



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:49 AM UTC

PDB ID : 4B1U / pdb_00004b1u
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)

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

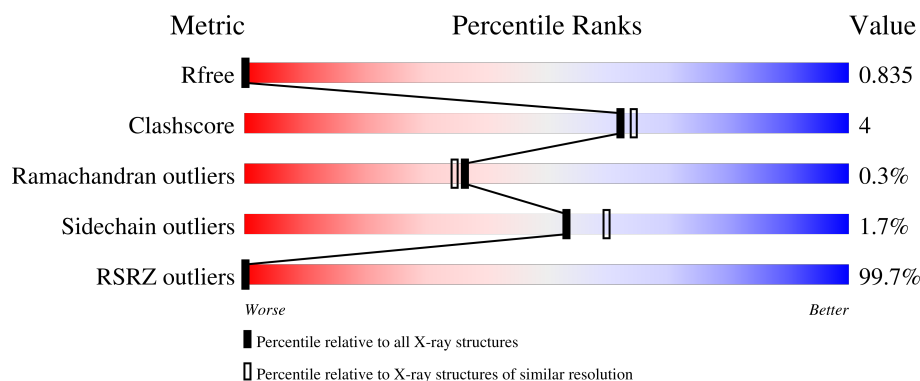
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of 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 $\leq 5\%$. 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	B	376	93% 84% 9% 7%
2	M	32	94% 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
6	TRS	B	1379	-	X	-	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.

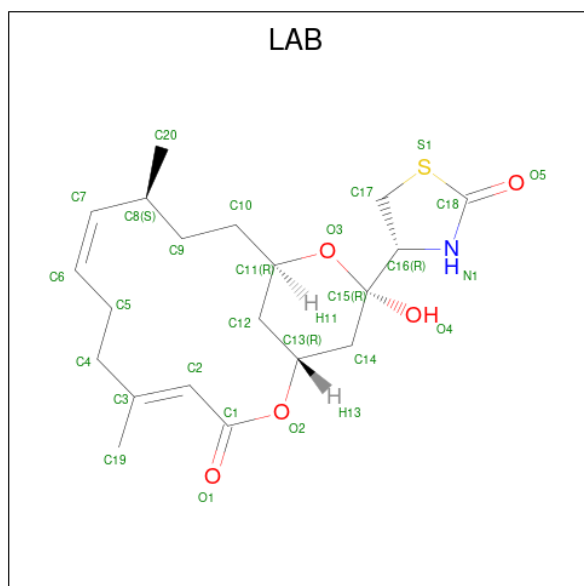
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

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.

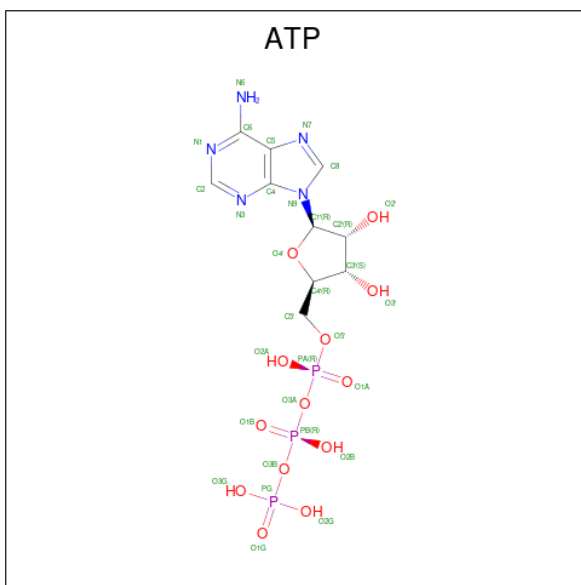
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	30	Total	C	N	O	S	0	1	0
			228	145	44	38	1			

- Molecule 3 is LATRUNCULIN B (CCD ID: 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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

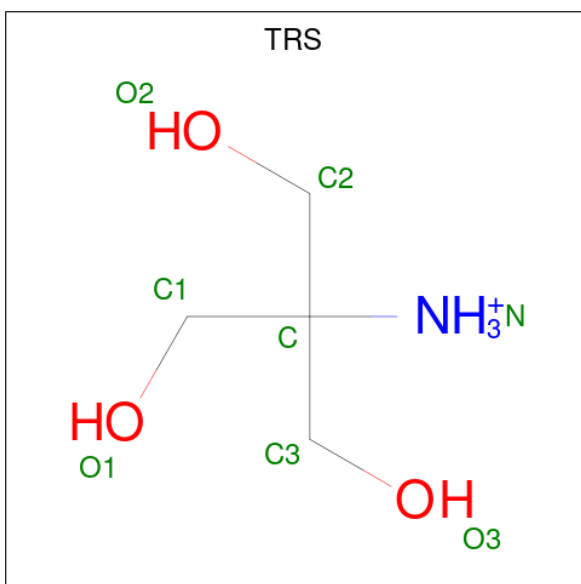


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is water.

