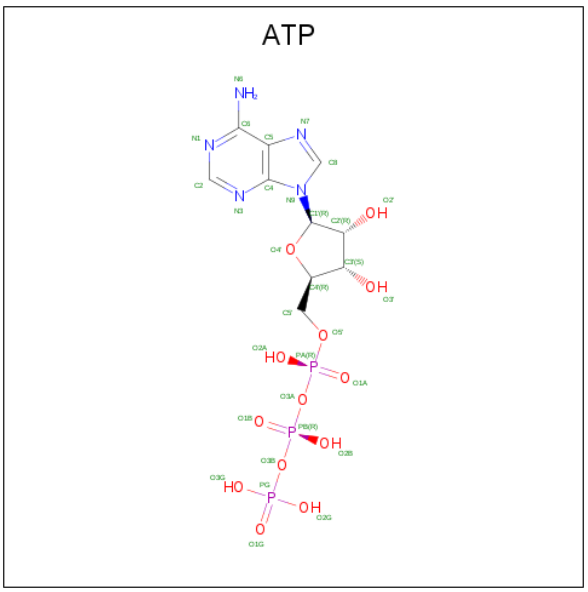
- Molecule 3 is LATRUNCULIN B (three-letter code: LAB) (formula: $C_{20}H_{29}NO_5S$).



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:

$C_{10}H_{16}N_5O_{13}P_3$).

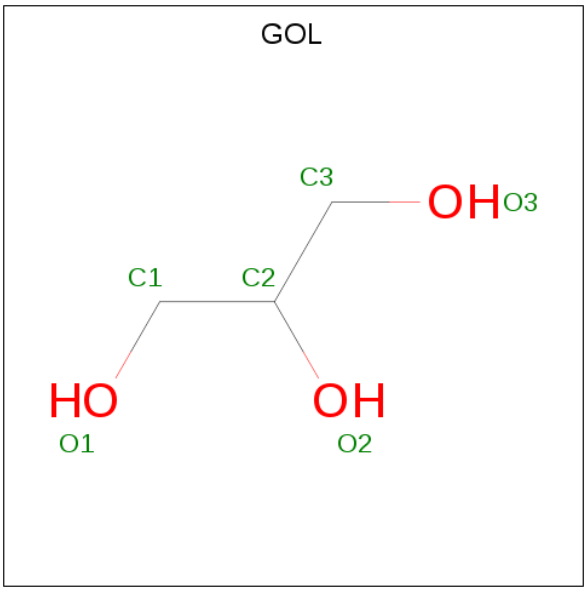


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- 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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

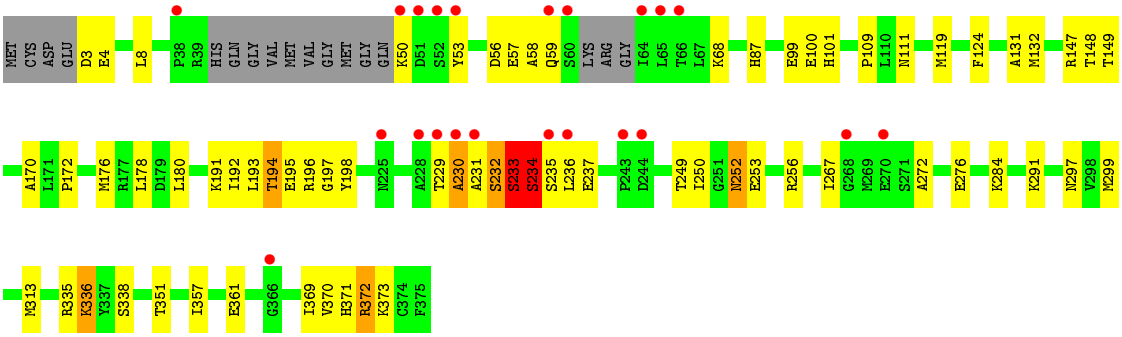
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	334	Total O 334 334	0	2
7	M	25	Total O 25 25	0	0

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: ACTIN, ALPHA SKELETAL MUSCLE

Chain B:



- Molecule 2: MKL/MYOCARDIN-LIKE PROTEIN 1

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.75Å 55.44Å 138.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 1.45 29.35 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.35-1.45) 99.3 (29.35-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.147 , 0.188 0.143 , 0.183	Depositor DCC
R_{free} test set	3769 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3738	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, LAB, 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	B	1.44	55/3138 (1.8%)	1.03	11/4245 (0.3%)
2	M	1.79	4/319 (1.3%)	1.10	3/420 (0.7%)
All	All	1.48	59/3457 (1.7%)	1.04	14/4665 (0.3%)

