



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 8, 2026 – 01:55 PM UTC

PDB ID : 2ZWH / pdb_00002zwh
Title : Model for the F-actin structure
Authors : Oda, T.; Iwasa, M.; Aihara, T.; Maeda, Y.; Narita, A.
Deposited on : 2008-12-05
Resolution : 3.30 Å(reported)

This is a Full wwPDB Geometry-Only 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)
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

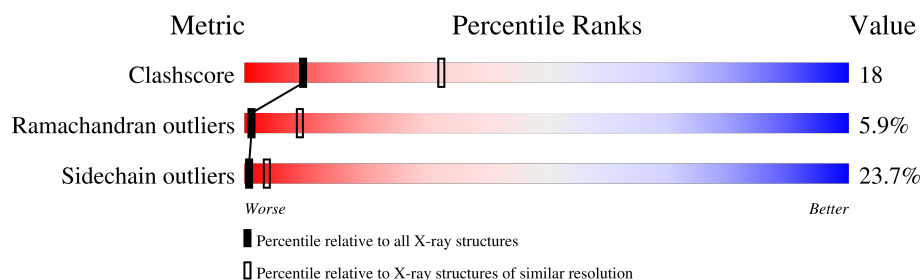
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

FIBER DIFFRACTION

The reported resolution of this entry is 3.30 Å.

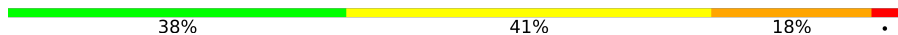
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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	A	375	

2 Entry composition [i](#)

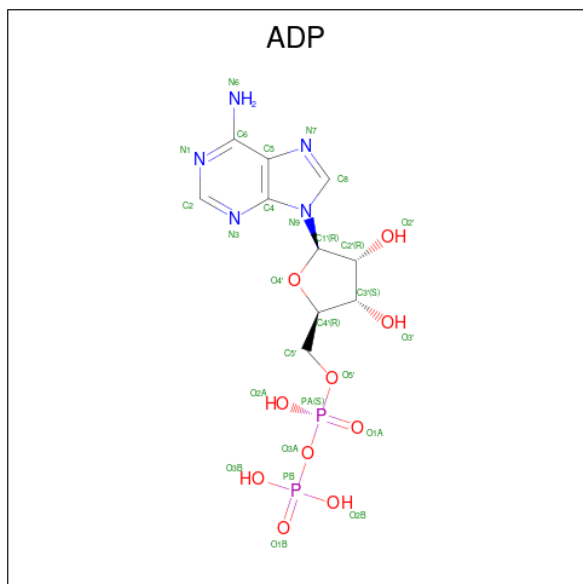
There are 3 unique types of molecules in this entry. The entry contains 2961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	375	Total	C	N	O	S	0	0	0
			2933	1855	493	564	21			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

