



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:31 PM UTC

PDB ID : 1ESV / pdb_00001esv
Title : COMPLEX BETWEEN LATRUNCULIN A:RABBIT MUSCLE ALPHA
ACTIN:HUMAN GELSOLIN DOMAIN 1
Authors : Morton, W.M.; Ayscough, K.A.; McLaughlin, P.J.
Deposited on : 2000-04-11
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

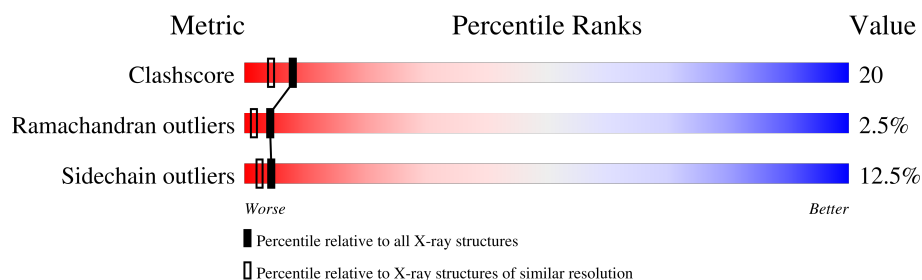
1 Overall quality at a glance

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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	S	125	
2	A	377	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4176 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 GELSOLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	125	Total	C	N	O	S	0	0	0
			984	636	164	182	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	33	CYS	ASN	engineered mutation	UNP P06396

- Molecule 2 is a protein called ALPHA ACTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	359	Total	C	N	O	S	0	0	0
			2685	1707	462	498	18			

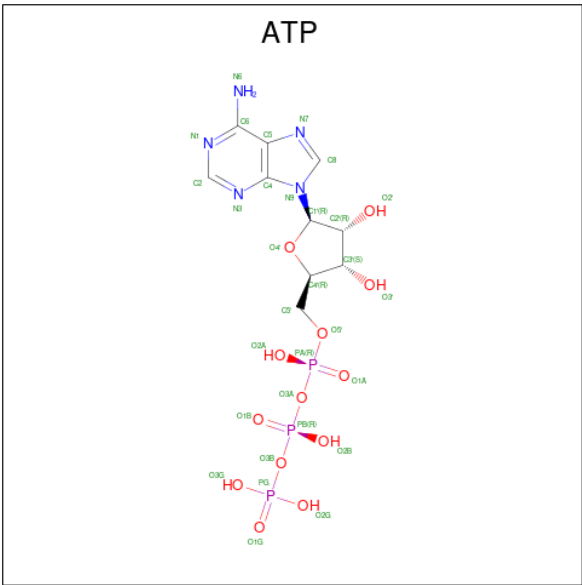
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	modified residue	UNP P68135

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

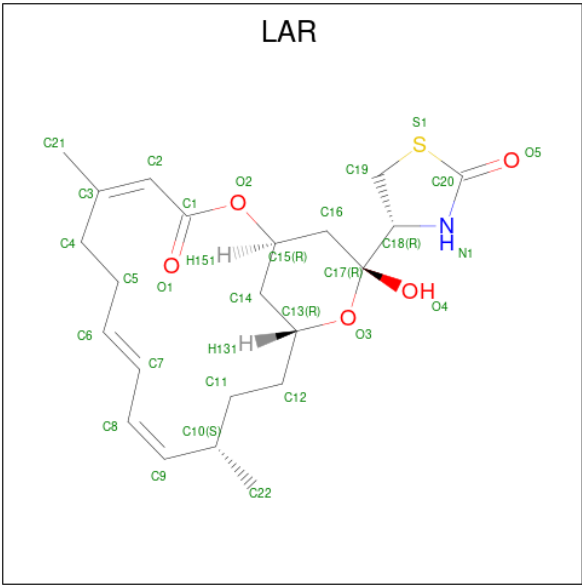
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	2	Total	Ca	0	0
			2	2		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is LATRUNCULIN A (CCD ID: LAR) (formula: C₂₂H₃₁NO₅S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	155	Total 155	O 155	0	0
6	A	289	Total 289	O 289	0	0

