Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 11:13 PM EDT

PDB ID	:	4Z94
Title	:	Actin Complex With a Chimera of Tropomodulin-1 and Leiomodin-1 Actin-Binding Site 2
Authors	:	Rebowski, G.; Boczkowska, M.; Dominguez, R.
Deposited on	:	2015-04-09
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

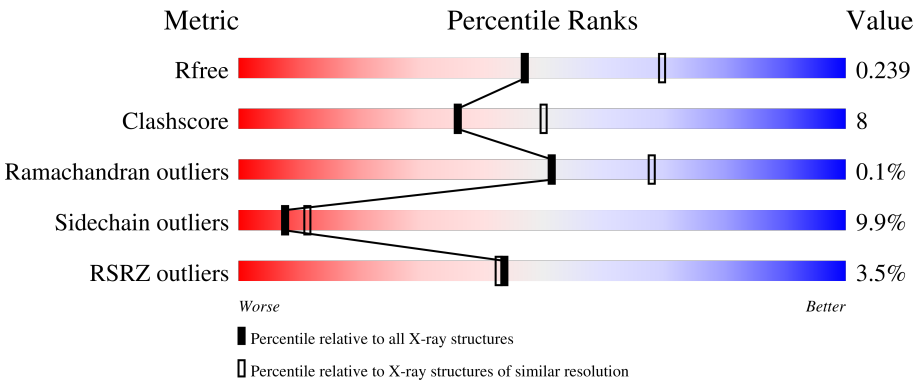
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	377	2% 77% 18% • • •
2	G	326	5% 71% 19% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10954 atoms, of which 5372 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
			Total	C	H	N	O	S			
1	A	371	5804	1846	2893	489	554	22	0	3	0

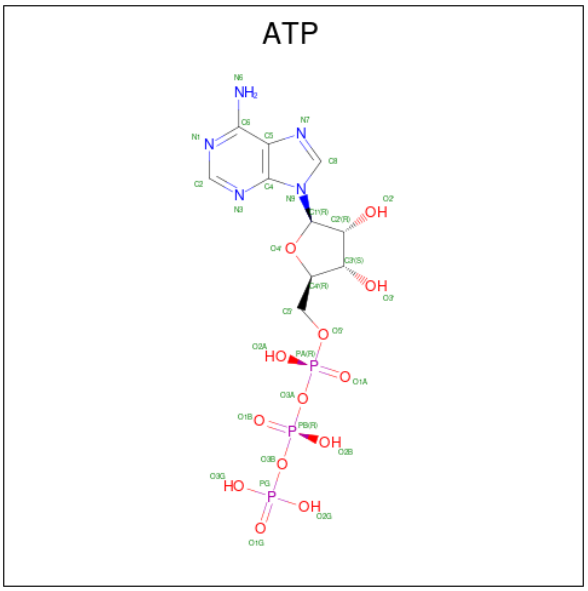
- Molecule 2 is a protein called Gelsolin, Tropomodulin-1, Leiomodin-1 chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	G	307	4923	1556	2468	432	459	8	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	126	GLY	-	linker	UNP P06396
G	1152	GLY	-	linker	UNP P06396
G	1153	SER	-	linker	UNP P06396
G	1154	GLY	-	linker	UNP P06396
G	1155	GLY	-	linker	UNP P06396
G	1156	SER	-	linker	UNP P06396
G	1157	GLY	-	linker	UNP P06396
G	1158	GLY	-	linker	UNP P06396
G	1159	SER	-	linker	UNP P06396

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	42	10	11	5	13	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	2	2	2	0	0
4	G	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	118	118	118	0	0
5	G	64	64	64	0	0

3 Residue-property plots (i)

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

Chain A: 2% 77% 18%

MET CYS ASP GLU ASP GLU T5 V17 R28 R39 H40 Q41 G42 V43 M44 V45 G46 M47 K50 K61 R62 T66 H73 R95 T106 E107 A108 K113 A131 Q137 D154 D157 H161 Y166 Y169 P172 I175 M176 R177 L180

