Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:59 am BST

PDB ID	:	4GY2
Title	:	Crystal structure of apo-Ia-actin complex
Authors	:	Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.
Deposited on	:	2012-09-05
Resolution	:	2.71 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:

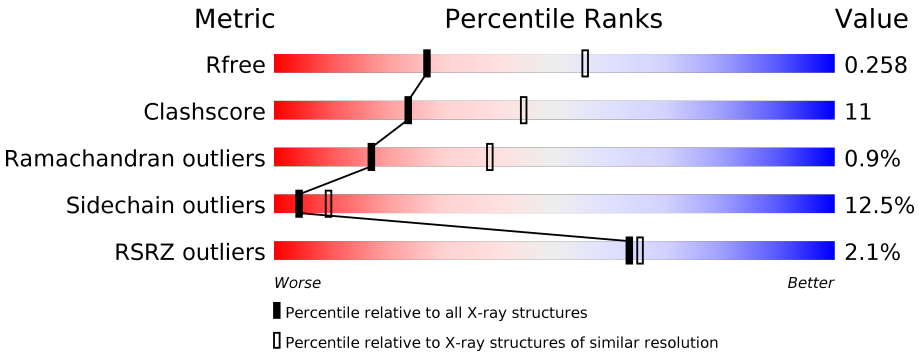
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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

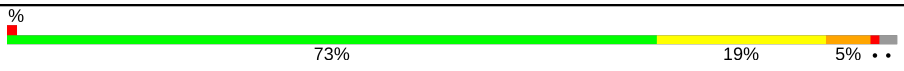
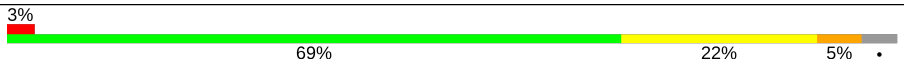
The reported resolution of this entry is 2.71 Å.

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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	A	418	
2	B	375	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6373 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 Iota toxin component Ia.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3347	2134	551	659	3			

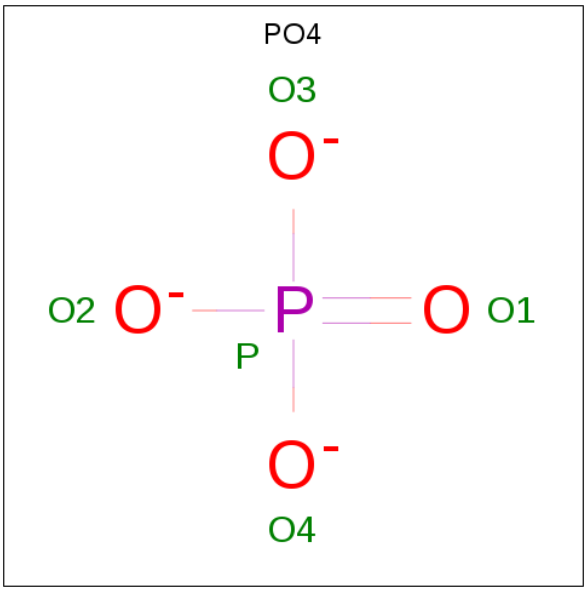
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ARG	-	EXPRESSION TAG	UNP Q46220
A	-3	GLY	-	EXPRESSION TAG	UNP Q46220
A	-2	SER	-	EXPRESSION TAG	UNP Q46220
A	-1	HIS	-	EXPRESSION TAG	UNP Q46220
A	0	MET	-	EXPRESSION TAG	UNP Q46220

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	360	Total	C	N	O	S	0	0	0
			2817	1785	474	539	19			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

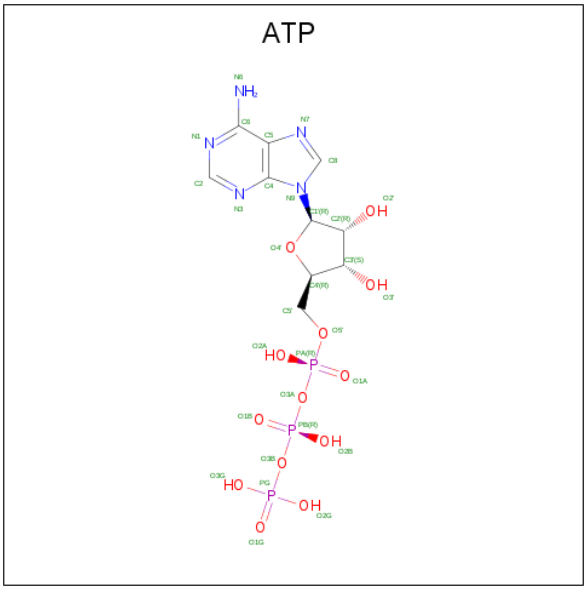


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

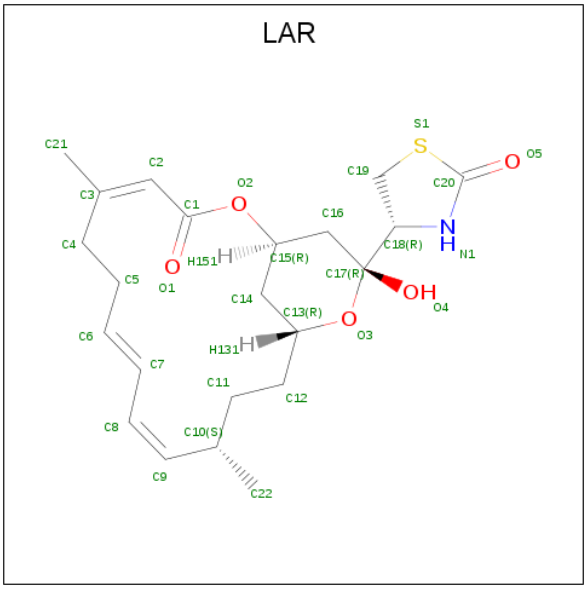
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

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



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

- Molecule 6 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).