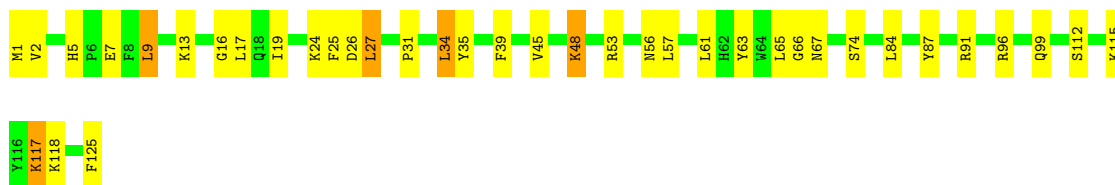
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

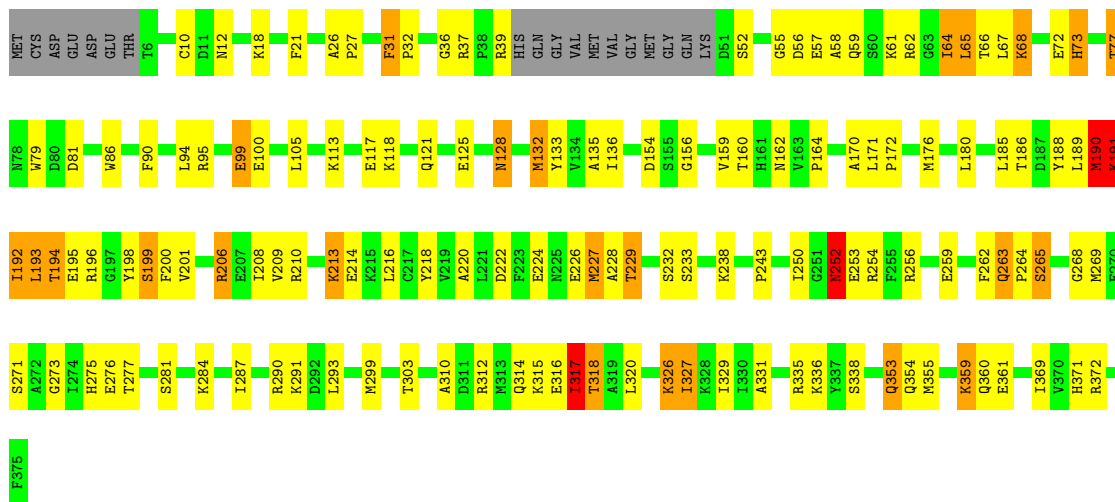
• Molecule 1: GELSOLIN

Chain S: 



• Molecule 2: ALPHA ACTIN

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.75Å 69.25Å 182.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.70 – 2.00	Depositor
% Data completeness (in resolution range)	85.6 (25.70-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.228 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4176	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	S	0.43	0/1010	1.41	6/1365 (0.4%)
2	A	0.43	0/2731	1.38	10/3710 (0.3%)
All	All	0.43	0/3741	1.39	16/5075 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	21	PHE	CA-CB-CG	-6.70	107.10	113.80
1	S	125	PHE	CA-CB-CG	6.10	119.90	113.80
2	A	252	ASN	CA-C-N	5.92	129.03	120.38
2	A	252	ASN	C-N-CA	5.92	129.03	120.38
2	A	90	PHE	CA-CB-CG	5.67	119.47	113.80
2	A	317	ILE	CA-C-N	-5.33	111.82	120.72
2	A	317	ILE	C-N-CA	-5.33	111.82	120.72
2	A	31	PHE	CA-CB-CG	5.33	119.13	113.80
1	S	87	TYR	O-C-N	5.21	127.64	122.12
1	S	66	GLY	CA-C-N	5.20	127.97	120.38
1	S	66	GLY	C-N-CA	5.20	127.97	120.38
1	S	45	VAL	CA-C-N	-5.16	116.38	123.14
1	S	45	VAL	C-N-CA	-5.16	116.38	123.14
2	A	133	TYR	CA-C-O	-5.07	115.31	120.89
2	A	291	LYS	CA-C-N	5.07	127.58	120.28
2	A	291	LYS	C-N-CA	5.07	127.58	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	S	984	0	938	25	0
2	A	2685	0	2544	115	0
3	A	1	0	0	0	0
3	S	2	0	0	0	0
4	A	31	0	12	3	0
5	A	29	0	31	2	0
6	A	289	0	0	25	0
6	S	155	0	0	4	0
All	All	4176	0	3525	142	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 20.