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

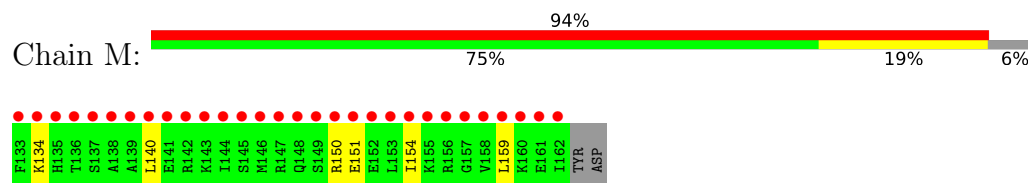
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



4 Data and refinement statistics

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) 95.9 (28.93-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.13 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.195 , 0.236 0.817 , 0.835	Depositor DCC
R_{free} test set	1529 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.237 for -h,-k,l	Xtriage
F_o, F_c correlation	0.62	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 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CA, ATP, TRS, MG, 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	0.55	0/2772	0.83	2/3764 (0.1%)
2	M	0.39	0/235	0.74	0/312
All	All	0.54	0/3007	0.82	2/4076 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	GLY	CA-C-N	5.86	126.27	119.47
1	B	366	GLY	C-N-CA	5.86	126.27	119.47

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	21	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	1	0
7	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	148	0	0	0	0
8	M	7	0	0	0	0
All	All	3149	0	2903	24	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 4.

All (24) 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)
6:B:1379:TRS:O1	6:B:1379:TRS:O2	1.88	0.82
1:B:71:ILE:HG13	1:B:82:MET:HE1	1.67	0.74
1:B:70:PRO:HB2	1:B:82:MET:HE2	1.76	0.67
1:B:274:ILE:HG13	1:B:313:MET:HE1	1.83	0.59
1:B:76:ILE:HG23	1:B:82:MET:HE3	1.86	0.56
1:B:10[B]:CYS:HB2	1:B:105:LEU:HD23	1.87	0.56
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: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:79:TRP:CE2	1:B:118:LYS:HE3	2.48	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.13	0.48
1:B:294:TYR:CD2	1:B:325:MET:HG2	2.50	0.47
1:B:71:ILE:HG13	1:B:82:MET:CE	2.40	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:53:TYR:C	1:B:58:ALA:HB2	2.44	0.42
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:70:PRO:HB2	1:B:82:MET:CE	2.46	0.42
1:B:53:TYR:HB3	1:B:58:ALA:HA	2.03	0.41
1:B:269:MET:HE2	1:B:269:MET:HB3	1.90	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

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	B	349/376 (93%)	342 (98%)	7 (2%)	0	100	100
2	M	29/32 (91%)	28 (97%)	0	1 (3%)	3	1
All	All	378/408 (93%)	370 (98%)	7 (2%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	134	LYS

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	B	286/319 (90%)	282 (99%)	4 (1%)	59	66
2	M	21/29 (72%)	20 (95%)	1 (5%)	23	21
All	All	307/348 (88%)	302 (98%)	5 (2%)	53	62

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	297	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 oligosaccharides 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	$\# Z > 2$
4	ATP	B	1377	5	32,33,33	1.56	7 (21%)	48,52,52	1.72	10 (20%)
6	TRS	B	1379	-	7,7,7	0.51	0	9,9,9	0.92	1 (11%)
3	LAB	B	1376	-	28,29,29	1.92	9 (32%)	29,41,41	2.22	6 (20%)

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
4	ATP	B	1377	5	-	1/22/38/38	0/3/3/3
6	TRS	B	1379	-	-	9/9/9/9	-
3	LAB	B	1376	-	-	4/21/49/49	0/2/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1376	LAB	C2-C3	4.51	1.41	1.33
4	B	1377	ATP	C5-C4	3.94	1.46	1.39
4	B	1377	ATP	PA-O3A	3.46	1.63	1.59
3	B	1376	LAB	C17-S1	-3.41	1.73	1.81
3	B	1376	LAB	O2-C13	-3.29	1.38	1.46
3	B	1376	LAB	O3-C11	-3.25	1.37	1.44
4	B	1377	ATP	PB-O3A	2.95	1.62	1.59
4	B	1377	ATP	PB-O3B	2.78	1.62	1.59
3	B	1376	LAB	C2-C1	2.74	1.53	1.46
4	B	1377	ATP	C4-N9	-2.63	1.32	1.37
4	B	1377	ATP	C5-C6	2.58	1.48	1.41
4	B	1377	ATP	C5-N7	-2.57	1.34	1.39
3	B	1376	LAB	O2-C1	2.49	1.39	1.34
3	B	1376	LAB	C16-N1	2.43	1.49	1.46
3	B	1376	LAB	C7-C6	2.42	1.41	1.31
3	B	1376	LAB	O3-C15	-2.10	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1376	LAB	C17-S1-C18	7.68	96.49	92.04
4	B	1377	ATP	C5-C4-N3	-4.87	120.01	126.72
4	B	1377	ATP	N3-C4-N9	4.18	134.28	127.17
3	B	1376	LAB	O3-C15-C16	3.97	109.34	104.25
3	B	1376	LAB	O2-C1-C2	3.79	119.98	111.20
4	B	1377	ATP	C4-N9-C8	3.74	109.66	105.74
4	B	1377	ATP	N3-C2-N1	-3.43	123.39	128.58
3	B	1376	LAB	C13-O2-C1	3.39	125.98	117.35
4	B	1377	ATP	C2-N3-C4	3.35	120.01	111.83
3	B	1376	LAB	O2-C1-O1	-3.32	118.02	123.34
4	B	1377	ATP	C4-C5-N7	-3.06	107.09	110.58
4	B	1377	ATP	N9-C8-N7	-2.79	109.97	113.94
4	B	1377	ATP	C5-N7-C8	2.62	107.56	103.45
4	B	1377	ATP	C2-N1-C6	2.28	122.47	118.73
4	B	1377	ATP	C6-C5-N7	2.17	136.27	132.09
3	B	1376	LAB	C9-C10-C11	-2.09	110.25	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1379	TRS	O2-C2-C	-2.04	105.20	110.88

