



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:45 AM UTC

PDB ID : 1HLU / pdb_00001hlu
Title : STRUCTURE OF BOVINE BETA-ACTIN-PROFILIN COMPLEX WITH
ACTIN BOUND ATP PHOSPHATES SOLVENT ACCESSIBLE
Authors : Chik, J.K.; Lindberg, U.; Schutt, C.E.
Deposited on : 1997-05-30
Resolution : 2.65 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

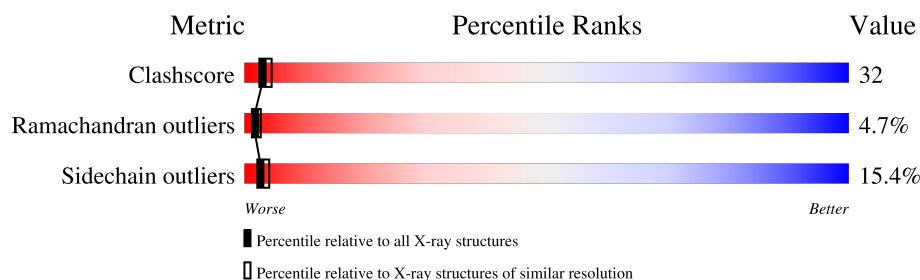
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

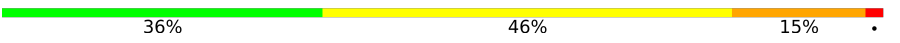
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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	P	140	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4001 atoms, of which 1 is hydrogen 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 BETA-ACTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2921	1848	490	561	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	modified residue	UNP P60712

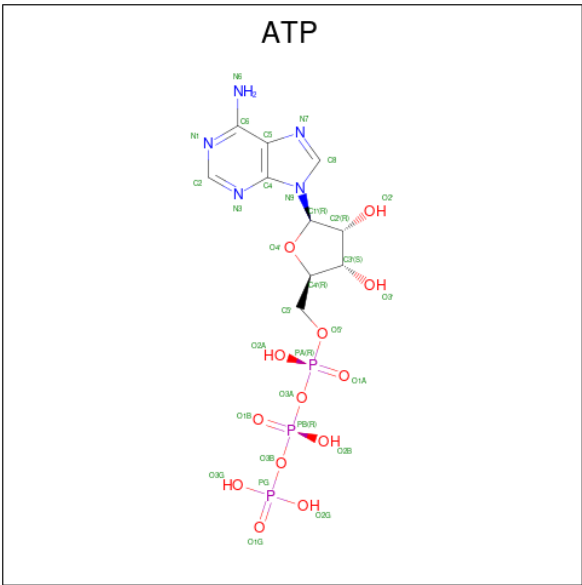
- Molecule 2 is a protein called PROFILIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	140	Total	C	N	O	S	0	0	0
			1047	659	179	200	9			