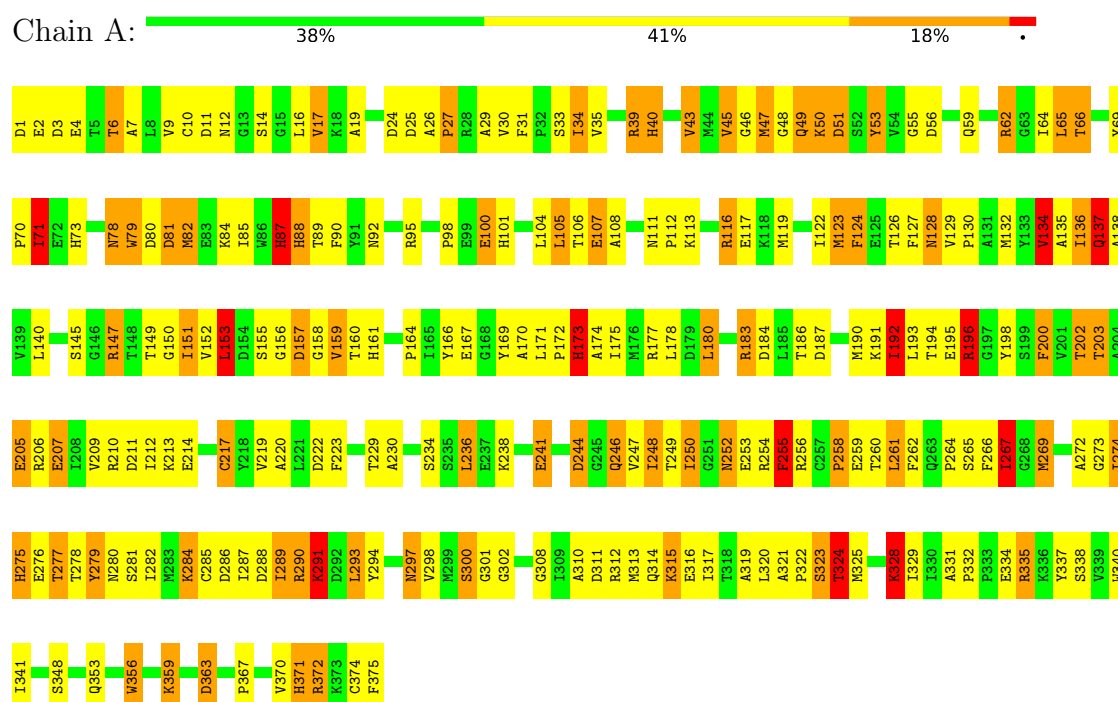
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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: Actin, alpha skeletal muscle



4 Model quality

4.1 Standard geometry

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

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	0.94	9/2983 (0.3%)	1.96	107/4040 (2.6%)

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	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	161	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	173	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	275	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	88	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	371	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	87	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	134	VAL	CA-CB	5.46	1.61	1.54
1	A	40	HIS	CD2-NE2	-5.40	1.31	1.37