R183 D184 L185 T186 D187 M190 K191 I192 L193 T194 E195 R196 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 L216 N225 S233 K238 S239 Y240 E241 L242 P243 Q246 V247 I248 T249 I250 G251 N252 E253 R254 F255 R256 T260 S265 E270 S271 H275

E276 I287 R290 K291 N296 I309 A310 I330 K336 T351 Q354 M355 W356 Q360 D363 H371 R372 K373 C374 F375

• Molecule 2: Gelsolin, Tropomodulin-1, Leiomodin-1 chimera

Chain G: 5% 71% 19% 6%

M1 V2 V3 E4 H5 Q18 T32 Y35 G36 D37 F38 L52 R53 N56 N67 E68 C69 S74 A78 D86 R91 R96 L107 K111 L114 K115 F125 G126 GLY SER GLY GLY SER GLY GLY SER GLY LEU ASN SER VAL ILE LYS PRO THR

GLN TYR K1171 P1172 V1173 P1174 D1175 E1176 E1177 R1189 I1190 N1193 D1194 P1195 E1199 L1202 N1203 N1204 I1205 R1206 N1207 I1208 P1209 I1210 P1211 T1212 K1221 E1222 N1223 S1224 Y1225 K1228 L1366 I1381 K1384 K1387 T1388 N1397 T1400 G1401 K1402 T1416 L1417 T1418 Q1425 R1426

H1427 I1428 G1431 K1432 T1433 E1434 M1435 E1436 L1441 N1444 T1445 T1446 L1447 E1455 P1459 R1475 R1478 L1479 Q1480 E1481 Q1482 R1483 Q1484 A1485 Q1486

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.23Å 70.80Å 81.32Å 90.00° 101.74° 90.00°	Depositor
Resolution (Å)	39.81 – 2.40 39.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.3 (39.81-2.40) 89.3 (39.81-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.243 0.194 , 0.239	Depositor DCC
R_{free} test set	1393 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10954	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: CA, HIC, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.74	1/2970 (0.0%)	0.83	3/4022 (0.1%)
2	G	0.65	1/2503 (0.0%)	0.82	2/3376 (0.1%)
All	All	0.70	2/5473 (0.0%)	0.82	5/7398 (0.1%)

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	A	0	2
2	G	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	VAL	CB-CG2	-5.52	1.41	1.52
2	G	78	ALA	CA-CB	-5.44	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ARG	NE-CZ-NH1	-7.16	116.72	120.30
2	G	1366	LEU	CB-CG-CD1	-6.20	100.47	111.00
2	G	1174	PRO	N-CA-C	5.77	127.09	112.10
1	A	44	MET	N-CA-C	5.20	125.04	111.00
1	A	154	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ASN	Mainchain
1	A	43	VAL	Peptide
2	G	1173	VAL	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	A	2911	2893	2893	45	0
2	G	2455	2468	2468	50	0
3	A	31	11	12	0	0
4	A	2	0	0	0	0
4	G	1	0	0	0	0
5	A	118	0	0	8	0
5	G	64	0	0	10	0
All	All	5582	5372	5373	86	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 8.