- 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		

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



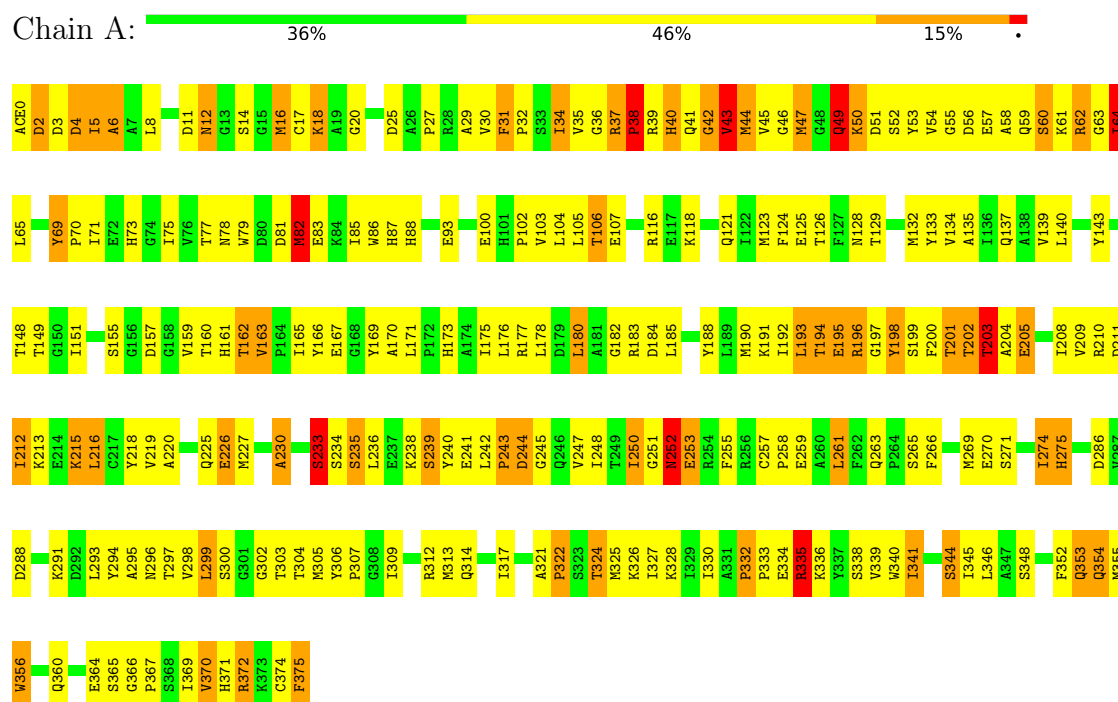
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			32	10	1	5	13	3		

3 Residue-property plots

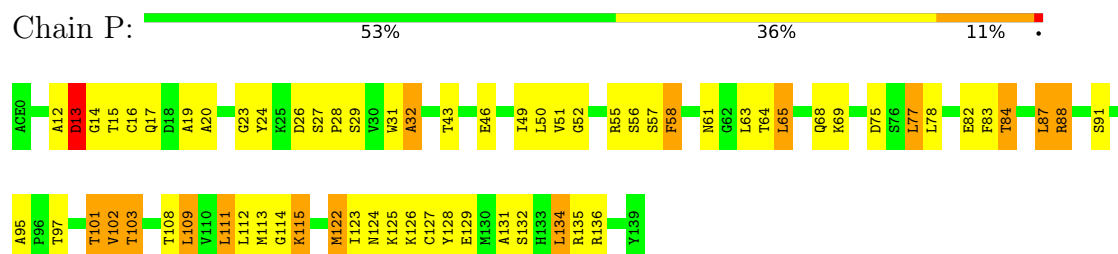
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: BETA-ACTIN