All (142) 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:A:39:ARG:CB	2:A:64:ILE:O	2.18	0.92
2:A:190:MET:HB2	2:A:209:VAL:HG11	1.50	0.91
2:A:360:GLN:HB2	6:A:1394:HOH:O	1.76	0.85
2:A:68:LYS:HD2	6:A:1224:HOH:O	1.81	0.80
2:A:210:ARG:O	2:A:214:GLU:HG3	1.83	0.79
2:A:12:ASN:HD21	2:A:86:TRP:HE1	1.32	0.78
2:A:252:ASN:HD22	2:A:252:ASN:H	1.30	0.77
2:A:190:MET:SD	2:A:206:ARG:HB3	2.24	0.77
1:S:67:ASN:H	1:S:99:GLN:NE2	1.84	0.76
2:A:336:LYS:HE2	6:A:1078:HOH:O	1.84	0.76
1:S:5:HIS:HD2	1:S:7:GLU:H	1.33	0.75
6:S:1243:HOH:O	2:A:355:MET:HE2	1.88	0.73
2:A:243:PRO:HG3	6:A:1335:HOH:O	1.89	0.73
2:A:359:LYS:HD2	6:A:1337:HOH:O	1.90	0.71
2:A:206:ARG:HD2	6:A:1347:HOH:O	1.91	0.70
2:A:59:GLN:HB2	5:A:401:LAR:H91	1.75	0.69
1:S:17:LEU:HD23	1:S:48:LYS:HD3	1.77	0.67
2:A:32:PRO:HG2	2:A:55:GLY:HA2	1.78	0.64
2:A:264:PRO:HG2	2:A:271:SER:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:189:LEU:HG	2:A:193:LEU:HD22	1.79	0.64
2:A:170:ALA:O	2:A:172:PRO:HD3	1.99	0.63
2:A:128:ASN:HA	6:A:1337:HOH:O	2.00	0.61
1:S:5:HIS:CD2	1:S:7:GLU:H	2.17	0.61
2:A:72:GLU:OE2	2:A:77:THR:HG21	2.01	0.61
2:A:253:GLU:HA	2:A:256:ARG:HB2	1.83	0.60
1:S:31:PRO:HA	6:S:1300:HOH:O	2.02	0.59
2:A:186:THR:OG1	2:A:213:LYS:HE3	2.02	0.59
2:A:64:ILE:HG13	2:A:65:LEU:N	2.17	0.59
2:A:113:LYS:HG2	2:A:371:HIS:CE1	2.38	0.58
2:A:36:GLY:HA3	2:A:67:LEU:HD23	1.85	0.58
2:A:121:GLN:O	2:A:125:GLU:HG3	2.02	0.58
2:A:136:ILE:HD12	6:A:1134:HOH:O	2.03	0.58
1:S:61:LEU:HD21	1:S:84:LEU:HD23	1.85	0.58
2:A:73:HIC:HE1	6:A:1006:HOH:O	2.03	0.58
1:S:96:ARG:HD3	6:A:1442:HOH:O	2.03	0.58
2:A:32:PRO:HG2	2:A:55:GLY:CA	2.34	0.57
2:A:189:LEU:HD23	2:A:209:VAL:HG13	1.86	0.57
2:A:58:ALA:HB1	2:A:67:LEU:HD22	1.86	0.57
2:A:252:ASN:HD22	2:A:252:ASN:N	2.02	0.57
1:S:39:PHE:CE1	1:S:117:LYS:HE3	2.41	0.56
2:A:128:ASN:HB2	6:A:1179:HOH:O	2.06	0.55
2:A:299:MET:HE1	2:A:310:ALA:HB2	1.88	0.55
2:A:77:THR:HG22	6:A:1176:HOH:O	2.05	0.55
2:A:113:LYS:O	2:A:117:GLU:HG3	2.06	0.55
5:A:401:LAR:H42	5:A:401:LAR:O2	2.05	0.55
2:A:193:LEU:O	2:A:196:ARG:HB2	2.07	0.55
2:A:299:MET:HE2	2:A:329:ILE:CG2	2.37	0.55
2:A:65:LEU:O	2:A:65:LEU:HD12	2.07	0.55
2:A:317:ILE:HD11	2:A:327:ILE:HG23	1.90	0.54
2:A:36:GLY:CA	2:A:67:LEU:HD23	2.37	0.54
2:A:361:GLU:HB3	2:A:369:ILE:CD1	2.37	0.54