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

- Molecule 7 is water.

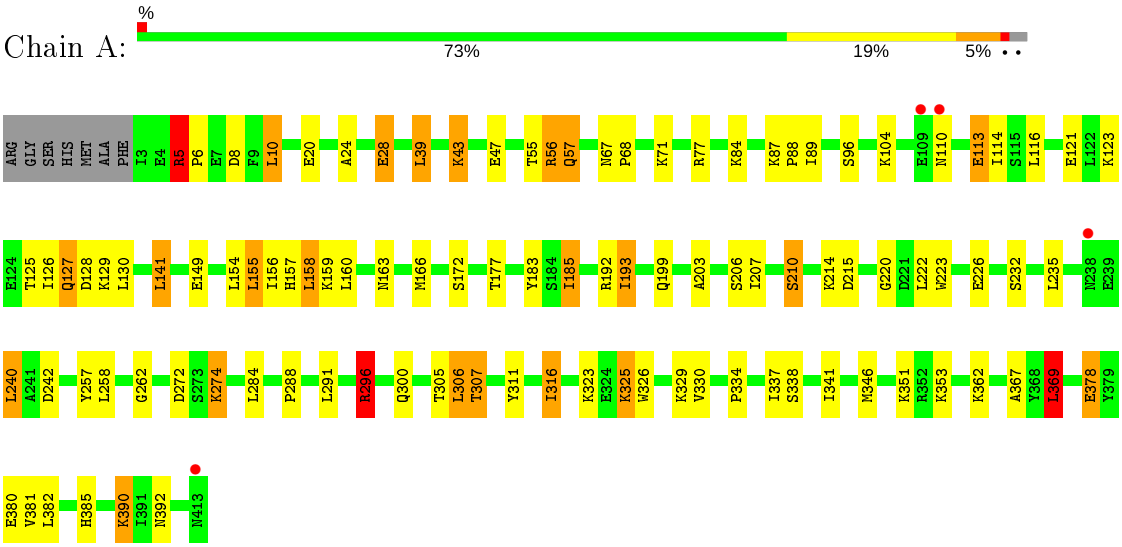
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	89	Total	O	0	0
			89	89		
7	B	54	Total	O	0	0
			54	54		

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.

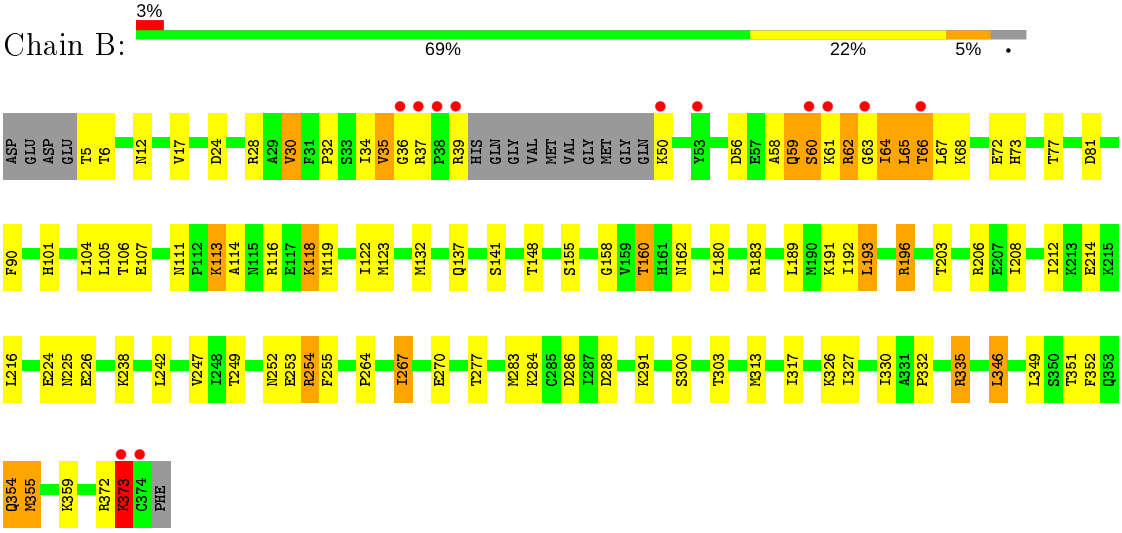
- Molecule 1: Iota toxin component Ia

Chain A:



- Molecule 2: Actin, alpha skeletal muscle

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.44Å 135.87Å 153.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 2.71 37.19 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.19-2.71) 99.6 (37.19-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.257 0.199 , 0.258	Depositor DCC
R_{free} test set	1605 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, PO4, CA, LAR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.70	1/3415 (0.0%)	0.91	8/4614 (0.2%)
2	B	0.76	0/2877	0.90	3/3899 (0.1%)
All	All	0.73	1/6292 (0.0%)	0.91	11/8513 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	TRP	CD2-CE2	5.49	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	335	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	296	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	B	335	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	296	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	116	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	353	LYS	CD-CE-NZ	-5.79	98.39	111.70
1	A	10	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	5	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	B	66	THR	N-CA-C	5.18	125.00	111.00
1	A	8	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	130	LEU	CA-CB-CG	5.13	127.09	115.30

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	3347	0	3329	67	0
2	B	2817	0	2793	70	0
3	A	5	0	0	1	0
4	B	1	0	0	0	0
5	B	31	0	12	2	0
6	B	29	0	31	2	0
7	A	89	0	0	11	0
7	B	54	0	0	8	0
All	All	6373	0	6165	137	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 11.