• Molecule 2: PROFILIN



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	38.14Å 72.24Å 185.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.65	Depositor
% Data completeness (in resolution range)	87.0 (8.00-2.65)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.201 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4001	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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, ACE, 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	A	0.82	2/2969 (0.1%)	1.43	52/4019 (1.3%)
2	P	0.88	1/1063 (0.1%)	1.23	6/1435 (0.4%)
All	All	0.84	3/4032 (0.1%)	1.38	58/5454 (1.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	122	MET	SD-CE	6.37	1.95	1.79
1	A	163	VAL	CA-CB	5.86	1.59	1.54
1	A	82	MET	SD-CE	-5.20	1.66	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	SER	N-CA-C	15.45	136.10	113.40
1	A	44	MET	N-CA-C	12.02	128.55	109.79
1	A	233	SER	N-CA-C	11.20	134.66	110.80
1	A	49	GLN	N-CA-C	9.22	122.22	110.24
1	A	69	TYR	CA-C-N	9.10	128.83	119.19
1	A	69	TYR	C-N-CA	9.10	128.83	119.19
1	A	235	SER	N-CA-C	-8.91	99.09	112.54
1	A	356	TRP	N-CA-C	8.76	122.56	109.95
1	A	82	MET	N-CA-C	-7.92	103.07	112.89
1	A	43	VAL	CA-C-N	7.75	134.65	121.86
1	A	43	VAL	C-N-CA	7.75	134.65	121.86
1	A	245	GLY	N-CA-C	7.61	120.71	110.43
1	A	354	GLN	N-CA-C	-7.60	103.99	112.57
1	A	321	ALA	N-CA-C	7.54	120.27	110.40
1	A	37	ARG	CA-C-N	7.46	129.16	119.84
1	A	37	ARG	C-N-CA	7.46	129.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	SER	N-CA-C	-7.36	103.19	111.14
2	P	108	THR	N-CA-C	7.10	120.97	110.46
1	A	212	ILE	N-CA-C	-7.04	103.92	110.53
1	A	196	ARG	N-CA-C	-6.88	103.37	112.72
1	A	198	TYR	N-CA-C	-6.83	104.94	113.28
2	P	27	SER	CA-C-N	6.80	126.84	119.90
2	P	27	SER	C-N-CA	6.80	126.84	119.90
1	A	215	LYS	N-CA-C	6.67	119.89	111.69
1	A	12	ASN	N-CA-C	6.66	119.69	108.23
1	A	265	SER	N-CA-C	-6.66	104.41	112.54
2	P	134	LEU	N-CA-C	-6.63	103.98	111.14
1	A	102	PRO	N-CA-C	-6.48	102.14	111.22
1	A	375	PHE	N-CA-C	6.26	128.54	111.00
1	A	270	GLU	N-CA-C	-6.23	99.85	109.76
2	P	13	ASP	N-CA-C	6.08	117.99	111.36
1	A	75	ILE	N-CA-C	6.02	117.25	108.58
1	A	241	GLU	N-CA-C	6.01	118.09	108.41
1	A	293	LEU	N-CA-C	-5.99	102.39	111.56
1	A	230	ALA	N-CA-C	-5.95	104.71	111.14
1	A	225	GLN	N-CA-C	5.94	118.54	111.71
1	A	60	SER	N-CA-C	-5.92	103.60	111.24
1	A	44	MET	N-CA-CB	-5.91	101.94	110.45
1	A	365	SER	N-CA-C	5.79	121.01	113.88
1	A	332	PRO	N-CA-C	5.75	117.72	110.70
1	A	226	GLU	N-CA-C	-5.71	105.03	112.23
1	A	247	VAL	N-CA-C	-5.65	99.09	107.51
1	A	44	MET	CA-C-N	5.57	129.53	121.52
1	A	44	MET	C-N-CA	5.57	129.53	121.52
1	A	6	ALA	N-CA-C	5.56	122.64	110.80
1	A	252	ASN	N-CA-C	-5.44	104.75	111.33
1	A	126	THR	N-CA-C	5.39	117.97	111.40
2	P	14	GLY	N-CA-C	-5.37	108.24	115.21
1	A	335	ARG	N-CA-C	5.32	122.13	110.80
1	A	216	LEU	N-CA-C	5.31	120.77	113.97
1	A	203	THR	N-CA-C	-5.26	99.59	110.80
1	A	305	MET	N-CA-C	5.21	119.39	113.19
1	A	339	VAL	N-CA-C	5.15	115.77	110.36
1	A	253	GLU	N-CA-C	5.13	117.61	111.71
1	A	162	THR	N-CA-C	-5.09	100.12	108.41
1	A	42	GLY	N-CA-C	-5.08	101.13	113.18
1	A	275	HIS	N-CA-C	5.06	116.49	110.97
1	A	261	LEU	N-CA-C	-5.04	105.67	111.07

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	A	2921	0	2884	209	0
2	P	1047	0	1050	48	0
3	A	1	0	0	0	0
4	A	31	1	12	3	0
All	All	4000	1	3946	255	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 32.