2:A:299:MET:HE3	2:A:331:ALA:HB2	1.89	0.54
2:A:37:ARG:HG2	2:A:52:SER:HB3	1.91	0.53
2:A:263:GLN:HB3	6:A:1313:HOH:O	2.10	0.52
2:A:154:ASP:O	2:A:160:THR:HA	2.10	0.52
2:A:31:PHE:HB2	2:A:32:PRO:HD2	1.91	0.51
2:A:189:LEU:CG	2:A:193:LEU:HD22	2.40	0.51
2:A:259:GLU:HG3	2:A:263:GLN:HG3	1.92	0.51
1:S:5:HIS:HE1	1:S:26:ASP:OD1	1.93	0.51
2:A:180:LEU:HB2	2:A:269:MET:SD	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:12:ASN:ND2	2:A:86:TRP:HE1	2.06	0.51
2:A:99:GLU:HG2	2:A:100:GLU:HG2	1.93	0.51
2:A:164:PRO:HG3	2:A:281:SER:OG	2.10	0.50
2:A:299:MET:CE	2:A:331:ALA:HB2	2.41	0.50
1:S:24:LYS:O	1:S:25:PHE:HB2	2.11	0.50
2:A:222:ASP:O	2:A:226:GLU:HB2	2.12	0.49
2:A:58:ALA:HB1	2:A:67:LEU:CD2	2.42	0.49
2:A:218:TYR:CE2	2:A:254:ARG:HB3	2.47	0.49
2:A:226:GLU:HA	2:A:226:GLU:OE1	2.12	0.49
1:S:13:LYS:HE3	6:S:1094:HOH:O	2.11	0.49
1:S:61:LEU:CD2	1:S:84:LEU:HD23	2.42	0.48
2:A:326:LYS:HE3	6:A:1272:HOH:O	2.13	0.48
2:A:172:PRO:HD2	6:A:1311:HOH:O	2.13	0.48
2:A:196:ARG:HH11	2:A:196:ARG:HG2	1.79	0.48
2:A:224:GLU:O	2:A:227:MET:N	2.47	0.48
2:A:79:TRP:CD2	2:A:118:LYS:HD3	2.49	0.47
2:A:36:GLY:HA2	2:A:66:THR:O	2.14	0.47
1:S:1:MET:HA	2:A:355:MET:SD	2.54	0.47
2:A:189:LEU:CD1	2:A:193:LEU:HD22	2.44	0.47
2:A:220:ALA:HB2	2:A:226:GLU:HG2	1.97	0.47
4:A:380:ATP:H2'	6:A:1336:HOH:O	2.15	0.47
2:A:176:MET:HE3	2:A:281:SER:N	2.30	0.47
2:A:277:THR:HG22	6:A:1140:HOH:O	2.13	0.47
2:A:113:LYS:HE2	2:A:371:HIS:CE1	2.49	0.46
2:A:326:LYS:HD3	6:A:1272:HOH:O	2.15	0.46
1:S:19:ILE:HD12	1:S:35:TYR:CG	2.50	0.46
2:A:369:ILE:HA	2:A:372:ARG:NH2	2.31	0.46
2:A:186:THR:O	2:A:190:MET:HB3	2.15	0.46
2:A:238:LYS:O	2:A:250:ILE:N	2.49	0.46
2:A:327:ILE:HD13	2:A:327:ILE:N	2.31	0.46
1:S:57:LEU:O	1:S:91:ARG:NH1	2.50	0.45
1:S:16:GLY:O	1:S:48:LYS:HD2	2.17	0.45
2:A:275:HIS:CE1	2:A:276:GLU:HG3	2.51	0.45
2:A:312:ARG:O	2:A:316:GLU:HG2	2.17	0.45
2:A:95:ARG:NH1	6:A:1253:HOH:O	2.50	0.45
2:A:353:GLN:OE1	2:A:354:GLN:NE2	2.50	0.45
2:A:105:LEU:HD12	2:A:132:MET:HE2	1.99	0.44
2:A:198:TYR:HD1	6:A:1331:HOH:O	2.00	0.44
4:A:380:ATP:H8	6:A:1336:HOH:O	2.00	0.44
2:A:156:GLY:O	2:A:303:THR:OG1	2.35	0.44
2:A:262:PHE:O	2:A:264:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:227:MET:O	2:A:229:THR:N	2.50	0.44