All (137) 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:156:ILE:HA	7:A:789:HOH:O	1.42	1.17
1:A:57:GLN:HE21	1:A:57:GLN:H	0.99	0.97
1:A:316:ILE:HD13	1:A:316:ILE:H	1.27	0.95
2:B:196:ARG:HH22	2:B:249:THR:HG22	1.36	0.89
1:A:89:ILE:HG21	1:A:166:MET:HE3	1.54	0.88
2:B:183:ARG:HD2	7:B:528:HOH:O	1.78	0.82
1:A:89:ILE:HG21	1:A:166:MET:CE	2.09	0.82
1:A:369:LEU:HD22	1:A:382:LEU:HB2	1.60	0.81
1:A:57:GLN:H	1:A:57:GLN:NE2	1.77	0.81
2:B:160:THR:CG2	2:B:180:LEU:O	2.36	0.73
2:B:332:PRO:O	2:B:335:ARG:HB2	1.88	0.73
1:A:57:GLN:HG2	1:A:214:LYS:HB3	1.71	0.72
1:A:316:ILE:CD1	1:A:316:ILE:H	2.03	0.72
2:B:160:THR:HG23	2:B:180:LEU:O	1.90	0.71
2:B:352:PHE:O	2:B:355:MET:HB2	1.90	0.71
1:A:20:GLU:OE1	1:A:177:THR:OG1	2.08	0.71
1:A:296:ARG:HD2	7:A:764:HOH:O	1.92	0.69
2:B:162:ASN:ND2	2:B:277:THR:OG1	2.25	0.69
2:B:35:VAL:HG22	2:B:36:GLY:N	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:HD13	1:A:316:ILE:N	2.07	0.67
2:B:346:LEU:HD22	2:B:352:PHE:CD1	2.31	0.66
2:B:32:PRO:HB3	6:B:403:LAR:H121	1.78	0.66
1:A:311:TYR:OH	7:A:752:HOH:O	2.10	0.66
2:B:313:MET:HG3	2:B:317:ILE:HD12	1.78	0.66
1:A:84:LYS:HD3	1:A:163:ASN:O	1.96	0.65
2:B:35:VAL:HG13	2:B:81:ASP:OD2	1.96	0.65
2:B:35:VAL:CG1	2:B:81:ASP:OD2	2.45	0.65
2:B:354:GLN:HE21	2:B:354:GLN:H	1.44	0.65
1:A:323:LYS:HE2	7:A:717:HOH:O	1.96	0.64
1:A:192:ARG:O	1:A:193:ILE:HD12	1.98	0.64
1:A:288:PRO:O	1:A:362:LYS:HE2	1.97	0.64
2:B:283:MET:CE	7:B:530:HOH:O	2.45	0.64
1:A:390:LYS:HG2	1:A:392:ASN:ND2	2.15	0.62
2:B:283:MET:HE3	7:B:530:HOH:O	2.00	0.62
1:A:5:ARG:NH1	1:A:88:PRO:O	2.34	0.61
1:A:20:GLU:CD	1:A:141:LEU:HD22	2.20	0.61
1:A:114:ILE:O	1:A:192:ARG:NH2	2.34	0.61
1:A:57:GLN:HE21	1:A:57:GLN:N	1.84	0.60
2:B:90:PHE:HZ	2:B:123:MET:CE	2.14	0.60
1:A:67:ASN:OD1	1:A:68:PRO:HD2	2.02	0.60
1:A:337:ILE:HD12	1:A:337:ILE:N	2.17	0.60
2:B:61:LYS:HD3	2:B:65:LEU:HG	1.84	0.60
2:B:216:LEU:O	2:B:254:ARG:HG3	2.03	0.59
1:A:28:GLU:HB2	7:A:739:HOH:O	2.03	0.58
2:B:12:ASN:ND2	7:B:507:HOH:O	2.36	0.58
1:A:203:ALA:O	7:A:789:HOH:O	2.17	0.58
2:B:72:GLU:HB2	7:B:529:HOH:O	2.04	0.57
2:B:72:GLU:HB3	7:B:526:HOH:O	2.04	0.57
2:B:77:THR:OG1	7:B:529:HOH:O	2.16	0.57
1:A:306:LEU:HB2	7:A:753:HOH:O	2.04	0.57
2:B:106:THR:HB	2:B:137:GLN:HG3	1.87	0.57
2:B:59:GLN:HE21	2:B:59:GLN:HA	1.70	0.56
2:B:300:SER:HA	2:B:335:ARG:HG2	1.88	0.56
2:B:104:LEU:HD23	2:B:104:LEU:C	2.26	0.56
1:A:155:LEU:O	7:A:789:HOH:O	2.18	0.55
2:B:317:ILE:HG22	2:B:327:ILE:HD13	1.88	0.55
2:B:73:HIS:HD2	2:B:158:GLY:O	1.90	0.55
2:B:155:SER:HA	2:B:160:THR:HB	1.89	0.55
2:B:118:LYS:O	2:B:122:ILE:HG13	2.07	0.55
2:B:196:ARG:NH2	2:B:249:THR:HG22	2.14	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:LEU:HD12	2:B:132:MET:HE2	1.88	0.55
1:A:378:GLU:HG3	7:A:771:HOH:O	2.05	0.54
1:A:192:ARG:O	1:A:193:ILE:CD1	2.55	0.54
2:B:17:VAL:O	2:B:30:VAL:HA	2.08	0.54
1:A:5:ARG:NH2	3:A:600:PO4:O4	2.40	0.54
1:A:242:ASP:OD1	1:A:274:LYS:HD2	2.08	0.53
1:A:220:GLY:HA3	1:A:341:ILE:HD13	1.89	0.53
2:B:62:ARG:O	2:B:66:THR:HA	2.09	0.53
2:B:62:ARG:O	2:B:66:THR:HG22	2.09	0.53
2:B:90:PHE:HZ	2:B:123:MET:HE3	1.73	0.53
1:A:183:TYR:CD2	1:A:207:ILE:HD12	2.44	0.52
2:B:107:GLU:OE2	2:B:116:ARG:HD3	2.09	0.52
1:A:89:ILE:HG21	1:A:166:MET:HE1	1.92	0.52
2:B:65:LEU:N	2:B:65:LEU:CD2	2.73	0.52
2:B:65:LEU:N	2:B:65:LEU:HD22	2.24	0.52
1:A:351:LYS:HB2	2:B:270:GLU:O	2.10	0.51
1:A:369:LEU:CD2	1:A:382:LEU:HB2	2.35	0.51
1:A:5:ARG:HG2	1:A:6:PRO:O	2.11	0.51
2:B:6:THR:O	2:B:101:HIS:HD2	1.94	0.51
1:A:158:LEU:HD13	1:A:160:LEU:HD23	1.93	0.50
1:A:257:TYR:OH	1:A:272:ASP:OD1	2.27	0.50
2:B:372:ARG:O	2:B:373:LYS:CB	2.59	0.50
2:B:90:PHE:CZ	2:B:123:MET:HE3	2.47	0.49
1:A:104:LYS:HE3	1:A:121:GLU:OE1	2.13	0.49
2:B:214:GLU:HG2	5:B:402:ATP:C5	2.48	0.49
1:A:334:PRO:O	1:A:385:HIS:HB2	2.13	0.48
2:B:35:VAL:HG11	2:B:81:ASP:OD2	2.14	0.48
2:B:24:ASP:OD2	2:B:28:ARG:NH2	2.36	0.47
2:B:283:MET:HE1	7:B:530:HOH:O	2.10	0.47
1:A:325:LYS:HB3	1:A:326:TRP:CD1	2.50	0.47
1:A:39:LEU:O	1:A:43:LYS:HG2	2.14	0.47
2:B:208:ILE:O	2:B:212:ILE:HG13	2.14	0.47
2:B:226:GLU:HB3	2:B:255:PHE:CE1	2.49	0.47
2:B:264:PRO:O	2:B:267:ILE:HG22	2.15	0.46
2:B:189:LEU:HG	2:B:193:LEU:HD22	1.98	0.46
1:A:305:THR:C	1:A:307:THR:H	2.19	0.46
1:A:337:ILE:HD12	1:A:337:ILE:H	1.77	0.46
1:A:57:GLN:HG2	1:A:214:LYS:HD3	1.98	0.46
1:A:24:ALA:O	1:A:28:GLU:HB2	2.16	0.46
2:B:58:ALA:C	2:B:60:SER:H	2.18	0.46
2:B:35:VAL:CG2	2:B:36:GLY:N	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:HIS:N	7:A:789:HOH:O	2.48	0.45
1:A:367:ALA:O	1:A:381:VAL:HA	2.16	0.45
2:B:214:GLU:HG2	5:B:402:ATP:C4	2.52	0.45
2:B:63:GLY:HA2	2:B:66:THR:HG23	1.98	0.45
1:A:338:SER:HB2	1:A:380:GLU:OE1	2.17	0.45
1:A:113:GLU:HA	1:A:199:GLN:HE21	1.81	0.45
2:B:32:PRO:HB2	2:B:34:ILE:HG13	1.99	0.45
2:B:39:ARG:H	2:B:65:LEU:HD13	1.82	0.45
6:B:403:LAR:H61	6:B:403:LAR:H91	1.49	0.45
1:A:235:LEU:HD13	1:A:240:LEU:HA	1.99	0.44
2:B:330:ILE:HG22	2:B:332:PRO:HD3	1.98	0.44
1:A:5:ARG:NH1	1:A:89:ILE:HB	2.32	0.44
2:B:192:ILE:HD12	2:B:253:GLU:HG3	1.99	0.43
1:A:125:THR:O	1:A:129:LYS:HE3	2.18	0.43
1:A:390:LYS:HG2	1:A:392:ASN:HD21	1.82	0.43
1:A:257:TYR:CE2	1:A:262:GLY:HA3	2.53	0.43
2:B:216:LEU:O	2:B:254:ARG:CG	2.66	0.43
1:A:326:TRP:O	1:A:329:LYS:HB2	2.19	0.43
2:B:59:GLN:O	2:B:59:GLN:HG3	2.18	0.43
1:A:306:LEU:HA	1:A:306:LEU:HD12	1.76	0.43
2:B:267:ILE:HD12	2:B:267:ILE:HG21	1.76	0.42
1:A:89:ILE:CG2	1:A:166:MET:HE3	2.38	0.42
2:B:64:ILE:C	2:B:65:LEU:HD22	2.40	0.42
1:A:123:LYS:O	1:A:127:GLN:HB2	2.19	0.42
2:B:113:LYS:O	2:B:114:ALA:C	2.58	0.41
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.62	0.41
2:B:372:ARG:O	2:B:373:LYS:HB3	2.21	0.41
1:A:183:TYR:CE2	1:A:207:ILE:HD12	2.55	0.41
1:A:346:MET:HE1	1:A:378:GLU:HB3	2.03	0.41
1:A:56:ARG:NH2	1:A:215:ASP:OD2	2.54	0.41
2:B:303:THR:HG22	2:B:303:THR:O	2.21	0.41
2:B:111:ASN:HD21	2:B:119:MET:HE3	1.85	0.41
1:A:210:SER:HB2	7:A:759:HOH:O	2.20	0.40
2:B:111:ASN:HD21	2:B:119:MET:CE	2.33	0.40
2:B:303:THR:O	2:B:303:THR:CG2	2.69	0.40
1:A:346:MET:CE	1:A:378:GLU:HB3	2.51	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	A	409/418 (98%)	390 (95%)	16 (4%)	3 (1%)	22 45
2	B	356/375 (95%)	335 (94%)	17 (5%)	4 (1%)	14 32
All	All	765/793 (96%)	725 (95%)	33 (4%)	7 (1%)	17 38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	373	LYS
1	A	172	SER
1	A	306	LEU
2	B	35	VAL
1	A	369	LEU
2	B	60	SER
2	B	64	ILE