All (255) 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:16:MET:HE2	1:A:32:PRO:HA	1.45	0.98
1:A:71:ILE:HD11	1:A:82:MET:HE3	1.44	0.97
1:A:216:LEU:HD23	1:A:250:ILE:HD11	1.48	0.96
1:A:257:CYS:SG	1:A:258:PRO:HD3	2.06	0.95
2:P:16:CYS:SG	2:P:112:LEU:HD11	2.07	0.94
2:P:101:THR:HG22	2:P:123:ILE:HG22	1.50	0.93
1:A:302:GLY:HA3	4:A:1:ATP:H5'2	1.51	0.91
1:A:5:ILE:HD12	1:A:5:ILE:H	1.40	0.85
1:A:70:PRO:HG2	1:A:85:ILE:HD11	1.60	0.83
1:A:192:ILE:O	1:A:195:GLU:HG2	1.78	0.82
1:A:185:LEU:HB2	1:A:213:LYS:NZ	1.96	0.80
1:A:185:LEU:HD21	1:A:261:LEU:HD21	1.64	0.78
2:P:102:VAL:HB	2:P:111:LEU:HD13	1.63	0.78
2:P:91:SER:HB2	2:P:95:ALA:HB3	1.66	0.77
1:A:36:GLY:HA3	1:A:65:LEU:HD23	1.65	0.77
1:A:216:LEU:CD2	1:A:250:ILE:HD11	2.14	0.77
2:P:101:THR:CG2	2:P:123:ILE:HG22	2.14	0.77
1:A:180:LEU:HD11	1:A:269:MET:SD	2.25	0.77
2:P:64:THR:HA	2:P:68:GLN:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG21	1:A:81:ASP:HB2	1.69	0.74
1:A:160:THR:HG23	1:A:180:LEU:O	1.89	0.72
1:A:31:PHE:HE2	1:A:88:HIS:CD2	2.08	0.72
1:A:53:TYR:HB2	1:A:65:LEU:HD21	1.70	0.72
2:P:114:GLY:HA3	2:P:123:ILE:HD11	1.72	0.71
1:A:157:ASP:OD1	1:A:183:ARG:HG3	1.90	0.71
1:A:170:ALA:H	1:A:375:PHE:HE2	1.40	0.69
1:A:16:MET:HG2	1:A:30:VAL:HG12	1.75	0.69
1:A:107:GLU:O	1:A:137:GLN:HG3	1.94	0.67
1:A:70:PRO:O	1:A:77:THR:HB	1.95	0.67
1:A:159:VAL:HG23	1:A:178:LEU:O	1.94	0.67
1:A:353:GLN:NE2	1:A:356:TRP:HZ2	1.93	0.66
1:A:334:GLU:O	1:A:334:GLU:HG3	1.96	0.65
1:A:257:CYS:SG	1:A:258:PRO:CD	2.83	0.65
1:A:341:ILE:O	1:A:345:ILE:HG13	1.97	0.64
1:A:190:MET:HE3	1:A:209:VAL:HG21	1.79	0.64
1:A:353:GLN:NE2	1:A:356:TRP:CZ2	2.65	0.64
1:A:374:CYS:O	1:A:375:PHE:HB2	1.98	0.63
1:A:372:ARG:HH21	2:P:84:THR:HG21	1.62	0.63
1:A:360:GLN:O	1:A:364:GLU:HG2	1.98	0.63
1:A:328:LYS:O	1:A:328:LYS:HG2	1.98	0.63
1:A:295:ALA:HB2	1:A:326:LYS:HG3	1.80	0.63
1:A:49:GLN:HG3	1:A:50:LYS:HE2	1.80	0.63
1:A:71:ILE:HD11	1:A:82:MET:CE	2.24	0.63
2:P:91:SER:HB3	2:P:97:THR:HG23	1.80	0.63
1:A:70:PRO:HG2	1:A:85:ILE:CD1	2.28	0.62
1:A:31:PHE:CE2	1:A:88:HIS:CD2	2.86	0.62
1:A:31:PHE:HE2	1:A:88:HIS:HD2	1.47	0.62
1:A:38:PRO:HB3	1:A:47:MET:SD	2.39	0.62