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	B	1	2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TYR	CD1-CE1	-17.19	1.13	1.39
1	B	195	GLU	CD-OE1	-13.18	1.11	1.25
2	M	130[A]	GLU	CB-CG	-12.80	1.27	1.52
2	M	130[B]	GLU	CB-CG	-12.80	1.27	1.52
1	B	99	GLU	CB-CG	-10.96	1.31	1.52
1	B	198	TYR	CD2-CE2	-10.89	1.23	1.39
1	B	237	GLU	CD-OE1	-10.68	1.14	1.25
2	M	130[A]	GLU	CD-OE1	-10.61	1.14	1.25
2	M	130[B]	GLU	CD-OE1	-10.61	1.14	1.25
1	B	99	GLU	CD-OE1	-10.40	1.14	1.25
1	B	99	GLU	CD-OE2	-9.92	1.14	1.25
1	B	149	THR	C-O	-9.90	1.04	1.23
1	B	197	GLY	C-O	-9.57	1.08	1.23
1	B	100	GLU	CD-OE2	-9.26	1.15	1.25
1	B	197	GLY	N-CA	-8.90	1.32	1.46
1	B	234	SER	CB-OG	-8.83	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GLU	CD-OE1	-8.68	1.16	1.25
1	B	148	THR	C-O	-8.65	1.06	1.23
1	B	297[A]	ASN	C-O	-8.39	1.07	1.23
1	B	297[B]	ASN	C-O	-8.39	1.07	1.23
1	B	99	GLU	CG-CD	8.13	1.64	1.51
1	B	230	ALA	CA-CB	-7.79	1.36	1.52
1	B	237	GLU	CB-CG	-7.70	1.37	1.52
1	B	192	ILE	C-O	-7.69	1.08	1.23
1	B	372	ARG	CB-CG	-7.44	1.32	1.52
1	B	198	TYR	CB-CG	-7.14	1.41	1.51
1	B	371	HIS	C-O	-7.07	1.09	1.23
1	B	100	GLU	C-O	-6.88	1.10	1.23
1	B	237	GLU	CG-CD	-6.86	1.41	1.51
1	B	53	TYR	CE1-CZ	-6.78	1.29	1.38
1	B	196	ARG	NE-CZ	-6.68	1.24	1.33
1	B	196	ARG	CZ-NH1	-6.66	1.24	1.33
1	B	4	GLU	CD-OE2	-6.55	1.18	1.25
1	B	196	ARG	CD-NE	-6.47	1.35	1.46
1	B	4	GLU	C-O	-6.44	1.11	1.23
1	B	373	LYS	C-O	-6.43	1.11	1.23
1	B	370	VAL	CB-CG1	-6.28	1.39	1.52
1	B	147	ARG	C-O	-6.28	1.11	1.23
1	B	100	GLU	CD-OE1	-6.20	1.18	1.25
1	B	237	GLU	CD-OE2	-6.16	1.18	1.25
1	B	57	GLU	CD-OE2	-6.15	1.18	1.25
1	B	195	GLU	CD-OE2	-6.14	1.18	1.25
1	B	87	HIS	C-O	-6.13	1.11	1.23
1	B	234	SER	C-O	-5.94	1.12	1.23
1	B	235	SER	N-CA	-5.81	1.34	1.46
1	B	57	GLU	CB-CG	-5.58	1.41	1.52
1	B	193	LEU	C-O	-5.56	1.12	1.23
1	B	232	SER	C-O	-5.52	1.12	1.23
1	B	194	THR	CB-CG2	-5.49	1.34	1.52
1	B	3	ASP	N-CA	-5.39	1.35	1.46
1	B	53	TYR	C-O	-5.39	1.13	1.23
1	B	194	THR	C-O	-5.35	1.13	1.23
1	B	99	GLU	C-O	-5.32	1.13	1.23
1	B	50	LYS	CA-CB	-5.29	1.42	1.53
1	B	370	VAL	C-O	-5.29	1.13	1.23
1	B	196	ARG	CZ-NH2	-5.25	1.26	1.33
1	B	147	ARG	CZ-NH2	-5.08	1.26	1.33
1	B	58	ALA	CA-CB	-5.05	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	C-O	-5.00	1.13	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	196	ARG	NE-CZ-NH1	-16.71	111.95	120.30
1	B	372	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	B	196	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	B	372	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	57	GLU	CG-CD-OE1	6.63	131.57	118.30
1	B	373	LYS	CD-CE-NZ	6.50	126.66	111.70
1	B	196	ARG	CD-NE-CZ	6.50	132.71	123.60
1	B	336[A]	LYS	CD-CE-NZ	5.94	125.36	111.70
1	B	336[B]	LYS	CD-CE-NZ	5.94	125.36	111.70
1	B	3	ASP	CB-CG-OD1	5.72	123.45	118.30
2	M	114	THR	CB-CA-C	-5.67	96.28	111.60
1	B	194	THR	OG1-CB-CG2	5.53	122.72	110.00
2	M	123[A]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	M	123[B]	ARG	NE-CZ-NH2	-5.28	117.66	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	194	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	233	SER	Peptide
1	B	234	SER	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	B	3003	0	3032	49	0
2	M	305	0	331	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	29	1	0
4	B	31	0	12	0	0
5	B	1	0	0	0	0
6	B	12	0	16	0	0
7	B	334	0	0	11	1
7	M	25	0	0	1	0
All	All	3738	0	3420	61	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 9.