All (86) 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:G:1189:ARG:O	5:G:2101:HOH:O	1.85	0.95
2:G:1402:LYS:NZ	5:G:2104:HOH:O	2.04	0.89
1:A:157:ASP:OD2	1:A:183:ARG:NH2	2.06	0.88
2:G:91:ARG:O	5:G:2102:HOH:O	1.93	0.85
1:A:351:THR:O	2:G:3:VAL:HG21	1.80	0.81
2:G:38:PHE:HD2	2:G:114:LEU:HD21	1.46	0.80
2:G:1193:ASN:N	5:G:2101:HOH:O	2.14	0.80
1:A:166:TYR:O	5:A:501:HOH:O	2.01	0.79
2:G:37:ASP:O	5:G:2103:HOH:O	2.01	0.79
1:A:363:ASP:O	2:G:1475:ARG:NH1	2.17	0.77
2:G:91:ARG:NH2	5:G:2105:HOH:O	2.15	0.77
1:A:187:ASP:OD2	5:A:502:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:OD1	5:A:503:HOH:O	2.03	0.75
2:G:1173:VAL:HG22	2:G:1174:PRO:HD3	1.68	0.73
2:G:1387:LYS:O	2:G:1416:THR:HG21	1.93	0.68
2:G:1173:VAL:HG13	2:G:1174:PRO:HD2	1.74	0.68
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.76	0.67
2:G:1223:ASN:OD1	2:G:1225:TYR:N	2.27	0.67
1:A:199:SER:O	5:A:504:HOH:O	2.13	0.66
2:G:1173:VAL:HG13	2:G:1174:PRO:CD	2.25	0.66
2:G:38:PHE:CD2	2:G:114:LEU:HD21	2.32	0.64
1:A:180:LEU:HD21	1:A:260:THR:HG22	1.82	0.61
1:A:28:ARG:NH2	5:A:508:HOH:O	2.32	0.61
1:A:206:ARG:NH2	5:A:510:HOH:O	2.33	0.61
2:G:96:ARG:NH1	5:G:2111:HOH:O	2.34	0.60
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.83	0.59
2:G:1202:LEU:HA	2:G:1205:ILE:HD12	1.85	0.58
1:A:275:HIS:CD2	1:A:276:GLU:HG3	2.42	0.55
2:G:18:GLN:OE1	5:G:2106:HOH:O	2.18	0.55
2:G:1400:THR:HG23	2:G:1401:GLY:N	2.21	0.55
1:A:354:GLN:HB2	2:G:3:VAL:HG23	1.90	0.52
2:G:1205:ILE:HG21	2:G:1208:ILE:HD11	1.90	0.52
1:A:208:ILE:HD11	1:A:243:PRO:HG2	1.91	0.52
2:G:1431:GLY:O	2:G:1435:MET:HG2	2.10	0.52
2:G:32:THR:HA	2:G:35:TYR:CE1	2.44	0.52
2:G:1193:ASN:CA	5:G:2101:HOH:O	2.58	0.51
2:G:107:LEU:HD23	2:G:114:LEU:HD12	1.92	0.50
2:G:1433:THR:OG1	5:G:2107:HOH:O	2.20	0.50
1:A:61:LYS:HG2	2:G:1173:VAL:HG23	1.93	0.50
2:G:1205:ILE:CG2	2:G:1208:ILE:HD11	2.42	0.50
1:A:202:THR:H	1:A:205:GLU:HB2	1.77	0.49
2:G:1190:ILE:HG23	2:G:1223:ASN:HD22	1.77	0.49
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.94	0.49
2:G:1195:PRO:HG3	2:G:1225:TYR:CE2	2.48	0.48
1:A:44:MET:HG3	1:A:46:GLY:H	1.79	0.48
2:G:1441:LEU:HD12	2:G:1444:ASN:HB3	1.95	0.48
1:A:275:HIS:NE2	1:A:276:GLU:HG3	2.28	0.47
1:A:169:TYR:OH	2:G:86:ASP:OD2	2.32	0.47
1:A:242:LEU:HD12	1:A:246:GLN:HB3	1.97	0.47
1:A:161:HIS:NE2	1:A:177:ARG:HG3	2.30	0.47
1:A:5:THR:OG1	5:A:505:HOH:O	2.18	0.47
2:G:1387:LYS:C	2:G:1416:THR:HG21	2.35	0.46
1:A:191:LYS:O	1:A:194:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HB	1:A:137:GLN:HG3	1.97	0.45
1:A:183:ARG:HH21	1:A:183:ARG:HG3	1.82	0.45
1:A:351:THR:HB	2:G:3:VAL:HG21	1.98	0.45
1:A:354:GLN:OE1	2:G:3:VAL:HG22	2.17	0.45
1:A:351:THR:O	2:G:3:VAL:CG2	2.59	0.45
2:G:1435:MET:SD	2:G:1459:PRO:HG3	2.57	0.45
2:G:1479:LEU:O	2:G:1483:ARG:N	2.50	0.44
1:A:202:THR:HB	1:A:205:GLU:HB2	2.00	0.44
1:A:208:ILE:HD11	1:A:243:PRO:CG	2.48	0.44
1:A:183:ARG:NH1	5:A:518:HOH:O	2.42	0.44
1:A:216:LEU:HD11	1:A:240:TYR:HB2	2.00	0.44
2:G:69:CYS:SG	2:G:74:SER:HB3	2.59	0.43
1:A:330:ILE:N	1:A:330:ILE:HD12	2.33	0.43
2:G:1485:ALA:C	2:G:1486:GLN:HG3	2.39	0.43
2:G:4:GLU:OE2	2:G:5:HIS:N	2.51	0.43
2:G:1397:ASN:O	2:G:1425:GLN:HA	2.19	0.43
1:A:252:ASN:O	1:A:256:ARG:HG3	2.18	0.43
1:A:44:MET:HA	1:A:44:MET:HE2	2.00	0.42
1:A:287:ILE:HG23	1:A:290:ARG:NH2	2.34	0.42
1:A:113:LYS:HD2	1:A:371:HIS:CE1	2.55	0.42
2:G:1210:ILE:N	2:G:1211:PRO:CD	2.82	0.42
2:G:1400:THR:CG2	2:G:1401:GLY:N	2.82	0.42
1:A:47:MET:HB3	2:G:1204:ASN:ND2	2.35	0.41
1:A:196:ARG:O	1:A:196:ARG:HG3	2.20	0.41
2:G:1205:ILE:HG22	2:G:1208:ILE:HG13	2.03	0.41
2:G:1479:LEU:O	2:G:1483:ARG:HB2	2.21	0.41
2:G:1418:THR:HA	2:G:1447:LEU:HA	2.03	0.41
1:A:192:ILE:HD12	1:A:253:GLU:HG3	2.03	0.40
1:A:309:ILE:HG23	1:A:310:ALA:N	2.36	0.40
2:G:52:LEU:HD12	2:G:56:ASN:ND2	2.36	0.40
2:G:1381:ILE:HA	2:G:1384:LYS:HD2	2.03	0.40
1:A:238:LYS:HD2	1:A:254:ARG:NH1	2.36	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	A	371/377 (98%)	362 (98%)	9 (2%)	0	100	100
2	G	304/326 (93%)	293 (96%)	10 (3%)	1 (0%)	41	55
All	All	675/703 (96%)	655 (97%)	19 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	5	HIS