There are no chirality outliers.

All (14) torsion outliers are listed below:

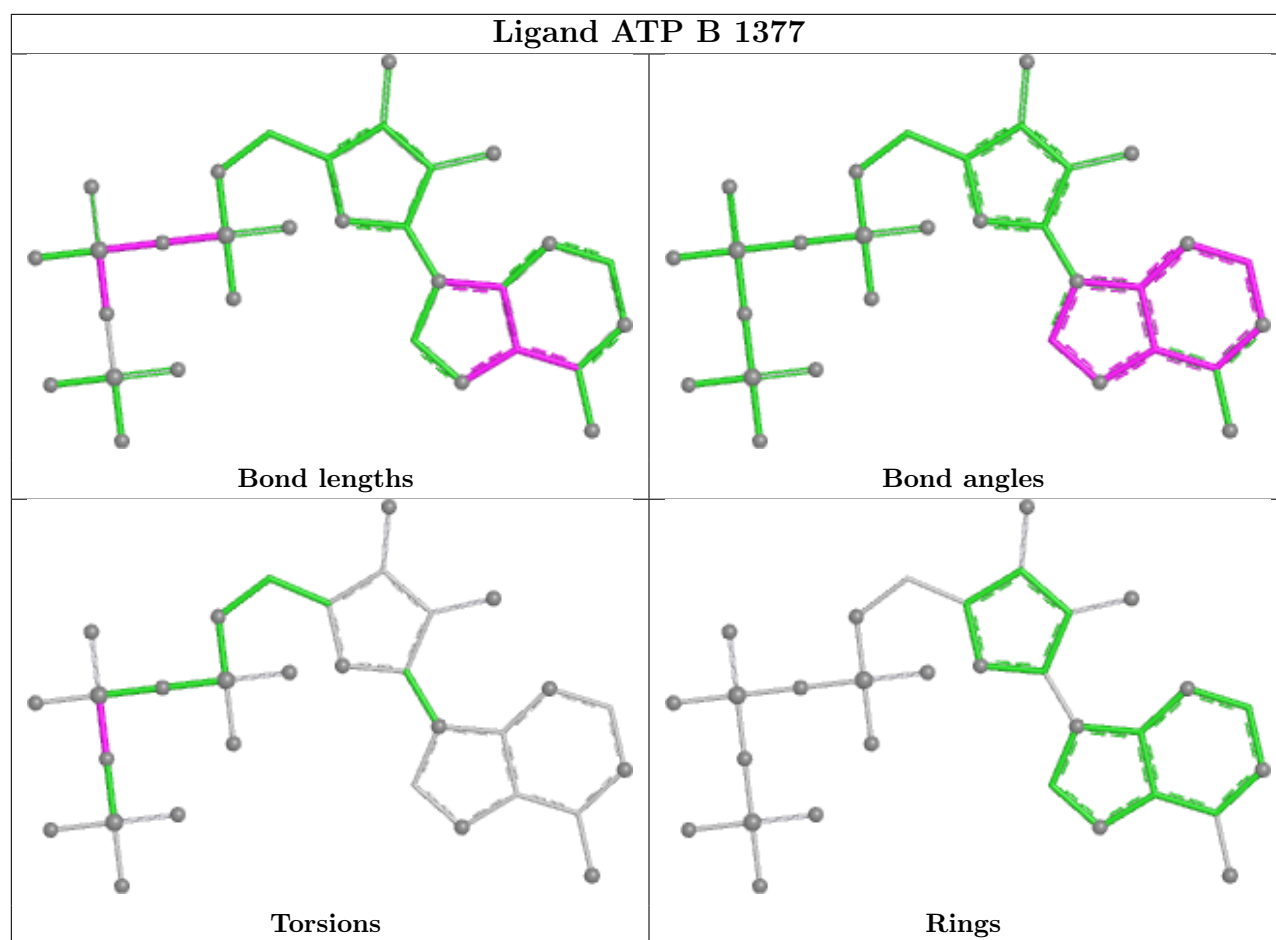
Mol	Chain	Res	Type	Atoms
3	B	1376	LAB	O3-C15-C16-C17
3	B	1376	LAB	C5-C6-C7-C8
6	B	1379	TRS	N-C-C1-O1
6	B	1379	TRS	C1-C-C2-O2
6	B	1379	TRS	C3-C-C2-O2
6	B	1379	TRS	N-C-C2-O2
6	B	1379	TRS	C2-C-C3-O3
6	B	1379	TRS	C2-C-C1-O1
6	B	1379	TRS	C1-C-C3-O3
6	B	1379	TRS	N-C-C3-O3
3	B	1376	LAB	C1-C2-C3-C4
6	B	1379	TRS	C3-C-C1-O1
3	B	1376	LAB	O2-C1-C2-C3
4	B	1377	ATP	PG-O3B-PB-O2B