All (61) 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)
2:M:123[B]:ARG:NH2	7:M:201:HOH:O	1.79	1.15
2:M:111[B]:ARG:HH11	2:M:111[B]:ARG:HG2	1.07	1.13
1:B:299:MET:CE	1:B:313[B]:MET:HG3	1.96	0.94
2:M:117:TYR:HD2	2:M:120[A]:ARG:HH22	1.05	0.93
1:B:111:ASN:HD21	1:B:119[B]:MET:CE	1.88	0.85
2:M:111[B]:ARG:NH1	2:M:111[B]:ARG:HG2	1.83	0.85
1:B:299:MET:HE1	1:B:313[B]:MET:HG3	1.61	0.82
2:M:117:TYR:HD2	2:M:120[A]:ARG:NH2	1.79	0.80
2:M:117:TYR:O	2:M:121[B]:LYS:HG2	1.83	0.79
2:M:111[B]:ARG:HH11	2:M:111[B]:ARG:CG	1.89	0.78
1:B:119[B]:MET:HE1	7:B:784:HOH:O	1.84	0.77
1:B:234:SER:HA	1:B:236:LEU:H	1.47	0.76
1:B:336[B]:LYS:HE2	7:B:633:HOH:O	1.85	0.75
1:B:68[B]:LYS:HD2	7:B:600:HOH:O	1.85	0.75
1:B:56:ASP:OD2	7:B:501:HOH:O	2.05	0.74
1:B:111:ASN:HD21	1:B:119[B]:MET:HE1	1.53	0.72
1:B:111:ASN:HD21	1:B:119[B]:MET:HE3	1.54	0.72
1:B:191:LYS:O	1:B:194:THR:HG22	1.90	0.71
1:B:233:SER:O	1:B:234:SER:CB	2.40	0.70
2:M:119[B]:LYS:HD3	2:M:123[B]:ARG:NH2	2.07	0.68
1:B:276[B]:GLU:OE2	7:B:502:HOH:O	2.13	0.67
1:B:299:MET:HE2	1:B:313[B]:MET:HG3	1.77	0.65
1:B:233:SER:OG	1:B:234:SER:N	2.30	0.61
1:B:176:MET:HE2	1:B:284:LYS:HD2	1.82	0.59
1:B:191:LYS:NZ	7:B:506:HOH:O	2.35	0.59
1:B:313[B]:MET:CE	7:B:578:HOH:O	2.49	0.59
1:B:272:ALA:HB1	1:B:276[B]:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276[A]:GLU:CD	7:B:529:HOH:O	2.45	0.54
1:B:233:SER:O	1:B:234:SER:HB2	2.07	0.54
1:B:230:ALA:C	1:B:232:SER:H	2.12	0.53
1:B:252:ASN:HD22	1:B:253:GLU:N	2.06	0.53
1:B:252:ASN:HD22	1:B:252:ASN:C	2.12	0.53
1:B:56:ASP:OD1	1:B:59:GLN:OE1	2.29	0.51
1:B:180[B]:LEU:HD13	1:B:267:ILE:HD11	1.92	0.51
1:B:361:GLU:HB3	1:B:369:ILE:CD1	2.40	0.51
1:B:336[B]:LYS:HG2	7:B:633:HOH:O	2.11	0.50
1:B:234:SER:CA	1:B:236:LEU:H	2.18	0.50
1:B:291[A]:LYS:HE2	7:B:773:HOH:O	2.12	0.49
1:B:111:ASN:ND2	1:B:119[B]:MET:CE	2.68	0.49
1:B:111:ASN:ND2	1:B:119[B]:MET:HE3	2.26	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.13	0.48
1:B:252:ASN:HD21	1:B:256:ARG:HH11	1.60	0.48
2:M:111[B]:ARG:NH1	2:M:111[B]:ARG:CG	2.58	0.48
1:B:124:PHE:CZ	1:B:132[A]:MET:HG3	2.49	0.48
1:B:351:THR:OG1	2:M:119[B]:LYS:HG3	2.13	0.48
1:B:109:PRO:HD3	7:B:539:HOH:O	2.13	0.48
1:B:252:ASN:ND2	1:B:256:ARG:HH11	2.12	0.47
3:B:401:LAB:H42	3:B:401:LAB:O2	2.15	0.46
1:B:111:ASN:ND2	1:B:119[B]:MET:HE1	2.29	0.44
1:B:250:ILE:HG13	1:B:253:GLU:HB2	2.00	0.44
2:M:120[A]:ARG:CZ	2:M:120[A]:ARG:HB2	2.48	0.44
1:B:8:LEU:HG	1:B:101:HIS:HB3	2.00	0.43
1:B:335:ARG:HA	1:B:338[A]:SER:OG	2.18	0.43
1:B:229:THR:O	1:B:232:SER:HB3	2.18	0.43
2:M:119[B]:LYS:HD3	2:M:123[B]:ARG:CZ	2.48	0.43
1:B:233:SER:OG	1:B:234:SER:CA	2.68	0.42
1:B:230:ALA:HB1	1:B:236:LEU:CD2	2.50	0.41
1:B:178[B]:LEU:HD23	1:B:178[B]:LEU:HA	1.68	0.41
1:B:131:ALA:HA	1:B:357:ILE:O	2.21	0.41
1:B:272:ALA:HB1	1:B:276[A]:GLU:HB2	2.03	0.41