1:A:242:LEU:CD1	1:A:243:PRO:HD2	2.30	0.61
1:A:166:TYR:CD1	1:A:167:GLU:HG2	2.35	0.61
1:A:31:PHE:CE2	1:A:88:HIS:HD2	2.19	0.61
1:A:31:PHE:HD1	1:A:31:PHE:H	1.48	0.61
1:A:41:GLN:CD	1:A:42:GLY:H	2.08	0.61
1:A:240:TYR:HB3	1:A:248:ILE:HG12	1.82	0.61
2:P:63:LEU:HD11	2:P:87:LEU:CD2	2.30	0.61
2:P:77:LEU:HD21	2:P:102:VAL:HG22	1.82	0.61
1:A:78:ASN:O	1:A:82:MET:HB2	2.01	0.61
1:A:132:MET:HE1	1:A:134:VAL:HG23	1.83	0.61
2:P:17:GLN:CD	2:P:113:MET:HE2	2.26	0.61
1:A:291:LYS:HG3	1:A:325:MET:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:82:GLU:O	2:P:83:PHE:HB2	2.00	0.60
1:A:139:VAL:HA	1:A:165:ILE:CD1	2.32	0.60
1:A:163:VAL:HG13	1:A:175:ILE:CD1	2.31	0.60
1:A:208:ILE:O	1:A:212:ILE:HG13	2.02	0.59
1:A:16:MET:CG	1:A:30:VAL:HG12	2.32	0.59
1:A:236:LEU:O	1:A:236:LEU:HD23	2.02	0.59
1:A:185:LEU:HB2	1:A:213:LYS:HZ1	1.68	0.58
2:P:125:LYS:O	2:P:129:GLU:HG2	2.04	0.58
1:A:193:LEU:HD11	1:A:250:ILE:CG2	2.33	0.58
1:A:198:TYR:CE2	1:A:248:ILE:HB	2.38	0.58
2:P:101:THR:HG22	2:P:123:ILE:CG2	2.30	0.58
1:A:64:ILE:HG23	1:A:65:LEU:HD13	1.85	0.58
1:A:139:VAL:HG12	1:A:143:TYR:CE2	2.39	0.58
1:A:180:LEU:CD1	1:A:269:MET:SD	2.91	0.58
1:A:322:PRO:O	1:A:325:MET:SD	2.62	0.57
1:A:166:TYR:CE1	1:A:167:GLU:HG2	2.39	0.57
1:A:140:LEU:HA	1:A:143:TYR:HD2	1.69	0.57
1:A:161:HIS:NE2	1:A:177:ARG:HG3	2.19	0.57
1:A:193:LEU:HD11	1:A:250:ILE:HG22	1.86	0.57
1:A:242:LEU:HD12	1:A:243:PRO:HD2	1.86	0.57
1:A:367:PRO:O	1:A:370:VAL:HG23	2.05	0.57
2:P:88:ARG:NH1	2:P:97:THR:OG1	2.37	0.56
1:A:196:ARG:O	1:A:196:ARG:HG3	2.06	0.56
1:A:193:LEU:HD12	1:A:253:GLU:HG2	1.88	0.56
2:P:103:THR:CG2	2:P:127:CYS:SG	2.94	0.56
1:A:47:MET:HE1	1:A:64:ILE:HD11	1.88	0.56
1:A:139:VAL:HA	1:A:165:ILE:HD13	1.89	0.55
1:A:198:TYR:HB3	1:A:200:PHE:CE1	2.42	0.55
1:A:44:MET:HG3	1:A:46:GLY:H	1.72	0.55
1:A:61:LYS:CB	1:A:65:LEU:HD22	2.37	0.55
1:A:53:TYR:HD1	1:A:57:GLU:OE1	1.89	0.55
1:A:61:LYS:O	1:A:63:GLY:N	2.40	0.55
1:A:54:VAL:HG22	1:A:55:GLY:N	2.22	0.54
2:P:23:GLY:O	2:P:28:PRO:HA	2.07	0.54
1:A:275:HIS:HA	1:A:313:MET:HE1	1.90	0.54
1:A:34:ILE:O	1:A:54:VAL:HG23	2.07	0.54
1:A:159:VAL:HG21	1:A:177:ARG:NH1	2.23	0.54