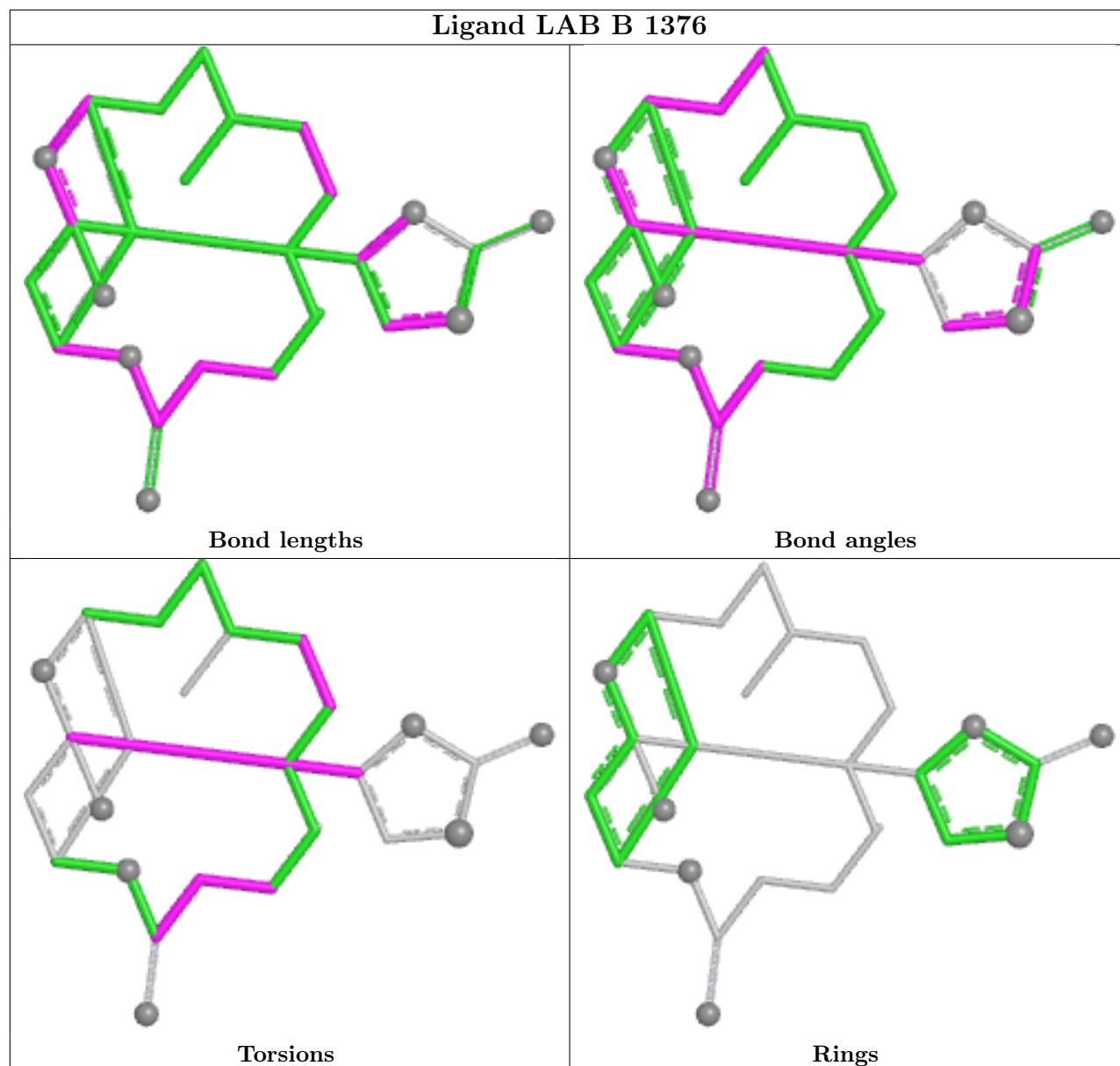
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1379	TRS	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 than 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.