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)
7:B:765:HOH:O	7:B:766:HOH:O[3_445]	2.11	0.09

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	389/377 (103%)	379 (97%)	7 (2%)	3 (1%)	19 4
2	M	34/32 (106%)	34 (100%)	0	0	100 100
All	All	423/409 (103%)	413 (98%)	7 (2%)	3 (1%)	19 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	SER
1	B	234	SER
1	B	231	ALA

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	337/320 (105%)	332 (98%)	5 (2%)	65 35
2	M	31/29 (107%)	28 (90%)	3 (10%)	8 0
All	All	368/349 (105%)	360 (98%)	8 (2%)	59 18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	233	SER
1	B	249[A]	THR
1	B	249[B]	THR

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Mol	Chain	Res	Type
1	B	252	ASN
1	B	372	ARG
2	M	111[A]	ARG
2	M	111[B]	ARG
2	M	114	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
1	B	252	ASN
1	B	280	ASN

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

Of 5 ligands modelled in this entry, 1 is 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	LAB	B	401	-	28,29,29	1.38	5 (17%)	30,41,41	1.96	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	B	402	5	26,33,33	0.98	0	31,52,52	1.22	4 (12%)
6	GOL	B	404	-	5,5,5	0.23	0	5,5,5	0.20	0
6	GOL	B	405	-	5,5,5	0.95	1 (20%)	5,5,5	1.75	2 (40%)

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	401	-	-	3/21/49/49	0/2/3/3
4	ATP	B	402	5	-	2/18/38/38	0/3/3/3
6	GOL	B	404	-	-	0/4/4/4	-
6	GOL	B	405	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	LAB	O2-C1	4.07	1.43	1.34
3	B	401	LAB	C17-C16	2.29	1.57	1.53
3	B	401	LAB	C14-C15	2.17	1.55	1.52
3	B	401	LAB	C18-S1	-2.16	1.73	1.77
3	B	401	LAB	C16-N1	-2.05	1.44	1.46
6	B	405	GOL	O2-C2	-2.02	1.37	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	LAB	C17-S1-C18	5.25	94.82	92.00
3	B	401	LAB	C4-C5-C6	-3.68	104.64	112.59
4	B	402	ATP	N3-C2-N1	-3.15	123.76	128.68
3	B	401	LAB	C19-C3-C4	3.05	120.41	115.27
3	B	401	LAB	C19-C3-C2	-3.00	113.73	122.77
3	B	401	LAB	O2-C1-C2	2.87	118.01	111.27
6	B	405	GOL	C3-C2-C1	2.45	121.22	111.70
6	B	405	GOL	O2-C2-C3	-2.25	99.22	109.12
3	B	401	LAB	O5-C18-N1	-2.22	124.38	126.81
3	B	401	LAB	C9-C10-C11	-2.18	109.98	114.03
4	B	402	ATP	C2-N1-C6	2.07	122.29	118.75
4	B	402	ATP	O3G-PG-O2G	2.06	115.50	107.64
4	B	402	ATP	N6-C6-N1	2.04	122.80	118.57