1:A:218:TYR:CE1	1:A:255:PHE:HB3	2.42	0.54
1:A:227:MET:HE1	1:A:252:ASN:OD1	2.07	0.54
1:A:191:LYS:O	1:A:194:THR:HG22	2.07	0.54
1:A:296:ASN:HA	1:A:330:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLN:O	1:A:266:PHE:HB2	2.07	0.53
1:A:185:LEU:CB	1:A:213:LYS:NZ	2.71	0.53
1:A:352:PHE:CE2	1:A:356:TRP:CZ3	2.97	0.53
1:A:132:MET:HE1	1:A:134:VAL:CG2	2.38	0.53
1:A:178:LEU:HD11	1:A:271:SER:OG	2.08	0.53
1:A:275:HIS:HA	1:A:313:MET:CE	2.38	0.53
1:A:169:TYR:HA	1:A:375:PHE:CZ	2.44	0.53
1:A:70:PRO:CG	1:A:85:ILE:HD11	2.36	0.52
1:A:218:TYR:HA	1:A:307:PRO:HD2	1.91	0.52
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.90	0.52
1:A:212:ILE:HG12	1:A:240:TYR:CE2	2.45	0.52
1:A:190:MET:HB2	1:A:209:VAL:HG21	1.92	0.52
1:A:121:GLN:O	1:A:125:GLU:HG3	2.10	0.52
1:A:201:THR:HG23	1:A:202:THR:H	1.75	0.52
1:A:219:VAL:HG23	1:A:306:TYR:HB3	1.90	0.51
2:P:63:LEU:O	2:P:63:LEU:HD12	2.10	0.51
1:A:151:ILE:HG23	1:A:297:THR:HA	1.93	0.51
1:A:133:TYR:HE2	1:A:135:ALA:HB2	1.74	0.51
1:A:60:SER:O	1:A:61:LYS:C	2.53	0.51
1:A:103:VAL:HG11	1:A:123:MET:HE2	1.92	0.51
2:P:132:SER:O	2:P:136:ARG:HG3	2.10	0.51
1:A:239:SER:HA	1:A:248:ILE:O	2.10	0.51
1:A:0:ACE:H3	1:A:6:ALA:CB	2.41	0.51
2:P:51:VAL:HG12	2:P:51:VAL:O	2.11	0.51
1:A:243:PRO:HG2	1:A:244:ASP:H	1.74	0.51
1:A:132:MET:O	1:A:356:TRP:HB2	2.11	0.50
1:A:356:TRP:CD1	1:A:356:TRP:C	2.88	0.50
1:A:0:ACE:H3	1:A:6:ALA:HB2	1.92	0.50
1:A:171:LEU:HB3	1:A:173:HIS:CE1	2.47	0.50
1:A:132:MET:CE	1:A:134:VAL:HG23	2.42	0.50
1:A:161:HIS:CD2	1:A:177:ARG:HG3	2.46	0.50
1:A:163:VAL:HG13	1:A:175:ILE:HD11	1.93	0.50
1:A:159:VAL:HG21	1:A:177:ARG:HH11	1.77	0.50
1:A:309:ILE:O	1:A:313:MET:HB2	2.12	0.50
1:A:116:ARG:HD3	1:A:371:HIS:CE1	2.47	0.49
1:A:159:VAL:HG22	1:A:160:THR:N	2.27	0.49
1:A:79:TRP:O	1:A:83:GLU:HB2	2.11	0.49
1:A:216:LEU:HD23	1:A:250:ILE:CD1	2.34	0.49
1:A:295:ALA:O	1:A:328:LYS:HE2	2.13	0.49
1:A:356:TRP:HD1	1:A:356:TRP:O	1.95	0.49
1:A:61:LYS:HB2	1:A:65:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG21	1:A:177:ARG:HG2	1.93	0.49
1:A:162:THR:OG1	1:A:176:LEU:HB2	2.13	0.49
2:P:103:THR:HG22	2:P:127:CYS:SG	2.52	0.49