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	MET	N-CA-C	11.04	124.43	108.86
1	A	203	THR	N-CA-C	10.51	122.43	110.97
1	A	275	HIS	CA-CB-CG	9.56	123.36	113.80
1	A	173	HIS	CA-CB-CG	9.39	123.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	PRO	N-CA-C	8.45	123.42	111.33
1	A	173	HIS	CB-CG-CD2	-8.17	120.57	131.20
1	A	82	MET	N-CA-C	8.17	121.22	111.33
1	A	334	GLU	N-CA-C	-7.98	95.51	108.52
1	A	319	ALA	N-CA-C	7.70	121.61	111.75
1	A	272	ALA	N-CA-C	-7.64	99.52	110.59
1	A	124	PHE	N-CA-C	7.61	121.50	111.75
1	A	280	ASN	CA-CB-CG	7.58	120.18	112.60
1	A	78	ASN	CA-CB-CG	7.57	120.17	112.60
1	A	356	TRP	N-CA-C	7.44	126.64	110.80
1	A	289	ILE	N-CA-C	7.28	122.46	113.00
1	A	297	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	A	244	ASP	N-CA-C	-7.21	95.44	110.80
1	A	290	ARG	N-CA-C	7.20	122.33	112.90
1	A	173	HIS	CB-CG-ND1	7.09	133.34	122.70
1	A	323	SER	N-CA-C	7.07	120.39	111.69
1	A	88	HIS	CA-CB-CG	7.04	120.83	113.80
1	A	81	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	80	ASP	N-CA-C	6.87	120.55	111.75
1	A	293	LEU	N-CA-C	-6.85	103.74	111.07
1	A	134	VAL	N-CA-C	-6.77	97.86	107.75
1	A	87	HIS	CA-CB-CG	6.68	120.48	113.80
1	A	137	GLN	OE1-CD-NE2	-6.62	115.98	122.60
1	A	217	CYS	CA-C-O	-6.61	113.51	121.05
1	A	255	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	101	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	A	371	HIS	CB-CG-CD2	-6.53	122.72	131.20
1	A	337	TYR	CA-C-N	6.50	129.31	120.54
1	A	337	TYR	C-N-CA	6.50	129.31	120.54
1	A	324	THR	N-CA-C	6.49	124.62	110.80
1	A	65	LEU	N-CA-C	6.44	120.53	110.17
1	A	17	VAL	N-CA-CB	6.43	117.73	110.72
1	A	49	GLN	N-CA-C	6.43	124.50	110.80
1	A	138	ALA	N-CA-C	6.40	119.94	111.75
1	A	147	ARG	CA-CB-CG	6.37	126.84	114.10
1	A	192	ILE	N-CA-CB	-6.23	100.15	110.56
1	A	297	ASN	CB-CG-ND2	6.20	125.71	116.40
1	A	11	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	297	ASN	CA-CB-CG	6.17	118.78	112.60
1	A	248	ILE	N-CA-C	-6.17	97.47	107.28
1	A	134	VAL	CB-CA-C	6.14	119.49	110.77
1	A	128	ASN	OD1-CG-ND2	-6.12	116.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	158	GLY	N-CA-C	6.05	127.51	113.18
1	A	338	SER	O-C-N	6.00	128.33	122.09
1	A	300	SER	N-CA-C	5.99	118.52	109.41
1	A	291	LYS	CA-CB-CG	5.99	126.07	114.10
1	A	328	LYS	N-CA-C	5.96	117.86	107.49
1	A	3	ASP	N-CA-C	5.95	120.01	112.87
1	A	375	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	212	ILE	O-C-N	5.89	127.68	121.91
1	A	46	GLY	N-CA-C	-5.89	102.00	112.54
1	A	252	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	280	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	340	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	A	169	TYR	N-CA-C	5.82	119.10	110.48
1	A	53	TYR	N-CA-C	-5.80	99.83	109.46
1	A	59	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	A	267	ILE	CB-CA-C	-5.74	104.55	112.24
1	A	310	ALA	CA-C-N	5.73	129.42	120.82
1	A	310	ALA	C-N-CA	5.73	129.42	120.82
1	A	287	ILE	CA-C-O	-5.73	114.77	120.85
1	A	90	PHE	N-CA-C	5.73	117.39	111.03
1	A	229	THR	CA-CB-OG1	-5.73	101.01	109.60
1	A	101	HIS	CB-CG-ND1	5.71	131.27	122.70
1	A	284	LYS	N-CA-C	5.69	119.32	112.38
1	A	45	VAL	N-CA-C	-5.66	97.57	109.34
1	A	78	ASN	N-CA-C	-5.63	98.80	110.80
1	A	11	ASP	N-CA-C	-5.63	100.01	109.07
1	A	56	ASP	CA-C-N	5.61	128.11	120.54
1	A	56	ASP	C-N-CA	5.61	128.11	120.54
1	A	56	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	16	LEU	N-CA-C	5.57	118.03	109.07
1	A	275	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	A	241	GLU	CB-CG-CD	5.53	122.00	112.60
1	A	291	LYS	N-CA-C	5.53	118.02	111.33
1	A	316	GLU	N-CA-C	5.49	117.97	111.33
1	A	62	ARG	N-CA-C	5.46	122.43	110.80
1	A	340	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	A	340	TRP	CB-CG-CD1	-5.42	118.76	126.90
1	A	40	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	31	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	192	ILE	CB-CA-C	5.37	119.44	112.24
1	A	184	ASP	CA-CB-CG	-5.36	107.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLU	CA-CB-CG	5.33	124.76	114.10
1	A	196	ARG	N-CA-C	-5.28	104.43	112.04
1	A	79	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	A	289	ILE	CA-CB-CG1	-5.26	101.47	110.40
1	A	157	ASP	CA-CB-CG	5.25	117.86	112.60
1	A	17	VAL	N-CA-C	-5.25	101.02	108.58
1	A	79	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	A	87	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	184	ASP	N-CA-C	-5.20	105.69	111.36
1	A	278	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	200	PHE	N-CA-C	-5.19	99.75	110.80
1	A	214	GLU	N-CA-C	5.16	118.68	112.38
1	A	359	LYS	N-CA-C	5.15	119.86	111.37
1	A	92	ASN	OD1-CG-ND2	-5.14	117.45	122.60
1	A	353	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	14	SER	N-CA-CB	-5.09	102.46	110.30
1	A	279	TYR	N-CA-C	-5.05	105.85	111.36
1	A	153	LEU	N-CA-C	-5.01	99.10	108.02
1	A	50	LYS	N-CA-C	5.01	116.45	108.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ALA	Peptide
1	A	116	ARG	Sidechain
1	A	321	ALA	Peptide

4.2 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	A	2933	0	2895	104	0
2	A	27	0	12	1	0
3	A	1	0	0	0	0
All	All	2961	0	2907	104	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 18.