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	LAB	O3-C15-C16-C17
4	B	402	ATP	PG-O3B-PB-O1B
3	B	401	LAB	O2-C1-C2-C3
4	B	402	ATP	PB-O3B-PG-O2G
6	B	405	GOL	O1-C1-C2-O2
6	B	405	GOL	C1-C2-C3-O3
3	B	401	LAB	O1-C1-C2-C3

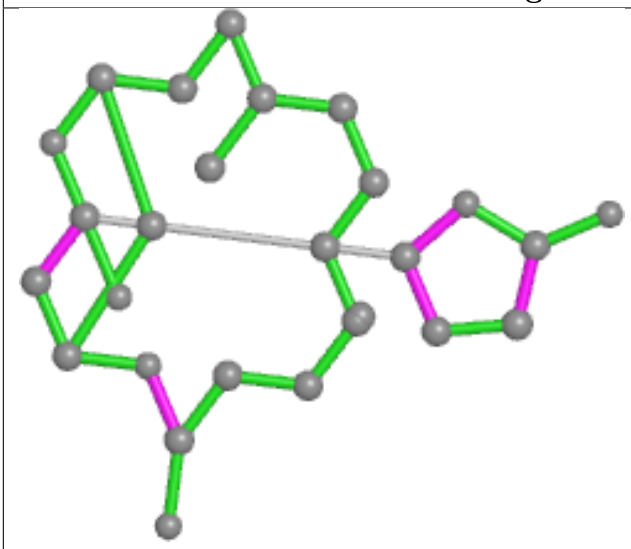
There are no ring outliers.

1 monomer is involved in 1 short contact:

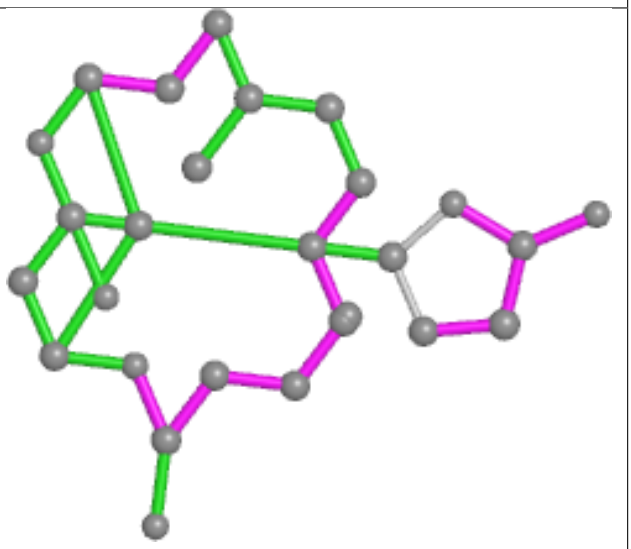
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	LAB	1	0

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.