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	375/380 (99%)	330 (88%)	45 (12%)	5 11
2	B	306/318 (96%)	266 (87%)	40 (13%)	4 9
All	All	681/698 (98%)	596 (88%)	85 (12%)	4 10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	10	LEU
1	A	28	GLU
1	A	39	LEU
1	A	43	LYS
1	A	47	GLU
1	A	55	THR
1	A	56	ARG
1	A	57	GLN
1	A	71	LYS
1	A	77	ARG
1	A	87	LYS
1	A	96	SER
1	A	110	ASN
1	A	113	GLU
1	A	126	ILE
1	A	127	GLN
1	A	128	ASP
1	A	141	LEU
1	A	149	GLU
1	A	154	LEU
1	A	155	LEU
1	A	158	LEU
1	A	159	LYS
1	A	185	ILE
1	A	193	ILE
1	A	206	SER
1	A	210	SER
1	A	222	LEU
1	A	226	GLU
1	A	232	SER
1	A	240	LEU
1	A	258	LEU
1	A	274	LYS
1	A	284	LEU
1	A	291	LEU
1	A	296	ARG
1	A	300	GLN
1	A	307	THR
1	A	316	ILE
1	A	325	LYS
1	A	330	VAL
1	A	369	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	378	GLU
1	A	390	LYS
2	B	5	THR
2	B	30	VAL
2	B	37	ARG
2	B	50	LYS
2	B	56	ASP
2	B	59	GLN
2	B	62	ARG
2	B	65	LEU
2	B	67	LEU
2	B	68	LYS
2	B	113	LYS
2	B	118	LYS
2	B	141	SER
2	B	148	THR
2	B	160	THR
2	B	191	LYS
2	B	193	LEU
2	B	196	ARG
2	B	203	THR
2	B	206	ARG
2	B	224	GLU
2	B	225	ASN
2	B	238	LYS
2	B	242	LEU
2	B	247	VAL
2	B	252	ASN
2	B	254	ARG
2	B	267	ILE
2	B	284	LYS
2	B	286	ASP
2	B	288	ASP
2	B	291	LYS
2	B	326	LYS
2	B	346	LEU
2	B	349	LEU
2	B	351	THR
2	B	354	GLN
2	B	355	MET
2	B	359	LYS
2	B	373	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	30	ASN
1	A	51	ASN
1	A	57	GLN
1	A	78	ASN
1	A	120	ASN
1	A	127	GLN
1	A	146	ASN
1	A	199	GLN
1	A	244	ASN
1	A	261	ASN
1	A	265	ASN
1	A	280	ASN
1	A	392	ASN
2	B	12	ASN
2	B	59	GLN
2	B	73	HIS
2	B	88	HIS
2	B	92	ASN
2	B	101	HIS
2	B	111	ASN
2	B	121	GLN
2	B	162	ASN
2	B	246	GLN
2	B	252	ASN
2	B	354	GLN