2:A:269:MET:HE3	2:A:269:MET:HB2	1.94	0.44
2:A:318:THR:HG21	6:A:1409:HOH:O	2.17	0.44
2:A:188:TYR:O	2:A:192:ILE:HB	2.18	0.44
1:S:48:LYS:HD2	1:S:48:LYS:HA	1.70	0.44
2:A:10:CYS:HB3	2:A:105:LEU:HD23	1.98	0.44
2:A:190:MET:HB2	2:A:209:VAL:CG1	2.35	0.44
1:S:115:LYS:NZ	6:S:1349:HOH:O	2.50	0.43
1:S:26:ASP:OD1	1:S:27:LEU:N	2.50	0.43
2:A:164:PRO:HB2	2:A:171:LEU:HD12	2.00	0.43
2:A:336:LYS:HE3	4:A:380:ATP:C8	2.53	0.43
2:A:37:ARG:CG	2:A:52:SER:HB3	2.48	0.43
2:A:189:LEU:HD11	2:A:193:LEU:HD22	2.00	0.43
1:S:39:PHE:CZ	1:S:117:LYS:HE3	2.54	0.43
2:A:354:GLN:HB2	6:A:1113:HOH:O	2.19	0.43
2:A:135:ALA:HA	6:A:1089:HOH:O	2.19	0.42
2:A:335:ARG:HA	2:A:338:SER:OG	2.18	0.42
1:S:34:LEU:HD12	1:S:34:LEU:HA	1.78	0.42
2:A:62:ARG:CB	2:A:67:LEU:HD11	2.49	0.42
2:A:265:SER:O	2:A:268:GLY:N	2.49	0.42
1:S:67:ASN:H	1:S:99:GLN:HE21	1.64	0.42
1:S:9:LEU:HD12	1:S:9:LEU:HA	1.89	0.42
2:A:259:GLU:CG	2:A:263:GLN:HE21	2.33	0.42
2:A:196:ARG:HG2	2:A:196:ARG:NH1	2.35	0.41
2:A:273:GLY:O	2:A:276:GLU:N	2.52	0.41
2:A:199:SER:O	2:A:200:PHE:HB2	2.21	0.41
2:A:303:THR:O	2:A:303:THR:HG22	2.20	0.41
2:A:192:ILE:HG23	2:A:256:ARG:NH2	2.34	0.41
2:A:253:GLU:CB	6:A:1316:HOH:O	2.68	0.41
2:A:191:LYS:HZ2	2:A:191:LYS:HG2	1.74	0.41
2:A:189:LEU:CD2	2:A:209:VAL:HG13	2.50	0.41
2:A:290:ARG:HH21	2:A:290:ARG:HD2	1.70	0.41
2:A:317:ILE:HD11	2:A:327:ILE:CG2	2.50	0.41
2:A:194:THR:HA	2:A:198:TYR:H	1.86	0.40
2:A:317:ILE:HA	2:A:320:LEU:HD12	2.03	0.40
1:S:56:ASN:OD1	1:S:57:LEU:N	2.50	0.40
2:A:26:ALA:HB1	2:A:27:PRO:HD2	2.03	0.40
2:A:162:ASN:HB2	2:A:176:MET:HB2	2.03	0.40
1:S:65:LEU:HD22	1:S:74:SER:HA	2.03	0.40
2:A:37:ARG:NH2	2:A:81:ASP:OD1	2.50	0.40
2:A:259:GLU:HG2	2:A:263:GLN:HE21	1.86	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	S	123/125 (98%)	118 (96%)	4 (3%)	1 (1%)	16	11
2	A	354/377 (94%)	319 (90%)	24 (7%)	11 (3%)	3	1
All	All	477/502 (95%)	437 (92%)	28 (6%)	12 (2%)	4	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	2	VAL
2	A	190	MET
2	A	199	SER
2	A	201	VAL
2	A	229	THR
2	A	232	SER
2	A	56	ASP
2	A	57	GLU
2	A	191	LYS
2	A	233	SER
2	A	314	GLN
2	A	228	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	S	99/103 (96%)	90 (91%)	9 (9%)	9	6
2	A	261/319 (82%)	225 (86%)	36 (14%)	3	2
All	All	360/422 (85%)	315 (88%)	45 (12%)	4	2