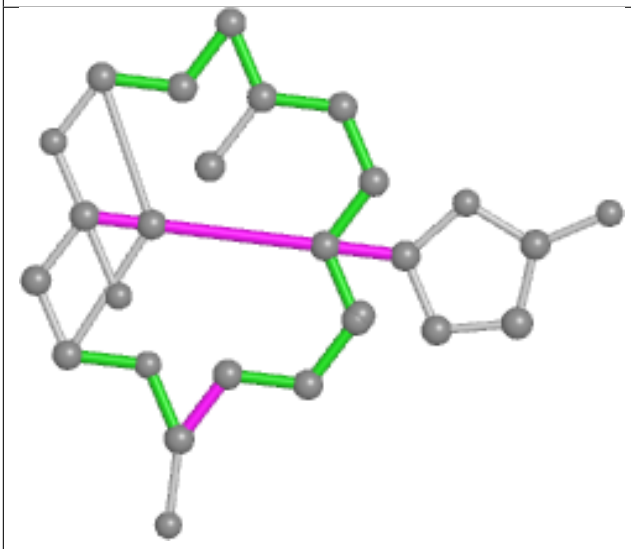
Ligand LAB B 401



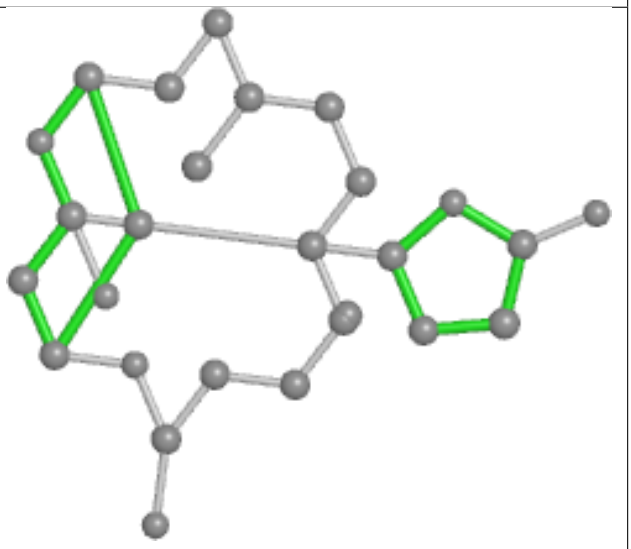
Bond lengths



Bond angles

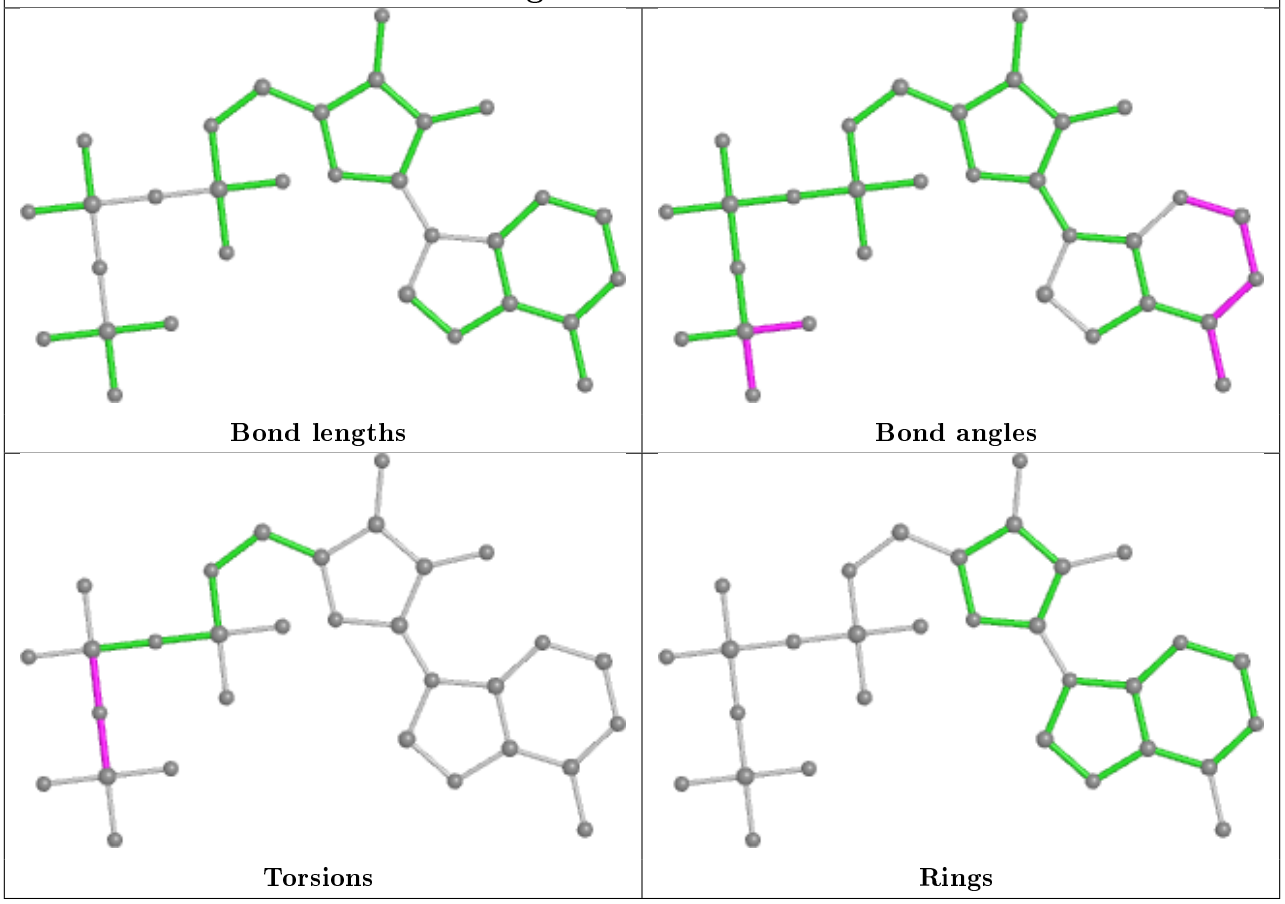


Torsions



Rings

Ligand ATP B 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	129:ALA	C	130[B]:GLU	N	1.19