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 (i)

Of 4 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
5	ATP	B	402	-	26,33,33	1.02	1 (3%)	31,52,52	1.71	6 (19%)
6	LAR	B	403	-	30,31,31	1.58	4 (13%)	32,43,43	1.99	11 (34%)
3	PO4	A	600	-	4,4,4	1.06	0	6,6,6	1.12	0

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
5	ATP	B	402	-	-	2/18/38/38	0/3/3/3
6	LAR	B	403	-	-	11/23/51/51	0/2/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	403	LAR	O2-C1	5.75	1.46	1.34
6	B	403	LAR	C20-S1	-3.99	1.68	1.77
5	B	402	ATP	C5-C4	2.48	1.47	1.40
6	B	403	LAR	C19-S1	-2.24	1.76	1.81
6	B	403	LAR	O4-C17	2.03	1.44	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	403	LAR	O3-C17-C18	4.60	110.15	104.25
5	B	402	ATP	O4'-C1'-C2'	-4.45	100.43	106.93
6	B	403	LAR	O2-C1-C2	4.44	121.70	111.27
6	B	403	LAR	O2-C15-C14	3.67	116.61	107.79
5	B	402	ATP	N3-C2-N1	-3.57	123.11	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	403	LAR	O1-C1-C2	-3.17	118.24	126.23
6	B	403	LAR	C4-C5-C6	-2.78	106.59	112.59
5	B	402	ATP	O2G-PG-O3B	2.74	113.83	104.64
6	B	403	LAR	C21-C3-C4	2.58	119.61	115.27
6	B	403	LAR	O5-C20-N1	-2.58	123.99	126.81
5	B	402	ATP	C2-N1-C6	2.54	123.11	118.75
5	B	402	ATP	PA-O3A-PB	-2.54	124.10	132.83
6	B	403	LAR	C14-C15-C16	2.54	116.59	111.00
6	B	403	LAR	C19-S1-C20	2.43	93.30	92.00
5	B	402	ATP	O3'-C3'-C2'	-2.18	104.76	111.82
6	B	403	LAR	C12-C11-C10	2.04	117.34	113.95
6	B	403	LAR	O2-C1-O1	-2.02	120.05	123.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	402	ATP	PB-O3B-PG-O2G
6	B	403	LAR	C14-C15-O2-C1
6	B	403	LAR	O3-C17-C18-C19
6	B	403	LAR	C6-C7-C8-C9
6	B	403	LAR	C3-C4-C5-C6
6	B	403	LAR	O2-C1-C2-C3
6	B	403	LAR	O1-C1-C2-C3
5	B	402	ATP	PB-O3B-PG-O3G
6	B	403	LAR	C9-C10-C11-C12
6	B	403	LAR	C22-C10-C9-C8
6	B	403	LAR	O1-C1-O2-C15
6	B	403	LAR	C11-C10-C9-C8
6	B	403	LAR	C10-C11-C12-C13

There are no ring outliers.