All (104) 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:82:MET:SD	1:A:85:ILE:HD12	2.28	0.74
1:A:153:LEU:HD11	1:A:274:ILE:HB	1.72	0.71
1:A:262:PHE:HA	1:A:273:GLY:HA3	1.76	0.68
1:A:149:THR:HG23	1:A:166:TYR:HA	1.76	0.68
1:A:116:ARG:HB3	1:A:370:VAL:HG11	1.75	0.68
1:A:219:VAL:HG22	1:A:258:PRO:HB3	1.79	0.64
1:A:331:ALA:HB1	1:A:335:ARG:HD3	1.81	0.63
1:A:17:VAL:HG23	1:A:33:SER:OG	2.00	0.61
1:A:62:ARG:HE	1:A:207:GLU:HB3	1.65	0.61
1:A:192:ILE:HG23	1:A:256:ARG:HH11	1.64	0.61
1:A:200:PHE:HB3	1:A:205:GLU:HB2	1.82	0.61
1:A:275:HIS:HB3	1:A:313:MET:SD	2.41	0.60
1:A:164:PRO:HD3	1:A:281:SER:HB2	1.85	0.59
1:A:124:PHE:CE2	1:A:359:LYS:HA	2.39	0.58
1:A:220:ALA:HB2	1:A:255:PHE:HD1	1.69	0.58
1:A:19:ALA:HB3	1:A:29:ALA:HB3	1.86	0.57
1:A:183:ARG:O	1:A:186:THR:HB	2.04	0.56
1:A:150:GLY:HA2	1:A:293:LEU:HA	1.89	0.55
1:A:217:CYS:SG	1:A:254:ARG:HA	2.47	0.54
1:A:119:MET:O	1:A:123:MET:SD	2.66	0.53
1:A:210:ARG:O	1:A:213:LYS:HB3	2.09	0.53
1:A:230:ALA:HA	1:A:236:LEU:HD22	1.91	0.53
1:A:372:ARG:CZ	1:A:372:ARG:HA	2.39	0.52
1:A:372:ARG:HA	1:A:372:ARG:NH1	2.23	0.52
1:A:160:THR:HB	1:A:178:LEU:HB3	1.92	0.52
1:A:12:ASN:HD21	1:A:71:ILE:HD13	1.75	0.52
1:A:152:VAL:HG22	1:A:298:VAL:HB	1.92	0.51
1:A:34:ILE:HG22	1:A:69:TYR:HA	1.91	0.51
1:A:47:MET:SD	1:A:48:GLY:N	2.84	0.51
1:A:279:TYR:CE1	1:A:320:LEU:HB2	2.45	0.51
1:A:187:ASP:O	1:A:190:MET:HG2	2.10	0.51
1:A:156:GLY:HA2	1:A:302:GLY:H	1.74	0.51
1:A:106:THR:OG1	1:A:137:GLN:NE2	2.44	0.50
1:A:124:PHE:HE2	1:A:359:LYS:HA	1.76	0.50
1:A:203:THR:O	1:A:206:ARG:HB3	2.12	0.50
1:A:196:ARG:HD3	1:A:198:TYR:CE2	2.47	0.50
1:A:219:VAL:HB	1:A:308:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HG12	1:A:374:CYS:SG	2.52	0.49
1:A:159:VAL:HG11	1:A:177:ARG:HH11	1.78	0.48
1:A:261:LEU:HD22	1:A:274:ILE:HG12	1.95	0.48
1:A:1:ASP:OD2	1:A:6:THR:HB	2.14	0.48
1:A:35:VAL:HB	1:A:81:ASP:HB2	1.95	0.48
1:A:117:GLU:OE1	1:A:370:VAL:HB	2.15	0.47
1:A:124:PHE:CE1	1:A:132:MET:SD	3.08	0.47
1:A:192:ILE:HG23	1:A:256:ARG:NH1	2.27	0.47
1:A:155:SER:OG	1:A:160:THR:HA	2.15	0.47
1:A:157:ASP:HB3	2:A:376:ADP:O2B	2.15	0.46
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.97	0.46
1:A:223:PHE:HB2	1:A:259:GLU:OE1	2.15	0.46
1:A:276:GLU:HA	1:A:279:TYR:CD1	2.51	0.46
1:A:9:VAL:HA	1:A:104:LEU:HB3	1.97	0.46
1:A:312:ARG:O	1:A:315:LYS:HD3	2.16	0.46
1:A:313:MET:HE3	1:A:317:ILE:HD11	1.98	0.45
1:A:252:ASN:HB3	1:A:256:ARG:HH21	1.81	0.45
1:A:122:ILE:O	1:A:126:THR:HB	2.16	0.45
1:A:191:LYS:NZ	1:A:266:PHE:O	2.50	0.45