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	B	360/377 (95%)	0.11	22 (6%)	21	23	11, 20, 43, 62	7 (1%)
2	M	30/32 (93%)	0.43	2 (6%)	17	19	18, 26, 45, 58	3 (10%)
All	All	390/409 (95%)	0.13	24 (6%)	20	22	11, 21, 43, 62	10 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	228	ALA	7.1
1	B	53	TYR	6.8
1	B	243	PRO	5.7
1	B	64	ILE	5.1
2	M	140	THR	4.8
1	B	231	ALA	4.0
1	B	235	SER	3.8
1	B	230	ALA	3.8
1	B	50	LYS	3.7
1	B	59	GLN	3.7
1	B	66	THR	3.7
1	B	38	PRO	3.5
1	B	51	ASP	3.3
1	B	229	THR	3.1
1	B	65	LEU	3.1
1	B	60	SER	3.1
1	B	244	ASP	2.9
2	M	138	GLU	2.4
1	B	52	SER	2.3
1	B	225	ASN	2.3
1	B	366	GLY	2.3
1	B	236	LEU	2.2
1	B	270	GLU	2.2
1	B	268	GLY	2.2

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)

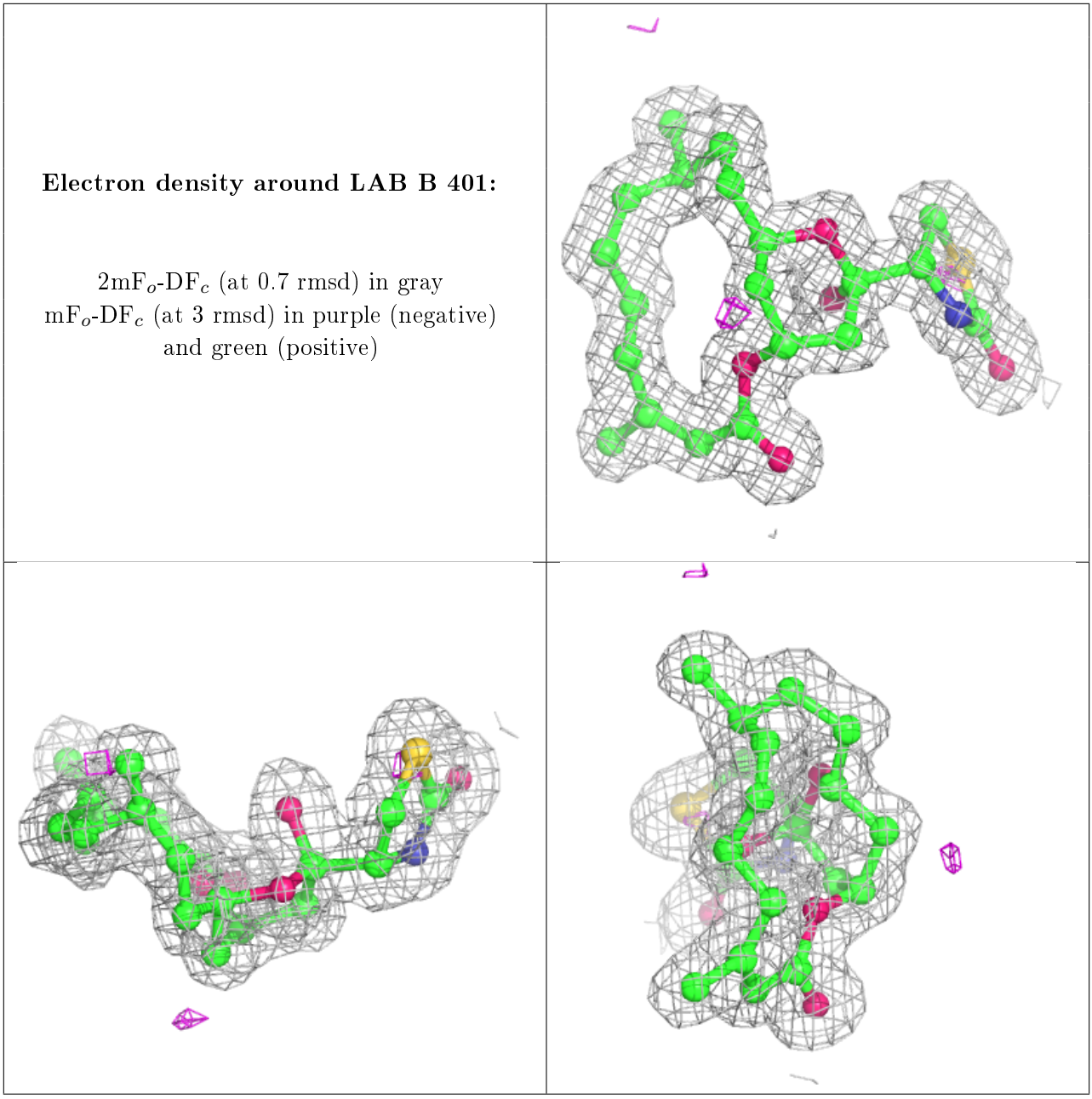
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GOL	B	405	6/6	0.84	0.15	46,49,51,51	0
6	GOL	B	404	6/6	0.90	0.11	34,35,37,37	0
3	LAB	B	401	27/27	0.98	0.06	14,17,20,23	0
4	ATP	B	402	31/31	0.99	0.08	11,13,15,16	4
5	MG	B	403	1/1	1.00	0.09	13,13,13,13	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.