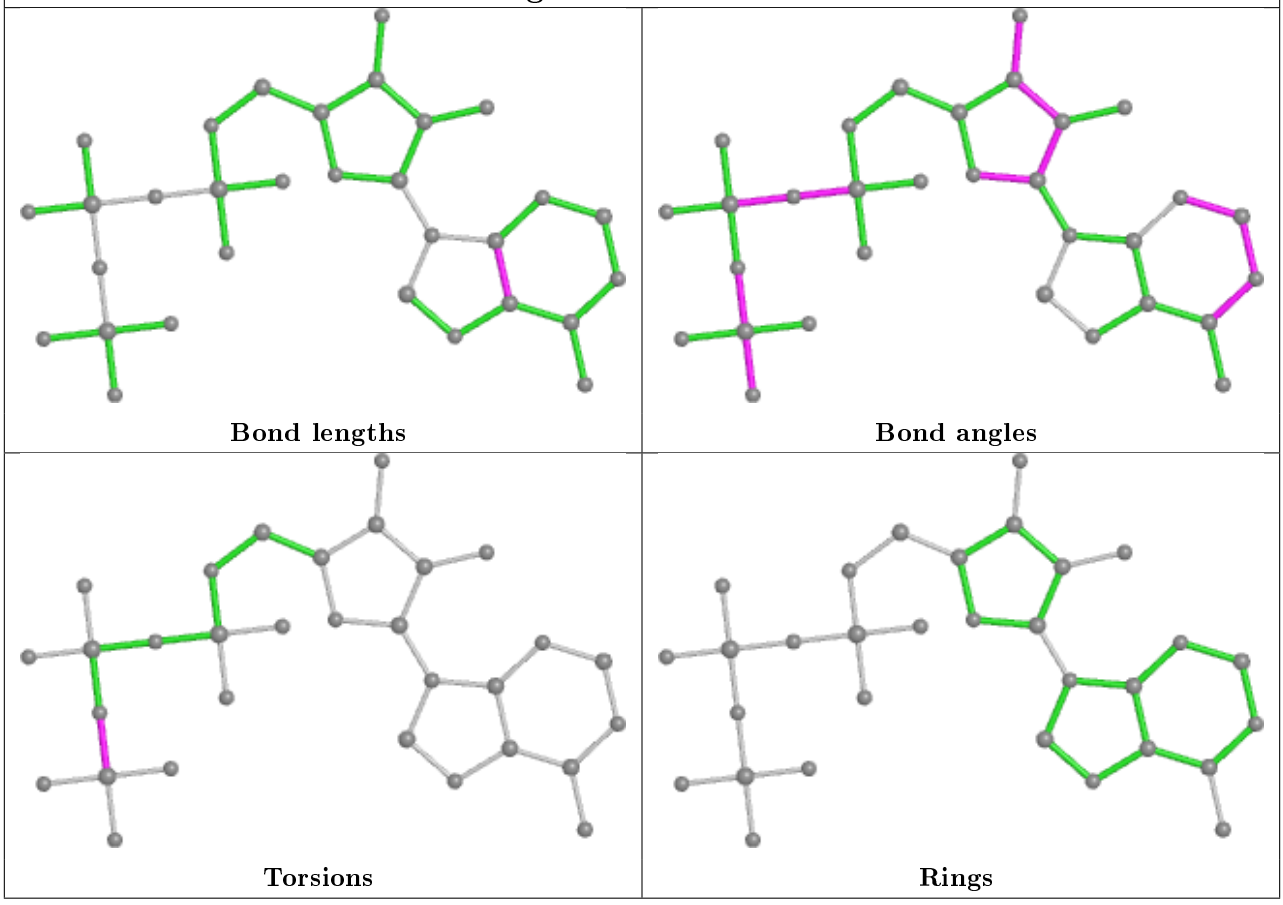
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	ATP	2	0
6	B	403	LAR	2	0
3	A	600	PO4	1	0