1:A:267:ILE:HD13	1:A:269:MET:SD	2.56	0.45
1:A:192:ILE:HD12	1:A:256:ARG:NH1	2.31	0.45
1:A:288:ASP:O	1:A:291:LYS:NZ	2.45	0.45
1:A:328:LYS:NZ	1:A:328:LYS:HB3	2.32	0.45
1:A:79:TRP:O	1:A:82:MET:HB2	2.17	0.44
1:A:164:PRO:O	1:A:170:ALA:HB2	2.16	0.44
1:A:282:ILE:HG23	1:A:293:LEU:HD12	1.99	0.44
1:A:1:ASP:N	1:A:4:GLU:O	2.49	0.44
1:A:164:PRO:HD2	1:A:175:ILE:HG22	1.98	0.44
1:A:174:ALA:HA	1:A:284:LYS:HD2	2.00	0.44
1:A:39:ARG:HG3	1:A:64:ILE:O	2.17	0.44
1:A:173:HIS:O	1:A:284:LYS:HD2	2.18	0.44
1:A:40:HIS:HB2	1:A:64:ILE:HA	2.00	0.44
1:A:151:ILE:HG21	1:A:282:ILE:HD11	1.99	0.44
1:A:145:SER:O	1:A:147:ARG:HD2	2.18	0.43
1:A:192:ILE:HD12	1:A:256:ARG:HH11	1.83	0.43
1:A:274:ILE:HA	1:A:277:THR:OG1	2.18	0.43
1:A:111:ASN:O	1:A:116:ARG:NH1	2.52	0.43
1:A:198:TYR:CZ	1:A:248:ILE:HA	2.54	0.43
1:A:98:PRO:HB2	1:A:129:VAL:HG22	2.01	0.43
1:A:107:GLU:CD	1:A:116:ARG:HH12	2.26	0.42
1:A:250:ILE:O	1:A:254:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ALA:O	1:A:312:ARG:HD2	2.18	0.42
1:A:359:LYS:NZ	1:A:363:ASP:OD1	2.52	0.42
1:A:123:MET:SD	1:A:132:MET:HE1	2.59	0.42
1:A:259:GLU:CD	1:A:312:ARG:HH12	2.28	0.42
1:A:127:PHE:O	1:A:129:VAL:HG23	2.19	0.42
1:A:276:GLU:HA	1:A:279:TYR:CE1	2.55	0.42
1:A:10:CYS:O	1:A:105:LEU:HA	2.20	0.42
1:A:107:GLU:HB3	1:A:136:ILE:HG13	2.02	0.42
1:A:84:LYS:HG2	1:A:87:HIS:HD2	1.85	0.42
1:A:290:ARG:HA	1:A:293:LEU:HG	2.01	0.42
1:A:290:ARG:HB3	1:A:294:TYR:CE2	2.55	0.42
1:A:71:ILE:HD11	1:A:82:MET:HE1	2.02	0.41
1:A:116:ARG:HD3	1:A:371:HIS:HE1	1.85	0.41
1:A:155:SER:O	1:A:301:GLY:HA3	2.20	0.41
1:A:202:THR:O	1:A:205:GLU:HG2	2.20	0.41
1:A:50:LYS:HG3	1:A:53:TYR:HA	2.01	0.41
1:A:51:ASP:OD1	1:A:84:LYS:NZ	2.53	0.41
1:A:297:ASN:HB2	1:A:329:ILE:HD13	2.03	0.41
1:A:106:THR:C	1:A:134:VAL:HG23	2.46	0.41
1:A:285:CYS:O	1:A:290:ARG:NH2	2.53	0.41
1:A:206:ARG:O	1:A:209:VAL:HB	2.21	0.41
1:A:39:ARG:HB3	1:A:66:THR:OG1	2.21	0.41
1:A:192:ILE:HA	1:A:192:ILE:HD13	1.83	0.41
1:A:26:ALA:HB1	1:A:27:PRO:HD2	2.03	0.40
1:A:262:PHE:HE1	1:A:313:MET:SD	2.45	0.40
1:A:64:ILE:HB	1:A:65:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 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	372/375 (99%)	288 (77%)	62 (17%)	22 (6%)	1 9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	128	ASN
1	A	137	GLN
1	A	173	HIS
1	A	324	THR
1	A	356	TRP
1	A	45	VAL
1	A	89	THR
1	A	100	GLU
1	A	43	VAL
1	A	180	LEU
1	A	236	LEU
1	A	244	ASP
1	A	246	GLN
1	A	123	MET
1	A	234	SER
1	A	167	GLU
1	A	348	SER
1	A	7	ALA
1	A	88	HIS
1	A	55	GLY
1	A	71	ILE