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	A	316/319 (99%)	286 (90%)	30 (10%)	8	12
2	G	264/276 (96%)	236 (89%)	28 (11%)	6	9
All	All	580/595 (98%)	522 (90%)	58 (10%)	8	11

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	28	ARG
1	A	39	ARG
1	A	44	MET
1	A	45	VAL
1	A	47	MET
1	A	50	LYS
1	A	62	ARG
1	A	66[A]	THR
1	A	66[B]	THR
1	A	95	ARG

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Mol	Chain	Res	Type
1	A	177	ARG
1	A	185	LEU
1	A	196	ARG
1	A	203	THR
1	A	205	GLU
1	A	206	ARG
1	A	233	SER
1	A	238	LYS
1	A	248	ILE
1	A	250	ILE
1	A	265	SER
1	A	270	GLU
1	A	271	SER
1	A	287	ILE
1	A	291	LYS
1	A	336	LYS
1	A	355	MET
1	A	360	GLN
1	A	373	LYS
2	G	1	MET
2	G	3	VAL
2	G	4	GLU
2	G	53	ARG
2	G	67	ASN
2	G	69	CYS
2	G	111	LYS
2	G	114	LEU
2	G	115	LYS
2	G	125	PHE
2	G	1199	GLU
2	G	1206	ARG
2	G	1212	THR
2	G	1221	LYS
2	G	1228	LYS
2	G	1366	LEU
2	G	1388	THR
2	G	1400	THR
2	G	1426	ARG
2	G	1428	ILE
2	G	1433	THR
2	G	1436	GLU
2	G	1445	THR

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Mol	Chain	Res	Type
2	G	1455	GLU
2	G	1478	ARG
2	G	1483	ARG
2	G	1484	GLN
2	G	1486	GLN