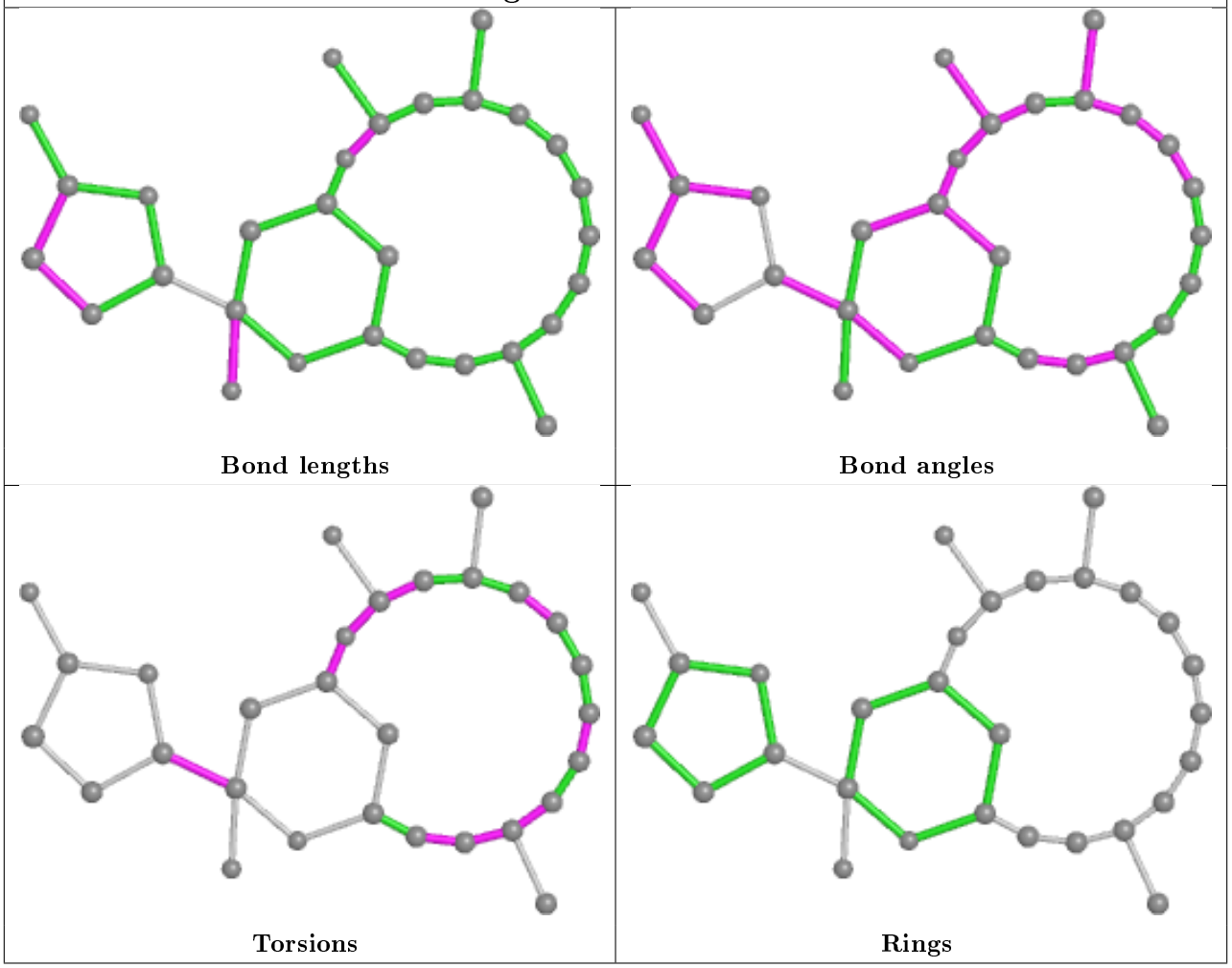
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ATP B 402



Ligand LAR B 403



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	411/418 (98%)	-0.38	4 (0%) 82 83	17, 31, 55, 81	0
2	B	360/375 (96%)	-0.23	12 (3%) 46 47	13, 26, 86, 158	0
All	All	771/793 (97%)	-0.31	16 (2%) 63 65	13, 29, 62, 158	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	38	PRO	8.5
2	B	37	ARG	7.5
2	B	66	THR	5.2
2	B	374	CYS	4.2
2	B	39	ARG	3.8
2	B	50	LYS	3.3
2	B	53	TYR	3.3
1	A	109	GLU	3.1
2	B	60	SER	3.1
2	B	373	LYS	2.8
2	B	63	GLY	2.8
1	A	413	ASN	2.4
2	B	61	LYS	2.4
1	A	110	ASN	2.4
2	B	36	GLY	2.2
1	A	238	ASN	2.1