4.3.2 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	317/317 (100%)	242 (76%)	75 (24%)	1 4

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	6	THR
1	A	25	ASP
1	A	30	VAL
1	A	34	ILE
1	A	39	ARG
1	A	43	VAL
1	A	47	MET
1	A	49	GLN
1	A	51	ASP
1	A	66	THR
1	A	71	ILE
1	A	78	ASN
1	A	87	HIS
1	A	95	ARG
1	A	105	LEU
1	A	107	GLU
1	A	112	PRO
1	A	113	LYS
1	A	130	PRO
1	A	134	VAL
1	A	136	ILE
1	A	137	GLN
1	A	151	ILE
1	A	153	LEU
1	A	159	VAL
1	A	171	LEU
1	A	172	PRO
1	A	173	HIS
1	A	180	LEU
1	A	183	ARG
1	A	192	ILE
1	A	193	LEU
1	A	194	THR
1	A	195	GLU
1	A	196	ARG
1	A	202	THR
1	A	205	GLU
1	A	207	GLU
1	A	211	ASP
1	A	222	ASP
1	A	238	LYS
1	A	241	GLU

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	247	VAL
1	A	249	THR
1	A	250	ILE
1	A	253	GLU
1	A	255	PHE
1	A	258	PRO
1	A	260	THR
1	A	261	LEU
1	A	264	PRO
1	A	265	SER
1	A	267	ILE
1	A	269	MET
1	A	274	ILE
1	A	277	THR
1	A	286	ASP
1	A	289	ILE
1	A	291	LYS
1	A	300	SER
1	A	311	ASP
1	A	314	GLN
1	A	315	LYS
1	A	322	PRO
1	A	323	SER
1	A	324	THR
1	A	328	LYS
1	A	332	PRO
1	A	335	ARG
1	A	341	ILE
1	A	363	ASP
1	A	367	PRO
1	A	372	ARG

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

Mol	Chain	Res	Type
1	A	12	ASN

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 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	$\# Z > 2$
1	HIC	A	73	1	10,11,12	1.81	2 (20%)	9,14,16	5.40	4 (44%)