Sometimes 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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
1	HIC	A	73	1	8,11,12	1.77	2 (25%)	6,14,16	1.14	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
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CZ-NE2	-3.62	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	3.04	1.40	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	401	4	26,33,33	1.18	2 (7%)	31,52,52	1.61	7 (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	ATP	A	401	4	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ATP	PG-O2G	-2.13	1.46	1.54
3	A	401	ATP	C2'-C1'	-2.08	1.50	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	ATP	O3'-C3'-C2'	-3.99	98.93	111.82
3	A	401	ATP	PA-O3A-PB	-2.86	123.00	132.83
3	A	401	ATP	N6-C6-N1	2.79	124.36	118.57
3	A	401	ATP	N3-C2-N1	-2.58	124.64	128.68
3	A	401	ATP	O2A-PA-O1A	2.40	124.11	112.24
3	A	401	ATP	O3G-PG-O2G	2.31	116.47	107.64
3	A	401	ATP	C3'-C2'-C1'	-2.10	97.81	100.98

There are no chirality outliers.

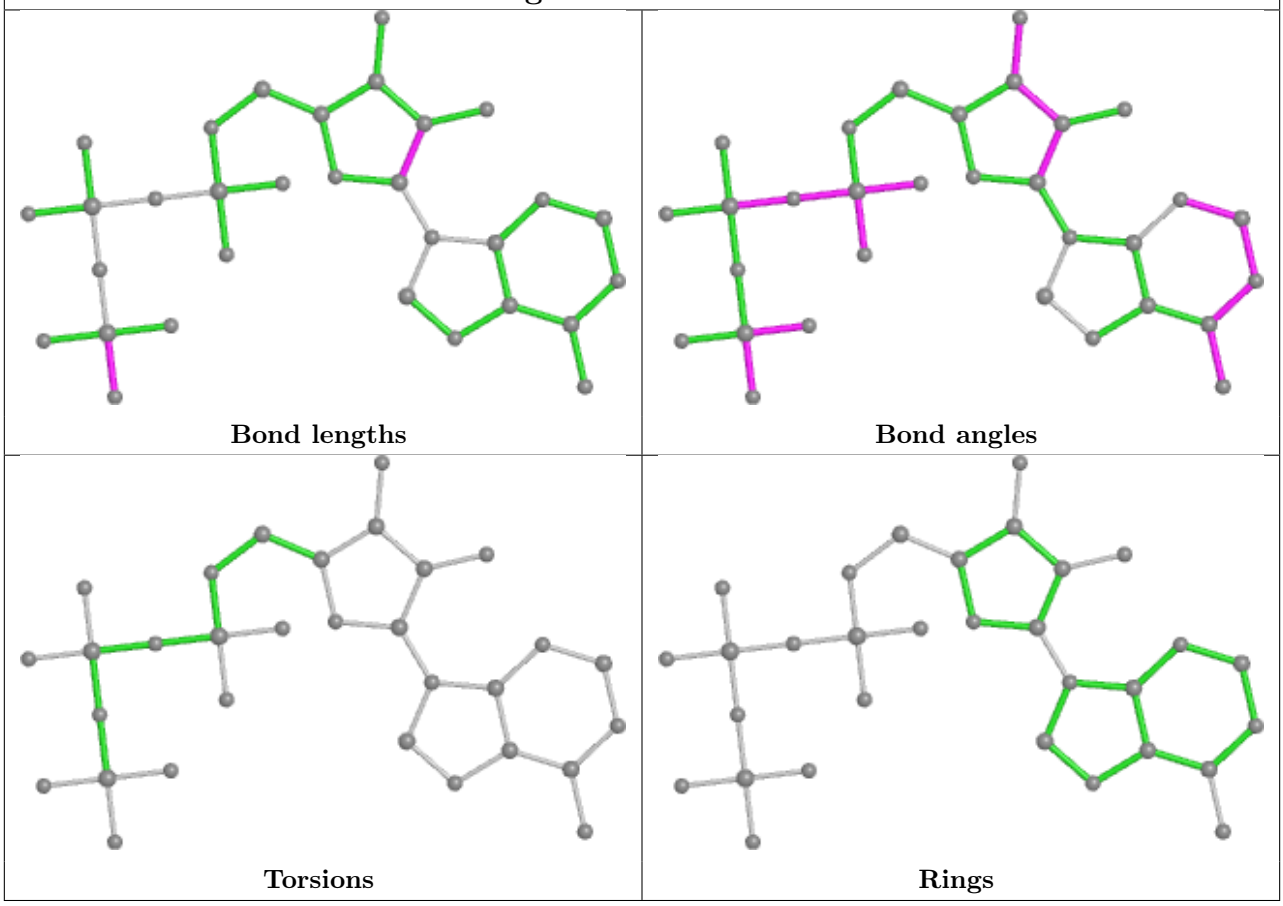
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 A 401