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, 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%)	6.47	348 (99%) 0 0	11, 32, 58, 73	6 (1%)
2	M	30/32 (93%)	9.20	30 (100%) 0 0	22, 48, 62, 74	1 (3%)
All	All	379/408 (92%)	6.69	378 (99%) 0 0	11, 33, 59, 74	7 (1%)

All (378) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	ASP	17.5
1	B	229	THR	17.4
1	B	77	THR	16.5
1	B	351	THR	14.6
1	B	358	THR	14.0
2	M	138	ALA	13.9
2	M	145	SER	13.9
2	M	144	ILE	13.7
1	B	222	ASP	13.4
1	B	350	SER	13.0
2	M	146	MET	12.1
1	B	5	THR	12.0
1	B	98	PRO	11.9
1	B	318	THR	11.9
2	M	151	GLU	11.8
1	B	197	GLY	11.6
2	M	154	ILE	11.5
1	B	258	PRO	11.4
1	B	324	THR	11.3
1	B	349	LEU	11.3
1	B	356	TRP	11.3
1	B	64	ILE	11.2
1	B	52	SER	11.2
1	B	62	ARG	10.9

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Mol	Chain	Res	Type	RSRZ
2	M	162	ILE	10.9
2	M	155	LYS	10.9
1	B	203	THR	10.8
1	B	53	TYR	10.7
1	B	251	GLY	10.6
2	M	149	SER	10.5
1	B	196	ARG	10.5
1	B	322	PRO	10.5
1	B	99	GLU	10.4
1	B	60	SER	10.4
1	B	375	PHE	10.3
2	M	142	ARG	10.3
1	B	364	GLU	10.2
1	B	198	TYR	10.2
1	B	204	ALA	10.0
2	M	134	LYS	10.0
1	B	321	ALA	10.0
2	M	133	PHE	10.0
1	B	228	ALA	10.0
1	B	67	LEU	9.9
1	B	325	MET	9.9
1	B	365	ALA	9.8
1	B	66	THR	9.8
1	B	79	TRP	9.8
1	B	266	PHE	9.7
1	B	56	ASP	9.7
2	M	148	GLN	9.5
1	B	297	ASN	9.5
1	B	102	PRO	9.5
1	B	104	LEU	9.4
1	B	131	ALA	9.4
1	B	212	ILE	9.3
1	B	130	PRO	9.3
1	B	368	SER	9.3
1	B	96	VAL	9.3
2	M	152	GLU	9.2
1	B	128	ASN	9.1
1	B	6	THR	9.1
1	B	354	GLN	9.1
2	M	156	ARG	9.0
1	B	361	GLU	9.0
1	B	113	LYS	9.0

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Mol	Chain	Res	Type	RSRZ
1	B	179	ASP	9.0
1	B	319	ALA	9.0
1	B	92	ASN	8.9
1	B	372	ARG	8.9
1	B	169	TYR	8.9
1	B	120	THR	8.8
1	B	97	ALA	8.8
2	M	159	LEU	8.8
1	B	295	ALA	8.7
2	M	153	LEU	8.7
1	B	314	GLN	8.7
1	B	362	TYR	8.7
2	M	141	GLU	8.6
1	B	58	ALA	8.6
1	B	184	ASP	8.6
1	B	194	THR	8.6
1	B	24	ASP	8.5
1	B	344	SER	8.5
1	B	237	GLU	8.5
1	B	192	ILE	8.5
1	B	287	ILE	8.5
2	M	135[A]	HIS	8.5
2	M	139	ALA	8.4
1	B	355	MET	8.4
1	B	307	PRO	8.4
1	B	126	THR	8.3
1	B	311	ASP	8.3
1	B	23	GLY	8.2
1	B	118	LYS	8.2
1	B	317	ILE	8.2
1	B	329	ILE	8.2
1	B	246	GLN	8.2
1	B	281	SER	8.2
1	B	13	GLY	8.2
1	B	225	ASN	8.2
2	M	161	GLU	8.1
1	B	100	GLU	8.1
1	B	224	GLU	8.0
1	B	326	LYS	8.0
1	B	63	GLY	8.0
1	B	78	ASN	8.0
1	B	249	THR	8.0