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	9	LEU
1	S	27	LEU
1	S	34	LEU
1	S	48	LYS
1	S	53	ARG
1	S	63	TYR
1	S	112	SER
1	S	117	LYS
1	S	118	LYS
2	A	18	LYS
2	A	61	LYS
2	A	64	ILE
2	A	65	LEU
2	A	68	LYS
2	A	77	THR
2	A	94	LEU
2	A	99	GLU
2	A	128	ASN
2	A	132	MET
2	A	159	VAL
2	A	185	LEU
2	A	190	MET
2	A	191	LYS
2	A	192	ILE
2	A	193	LEU
2	A	194	THR
2	A	195	GLU
2	A	206	ARG
2	A	208	ILE
2	A	213	LYS
2	A	216	LEU
2	A	227	MET
2	A	252	ASN
2	A	263	GLN
2	A	265	SER

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Mol	Chain	Res	Type
2	A	284	LYS
2	A	287	ILE
2	A	293	LEU
2	A	315	LYS
2	A	317	ILE
2	A	318	THR
2	A	326	LYS
2	A	327	ILE
2	A	353	GLN
2	A	359	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	5	HIS
1	S	99	GLN
2	A	12	ASN
2	A	92	ASN
2	A	252	ASN
2	A	263	GLN
2	A	280	ASN
2	A	354	GLN
2	A	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
2	HIC	A	73	2	10,11,12	0.65	0	9,14,16	2.98	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	A	73	2	-	0/5/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	73	HIC	NE2-CE1-ND1	-8.23	109.51	112.66
2	A	73	HIC	CE1-ND1-CG	2.45	109.73	105.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	A	380	3	32,33,33	1.25	6 (18%)	48,52,52	0.89	1 (2%)
5	LAR	A	401	-	30,31,31	1.20	2 (6%)	32,43,43	1.24	2 (6%)