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	A	370/377 (98%)	-0.09	8 (2%)	62	60	9, 27, 64, 98	0
2	G	307/326 (94%)	0.14	16 (5%)	27	26	14, 41, 79, 112	0
All	All	677/703 (96%)	0.01	24 (3%)	44	43	9, 34, 71, 112	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	3	VAL	9.6
2	G	1173	VAL	8.1
2	G	1172	PRO	5.8
2	G	1	MET	5.8
2	G	1482	GLN	5.3
2	G	2	VAL	5.2
2	G	1485	ALA	4.9
1	A	43	VAL	4.5
2	G	1486	GLN	4.4
2	G	1484	GLN	4.2
2	G	1483	ARG	4.1
2	G	1174	PRO	3.2
2	G	1175	ASP	3.1
1	A	45	VAL	3.0
2	G	1177	GLU	2.8
2	G	1221	LYS	2.6
2	G	1481	GLU	2.6
1	A	108	ALA	2.5
1	A	41	GLN	2.3
2	G	1171	LYS	2.2
1	A	46	GLY	2.2
1	A	201	VAL	2.2
1	A	204	ALA	2.1
1	A	42	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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(Å^2)	Q<0.9
1	HIC	A	73	11/12	0.97	0.20	9,13,23,23	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

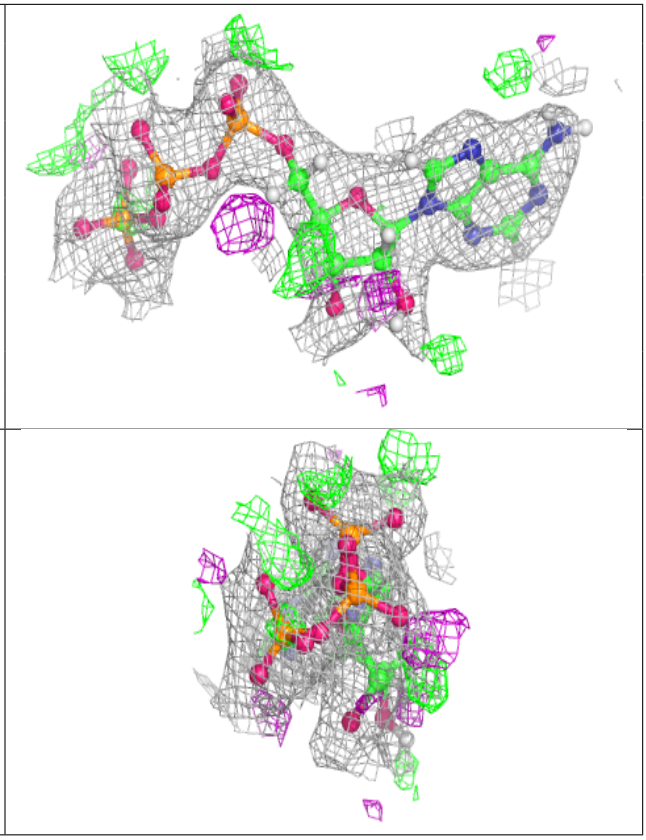
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	403	1/1	0.92	0.17	46,46,46,46	0
4	CA	A	402	1/1	0.93	0.31	26,26,26,26	0
3	ATP	A	401	31/31	0.96	0.18	6,21,34,58	0
4	CA	G	2000	1/1	0.98	0.10	31,31,31,31	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 ATP A 401:

$2mF_o$-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.