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Mol	Chain	Res	Type	RSRZ
1	B	127	PHE	8.0
1	B	65	LEU	8.0
1	B	262	PHE	8.0
1	B	267	ILE	7.9
1	B	276	GLU	7.9
1	B	373	LYS	7.9
2	M	157	GLY	7.9
1	B	271	SER	7.9
2	M	136	THR	7.9
1	B	359	LYS	7.8
1	B	180	LEU	7.8
1	B	250	ILE	7.8
1	B	61	LYS	7.7
1	B	247	VAL	7.6
1	B	294	TYR	7.6
1	B	223	PHE	7.5
1	B	146	GLY	7.5
1	B	54	VAL	7.5
1	B	323	SER	7.5
1	B	216	LEU	7.5
1	B	239	SER	7.5
1	B	172	PRO	7.5
1	B	121	GLN	7.4
1	B	105	LEU	7.4
1	B	221	LEU	7.4
1	B	360	GLN	7.4
1	B	227	MET	7.4
1	B	327	ILE	7.3
1	B	168	GLY	7.3
1	B	244	ASP	7.3
1	B	195	GLU	7.3
1	B	288	ASP	7.3
1	B	241	GLU	7.3
1	B	103	THR	7.3
1	B	57	GLU	7.2
1	B	374	CYS	7.2
1	B	75	ILE	7.2
1	B	91	TYR	7.1
1	B	59	GLN	7.1
1	B	8	LEU	7.1
1	B	200	PHE	7.1
1	B	242	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	B	201	VAL	7.1
1	B	124	PHE	7.1
1	B	190	MET	7.0
1	B	187	ASP	7.0
1	B	286	ASP	7.0
1	B	370	VAL	7.0
1	B	245	GLY	7.0
1	B	371	HIS	6.9
2	M	147	ARG	6.9
1	B	101	HIS	6.9
1	B	34	ILE	6.9
1	B	269	MET	6.8
2	M	137	SER	6.8
1	B	122	ILE	6.8
1	B	256	ARG	6.8
1	B	145	SER	6.8
1	B	348[A]	SER	6.8
1	B	95	ARG	6.8
1	B	218	TYR	6.8
1	B	265	SER	6.7
1	B	268	GLY	6.7
1	B	352	PHE	6.7
1	B	347	ALA	6.7
1	B	353	GLN	6.7
1	B	333	PRO	6.7
1	B	253	GLU	6.6
1	B	110	LEU	6.6
1	B	264	PRO	6.6
1	B	171	LEU	6.6
1	B	117	GLU	6.6
1	B	182	GLY	6.6
1	B	112	PRO	6.5
1	B	366	GLY	6.5
1	B	133	TYR	6.5
1	B	243	PRO	6.5
1	B	208	ILE	6.5
1	B	357	ILE	6.5
1	B	219	VAL	6.4
2	M	158	VAL	6.4
1	B	21	PHE	6.4
1	B	167	GLU	6.4
1	B	199[A]	SER	6.3