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	A	380	3	-	2/22/38/38	0/3/3/3
5	LAR	A	401	-	-	4/23/51/51	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	LAR	C18-N1	3.84	1.51	1.46
4	A	380	ATP	C5'-C4'	3.51	1.62	1.51
4	A	380	ATP	C2'-C3'	-2.54	1.46	1.53
4	A	380	ATP	PB-O3B	-2.20	1.57	1.59
4	A	380	ATP	C4-N9	2.15	1.42	1.37
5	A	401	LAR	C22-C10	2.12	1.60	1.53
4	A	380	ATP	O2'-C2'	2.03	1.48	1.43
4	A	380	ATP	C2-N1	2.03	1.37	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	LAR	C19-S1-C20	3.40	94.01	92.04
4	A	380	ATP	O3'-C3'-C4'	-2.61	103.58	111.08
5	A	401	LAR	C14-C15-C16	2.27	115.49	111.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	LAR	O3-C17-C18-C19
4	A	380	ATP	PG-O3B-PB-O1B

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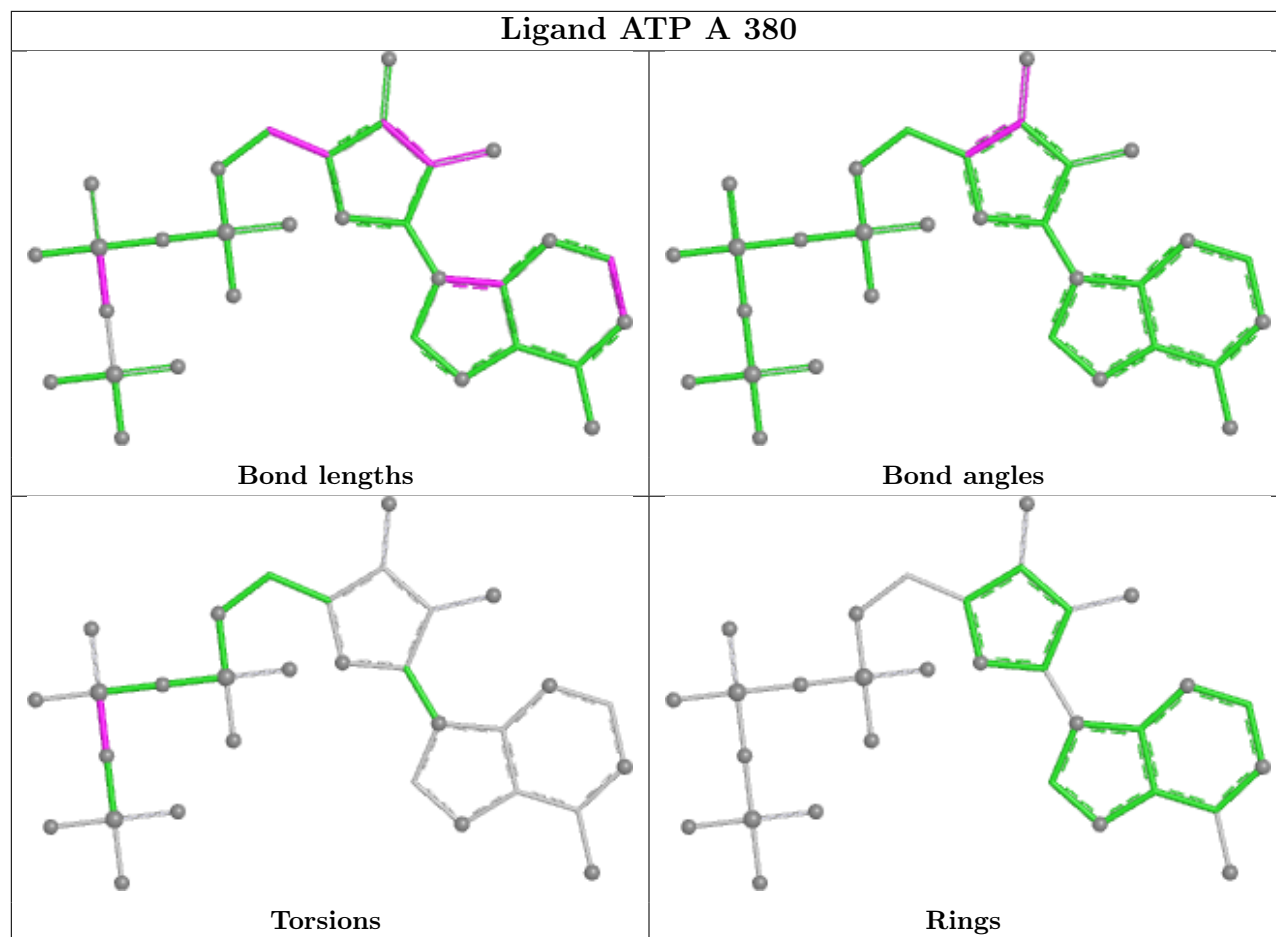
Mol	Chain	Res	Type	Atoms
4	A	380	ATP	PG-O3B-PB-O2B
5	A	401	LAR	O2-C1-C2-C3
5	A	401	LAR	O1-C1-C2-C3
5	A	401	LAR	C21-C3-C4-C5