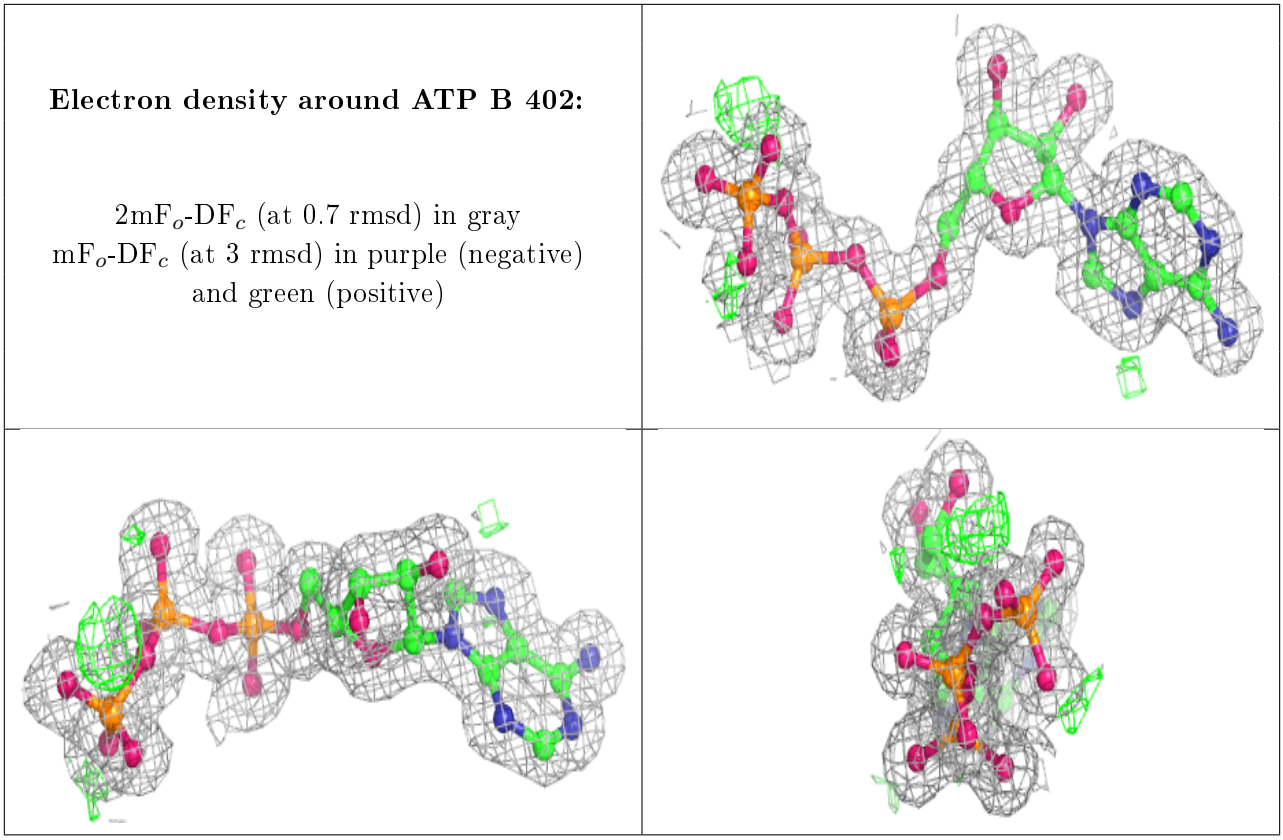
Electron density around LAB B 401:

$2mF_o$-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 B 402:

$2mF_o$-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 (i)

There are no such residues in this entry.