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Mol	Chain	Res	Type	RSRZ
1	B	367	PRO	6.3
1	B	90	PHE	6.3
1	B	189	LEU	6.3
1	B	156	GLY	6.3
1	B	240	TYR	6.3
1	B	369	ILE	6.2
1	B	10[A]	CYS	6.2
1	B	252	ASN	6.2
1	B	202	THR	6.2
1	B	345	ILE	6.2
1	B	76	ILE	6.1
1	B	188	TYR	6.0
1	B	166	TYR	6.0
1	B	135	ALA	6.0
1	B	148	THR	6.0
1	B	315	LYS	6.0
1	B	115	ASN	6.0
1	B	320	LEU	5.9
1	B	181	ALA	5.9
1	B	7	ALA	5.8
1	B	328	LYS	5.8
1	B	129	VAL	5.8
1	B	255	PHE	5.8
1	B	140	LEU	5.8
1	B	260	THR	5.8
1	B	36	GLY	5.8
1	B	282	ILE	5.7
2	M	143	LYS	5.7
1	B	14[A]	SER	5.7
1	B	71	ILE	5.7
1	B	69	TYR	5.6
1	B	277	THR	5.6
1	B	141	SER	5.6
1	B	337	TYR	5.6
1	B	174	ALA	5.6
1	B	153	LEU	5.5
1	B	28	ARG	5.5
1	B	238	LYS	5.5
1	B	31	PHE	5.5
1	B	149	THR	5.5
1	B	87	HIS	5.5
1	B	178	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	209	VAL	5.5
1	B	316	GLU	5.5
1	B	22	ALA	5.5
1	B	309	ILE	5.4
1	B	125	GLU	5.4
2	M	160	LYS	5.4
1	B	165	ILE	5.4
1	B	289	ILE	5.4
1	B	33	SER	5.4
1	B	248	ILE	5.4
1	B	108	ALA	5.3
1	B	270	GLU	5.3
1	B	139	VAL	5.3
1	B	303	THR	5.3
1	B	86	TRP	5.3
1	B	106	THR	5.3
1	B	332	PRO	5.3
1	B	175	ILE	5.3
1	B	284	LYS	5.3
1	B	340	TRP	5.3
2	M	140	LEU	5.3
1	B	177	ARG	5.2
2	M	150	ARG	5.2
1	B	298	VAL	5.2
1	B	304	THR	5.2
1	B	19	ALA	5.2
1	B	310	ALA	5.2
1	B	147	ARG	5.1
1	B	55	GLY	5.1
1	B	142	LEU	5.1
1	B	257	CYS	5.1
1	B	342	GLY	5.1
1	B	170	ALA	5.1
1	B	259	GLU	5.0
1	B	186	THR	5.0
1	B	94	LEU	5.0
1	B	160	THR	5.0
1	B	29	ALA	5.0
1	B	82	MET	4.9
1	B	292	ASP	4.9
1	B	72	GLU	4.9
1	B	191	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	4.9
1	B	163	VAL	4.9
1	B	107	GLU	4.8
1	B	144	ALA	4.8
1	B	220	ALA	4.8
1	B	158	GLY	4.8
1	B	215	LYS	4.8
1	B	119	MET	4.8
1	B	173	HIS	4.8
1	B	278	THR	4.8
1	B	226	GLU	4.7
1	B	12	ASN	4.7
1	B	193	LEU	4.7
1	B	159	VAL	4.7
1	B	312	ARG	4.7
1	B	205	GLU	4.6
1	B	132	MET	4.6
1	B	150	GLY	4.6
1	B	88	HIS	4.6
1	B	343	GLY	4.5
1	B	280	ASN	4.5
1	B	143	TYR	4.5
1	B	151	ILE	4.5
1	B	341	ILE	4.5
1	B	263	GLN	4.5
1	B	346	LEU	4.5
1	B	283	MET	4.4
1	B	85	ILE	4.4
1	B	136	ILE	4.4
1	B	293	LEU	4.4
1	B	210	ARG	4.4
1	B	20	GLY	4.4
1	B	25	ASP	4.4
1	B	211	ASP	4.4
1	B	111	ASN	4.3
1	B	80	ASP	4.3
1	B	299	MET	4.3
1	B	279	TYR	4.2
1	B	116	ARG	4.2
1	B	296	ASN	4.2
1	B	313	MET	4.2
1	B	70	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	114	ALA	4.2
1	B	308	GLY	4.1
1	B	207	GLU	4.1
1	B	272	ALA	4.1
1	B	306	TYR	4.1
1	B	81	ASP	4.0
1	B	214	GLU	4.0
1	B	68	LYS	4.0
1	B	9	VAL	4.0
1	B	152	VAL	4.0
1	B	164	PRO	3.9
1	B	123	MET	3.9
1	B	335	ARG	3.9
1	B	206	ARG	3.8
1	B	183	ARG	3.8
1	B	185	LEU	3.8
1	B	330	ILE	3.8
1	B	285	CYS	3.8
1	B	73	HIS	3.8
1	B	162	ASN	3.7
1	B	83	GLU	3.7
1	B	254	ARG	3.7
1	B	17	VAL	3.7
1	B	334	GLU	3.7
1	B	305	MET	3.6
1	B	134	VAL	3.6
1	B	274	ILE	3.6
1	B	261	LEU	3.6
1	B	300	SER	3.6
1	B	176	MET	3.5
1	B	339	VAL	3.5
1	B	275	HIS	3.5
1	B	291	LYS	3.5
1	B	15	GLY	3.4
1	B	93	GLU	3.4
1	B	161	HIS	3.3
1	B	84	LYS	3.3
1	B	32	PRO	3.2
1	B	290	ARG	3.1
1	B	273	GLY	3.1
1	B	26	ALA	3.1
1	B	109	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	16	LEU	3.1
1	B	217	CYS	3.0
1	B	30	VAL	3.0
1	B	336[A]	LYS	3.0
1	B	157	ASP	2.9
1	B	138	ALA	2.9
1	B	331	ALA	2.9
1	B	137	GLN	2.8
1	B	155	SER	2.8
1	B	213	LYS	2.8
1	B	74	GLY	2.8
1	B	302	GLY	2.6
1	B	11	ASP	2.5
1	B	89	THR	2.5
1	B	154	ASP	2.5
1	B	301	GLY	2.2
1	B	18	LYS	2.1
1	B	338[A]	SER	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

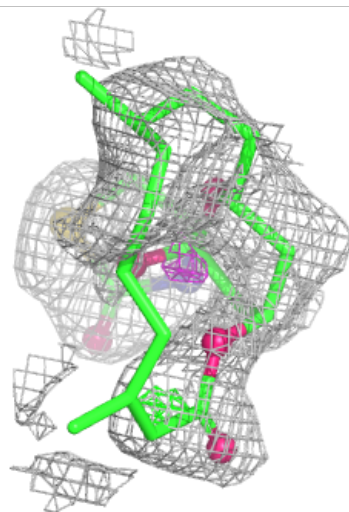
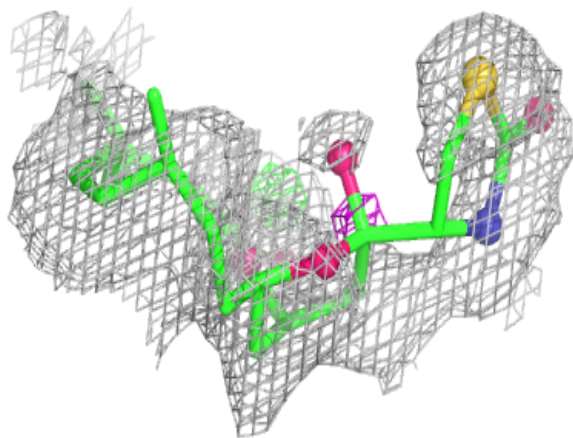
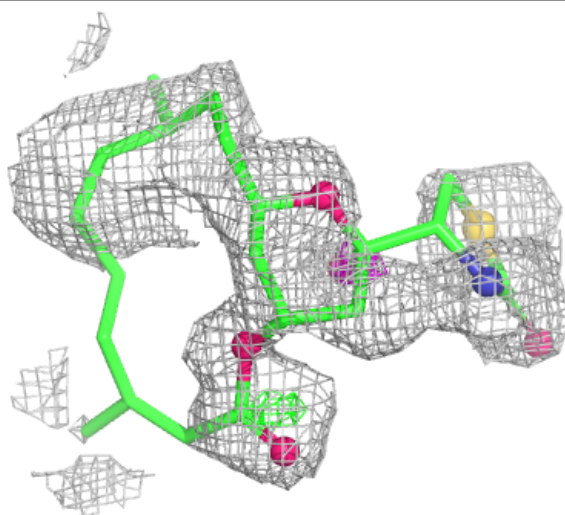
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