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

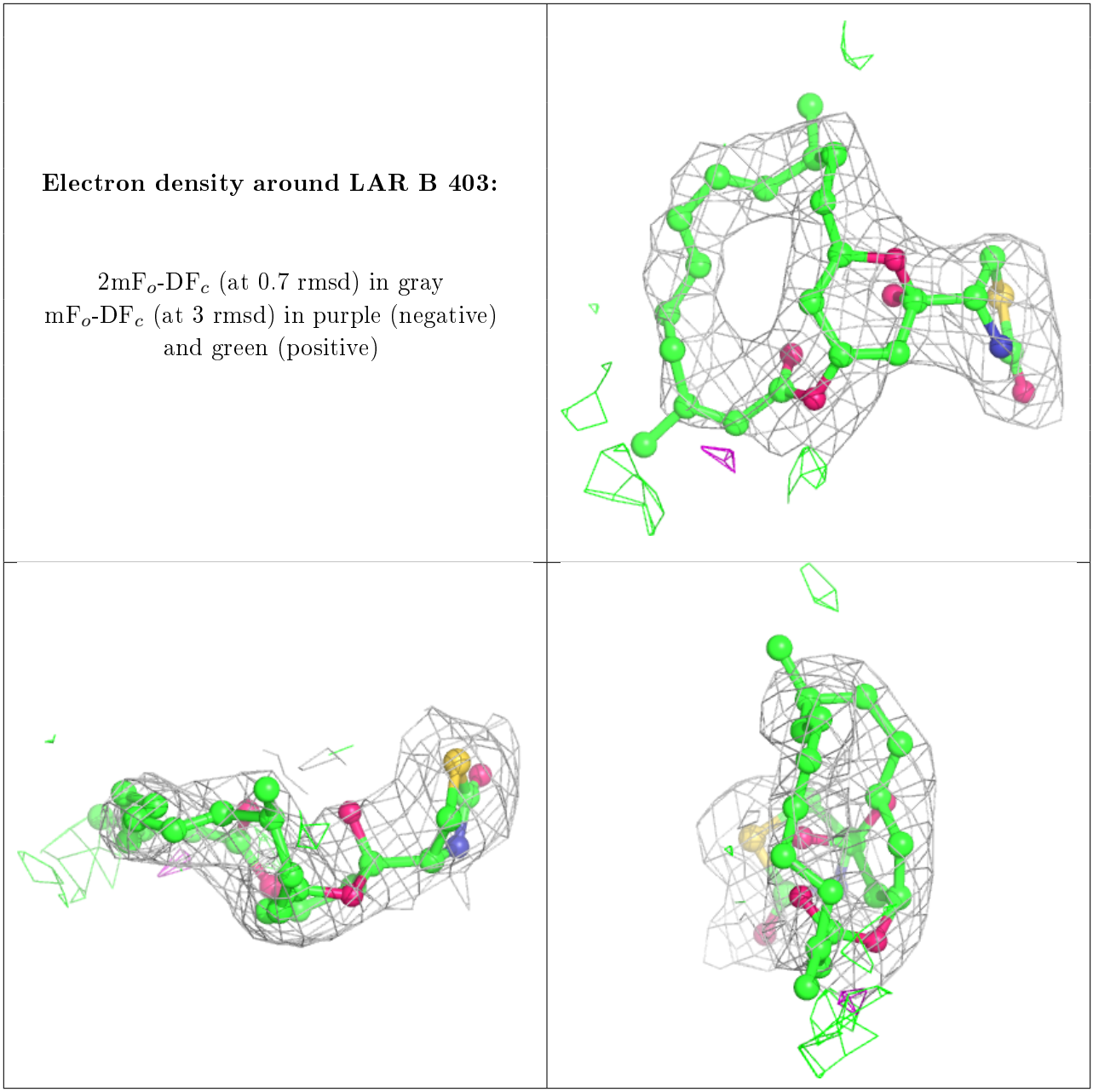
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	LAR	B	403	29/29	0.93	0.23	32,55,77,80	0
3	PO4	A	600	5/5	0.94	0.17	45,46,50,51	0
5	ATP	B	402	31/31	0.99	0.12	15,17,22,24	0
4	CA	B	401	1/1	0.99	0.10	21,21,21,21	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.

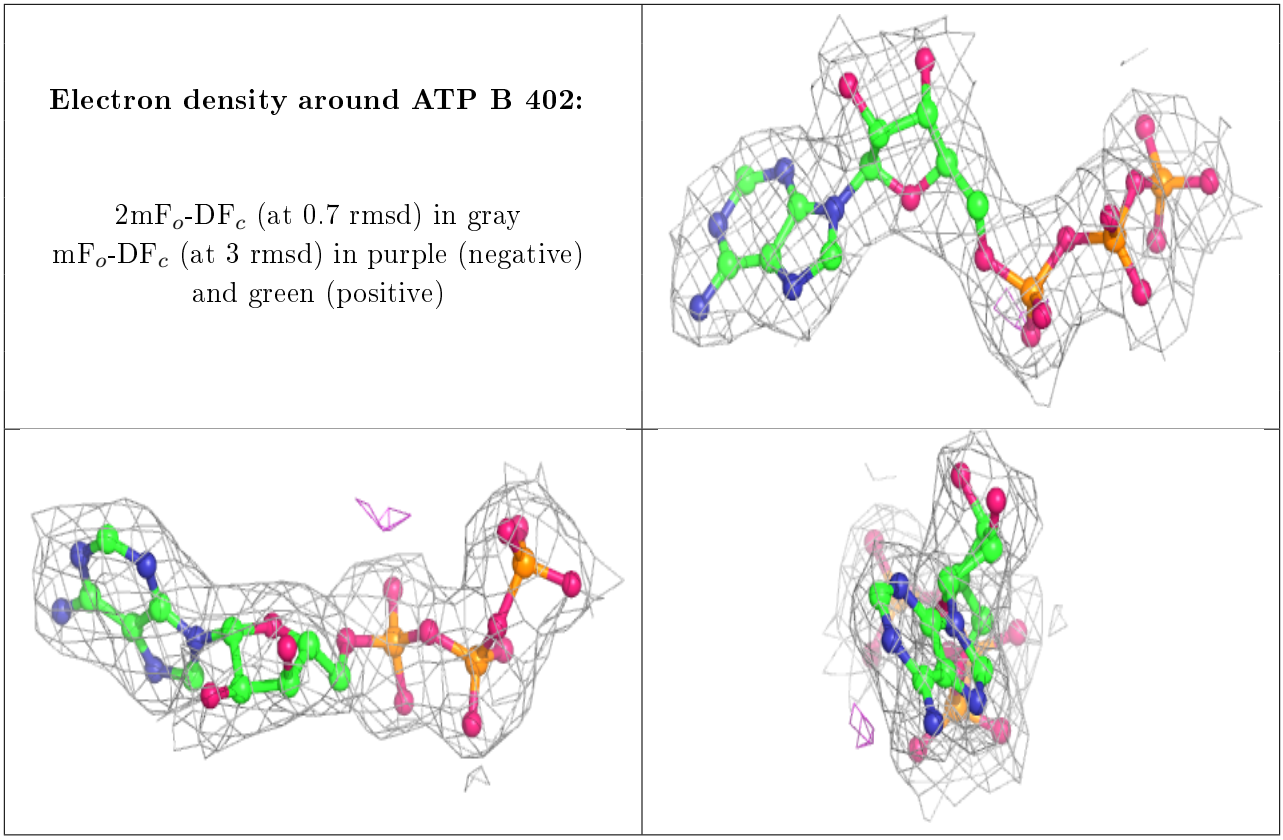
Electron density around LAR B 403:

$2mF_o$-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

There are no such residues in this entry.