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	-	2/5/6/8	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	CD2-NE2	-4.33	1.30	1.37
1	A	73	HIC	CG-ND1	-2.25	1.32	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	CZ-NE2-CD2	-10.00	112.91	126.03
1	A	73	HIC	CD2-NE2-CE1	8.44	110.05	106.71
1	A	73	HIC	NE2-CE1-ND1	-7.88	109.64	112.66
1	A	73	HIC	CZ-NE2-CE1	-4.87	115.22	126.71

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	ADP	A	376	3	28,29,29	1.30	3 (10%)	43,45,45	1.59	3 (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
2	ADP	A	376	3	-	2/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	376	ADP	PA-O3A	4.52	1.64	1.59
2	A	376	ADP	PB-O2B	-2.49	1.45	1.54
2	A	376	ADP	PB-O3B	2.24	1.63	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	376	ADP	O3B-PB-O1B	-5.81	88.20	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	376	ADP	O2B-PB-O3A	5.44	122.89	104.64
2	A	376	ADP	O3B-PB-O3A	4.14	118.53	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

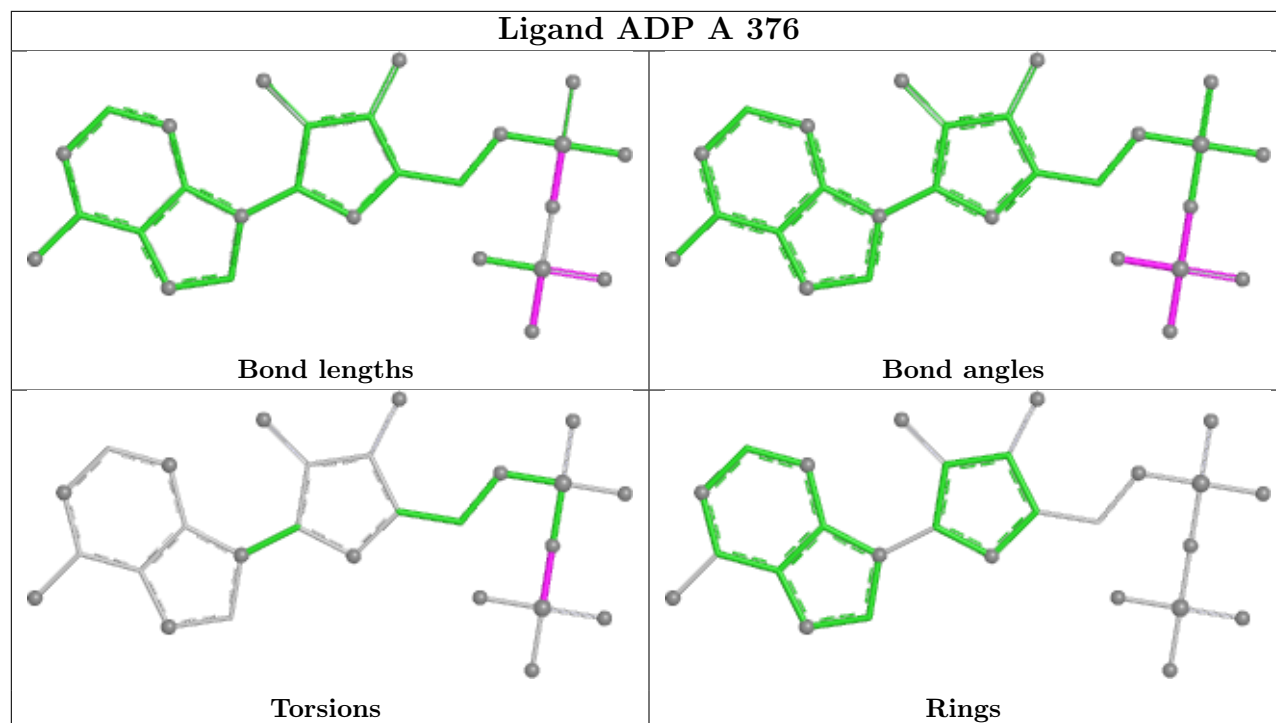
Mol	Chain	Res	Type	Atoms
2	A	376	ADP	PA-O3A-PB-O3B
2	A	376	ADP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	376	ADP	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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.