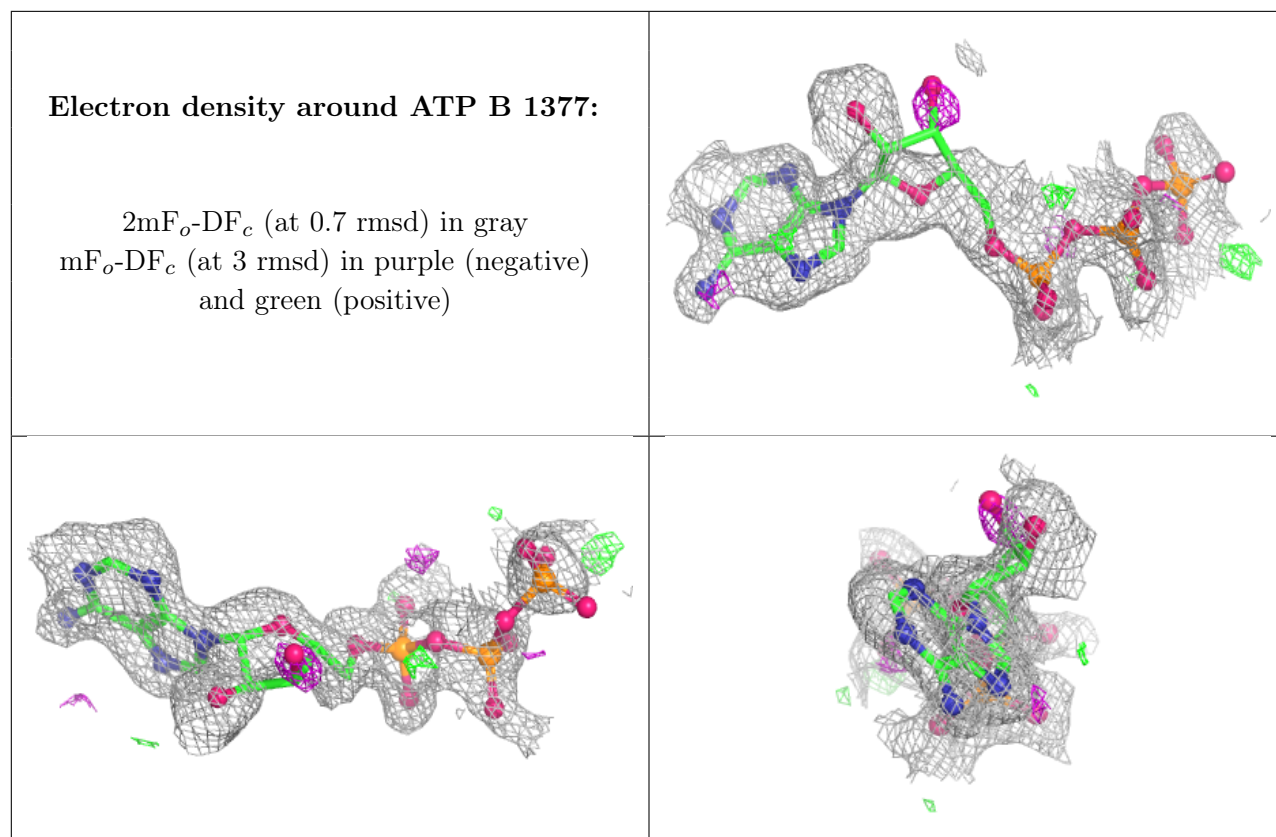
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LAB	B	1376	27/27	0.50	0.30	20,27,34,36	0
6	TRS	B	1379	8/8	0.73	0.50	21,45,56,60	0
4	ATP	B	1377	31/31	0.75	0.20	13,17,22,24	1
5	MG	B	1378	1/1	0.86	0.07	18,18,18,18	0
7	CA	M	1163	1/1	0.96	0.06	20,20,20,20	0

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 1376:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.