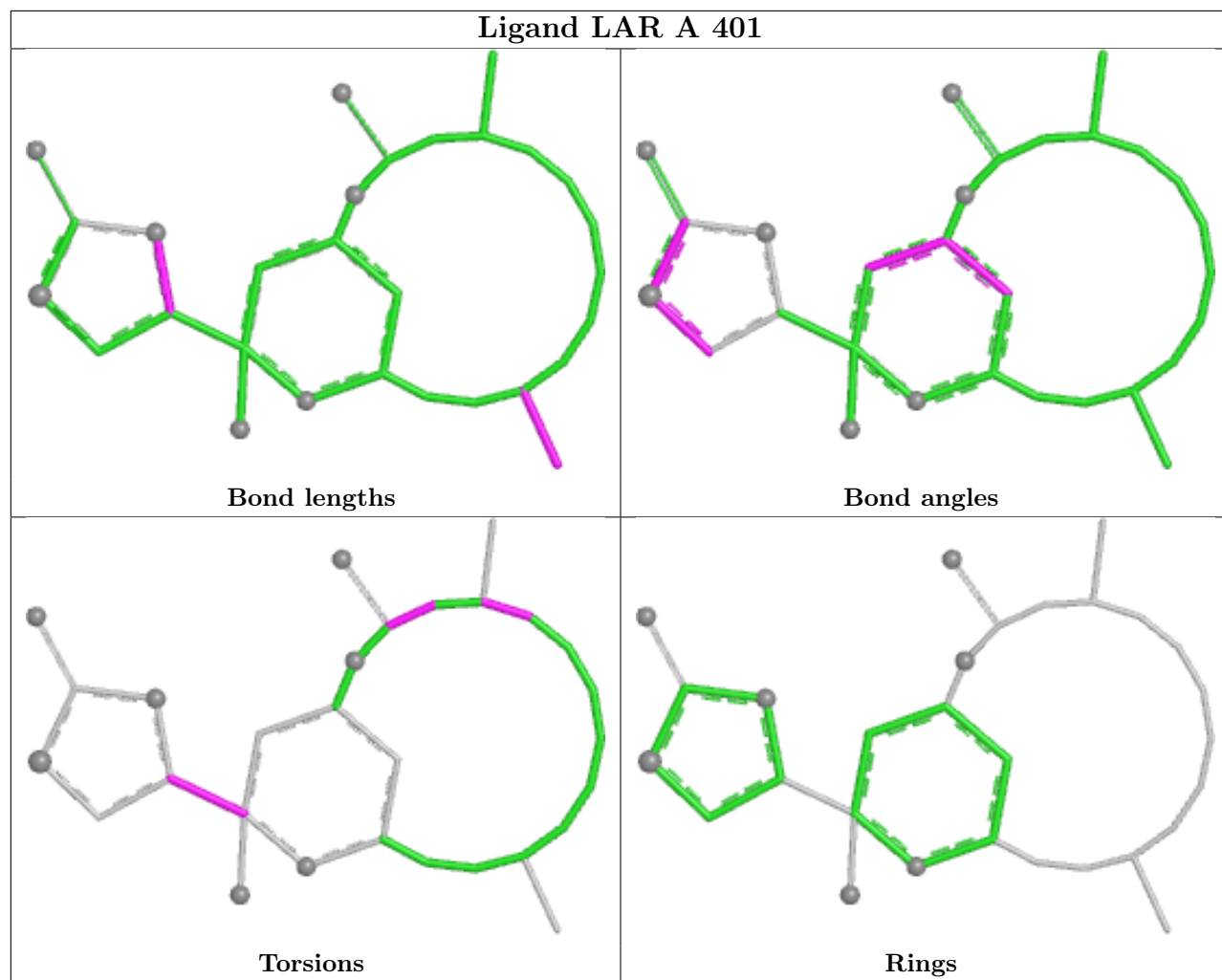
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	380	ATP	3	0
5	A	401	LAR	2	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.