1:A:39:ARG:HG2	1:A:64:ILE:O	2.13	0.49
1:A:325:MET:SD	1:A:325:MET:N	2.86	0.49
2:P:91:SER:HB2	2:P:95:ALA:CB	2.39	0.49
1:A:210:ARG:O	1:A:213:LYS:HB3	2.13	0.48
1:A:259:GLU:CD	1:A:312:ARG:HH22	2.21	0.48
1:A:3:ASP:O	1:A:4:ASP:HB2	2.13	0.48
1:A:313:MET:HE2	1:A:317:ILE:HD11	1.95	0.48
2:P:24:TYR:CD1	2:P:109:LEU:HD13	2.49	0.48
1:A:31:PHE:N	1:A:31:PHE:CD1	2.81	0.48
1:A:211:ASP:O	1:A:215:LYS:HB2	2.13	0.48
1:A:352:PHE:CE2	1:A:356:TRP:CE3	3.01	0.48
1:A:16:MET:HG2	1:A:30:VAL:CG1	2.43	0.48
1:A:31:PHE:HD1	1:A:31:PHE:N	2.11	0.48
1:A:50:LYS:C	1:A:52:SER:H	2.22	0.48
1:A:159:VAL:HG21	1:A:177:ARG:CG	2.43	0.47
1:A:88:HIS:CD2	1:A:93:GLU:HG2	2.49	0.47
1:A:341:ILE:HD13	1:A:341:ILE:HA	1.70	0.47
2:P:82:GLU:O	2:P:83:PHE:CB	2.63	0.47
1:A:296:ASN:HA	1:A:330:ILE:HD11	1.97	0.47
1:A:61:LYS:O	1:A:64:ILE:HG22	2.15	0.47
1:A:188:TYR:HD2	1:A:257:CYS:HA	1.79	0.47
1:A:212:ILE:HG12	1:A:240:TYR:CD2	2.50	0.47
2:P:31:TRP:O	2:P:32:ALA:HB2	2.15	0.47
1:A:41:GLN:CG	1:A:42:GLY:H	2.27	0.47
1:A:274:ILE:HG22	1:A:275:HIS:N	2.30	0.47
1:A:69:TYR:HA	1:A:70:PRO:HD3	1.58	0.46
1:A:12:ASN:H	1:A:106:THR:HG22	1.80	0.46
2:P:63:LEU:HD11	2:P:87:LEU:HD22	1.97	0.46
1:A:53:TYR:HD1	1:A:57:GLU:CD	2.23	0.46
1:A:124:PHE:O	1:A:128:ASN:HA	2.16	0.46
1:A:300:SER:HA	1:A:335:ARG:HB2	1.97	0.46
1:A:159:VAL:CG2	1:A:160:THR:N	2.79	0.46
2:P:131:ALA:O	2:P:135:ARG:HB2	2.16	0.46
1:A:41:GLN:CG	1:A:42:GLY:N	2.78	0.46
1:A:37:ARG:HD2	1:A:51:ASP:O	2.17	0.46
1:A:372:ARG:NH2	2:P:84:THR:HG21	2.31	0.46
1:A:200:PHE:HA	1:A:205:GLU:HG2	1.98	0.45
1:A:302:GLY:CA	4:A:1:ATP:H5'2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:O	1:A:43:VAL:HG23	2.16	0.45
2:P:101:THR:HG21	2:P:124:ASN:HA	1.97	0.45
1:A:294:TYR:O	1:A:327:ILE:HA	2.16	0.45
1:A:93:GLU:OE1	1:A:93:GLU:HA	2.17	0.45
1:A:195:GLU:C	1:A:197:GLY:H	2.24	0.45
1:A:159:VAL:CG2	1:A:177:ARG:HG2	2.47	0.45
1:A:116:ARG:NH1	1:A:116:ARG:HG2	2.31	0.45
1:A:35:VAL:CG2	1:A:81:ASP:HB2	2.44	0.44
1:A:334:GLU:O	1:A:334:GLU:CG	2.64	0.44
2:P:77:LEU:HD21	2:P:102:VAL:CG2	2.46	0.44
2:P:17:GLN:HB3	2:P:115:LYS:HD3	1.98	0.44
1:A:366:GLY:O	1:A:369:ILE:HG22	2.17	0.44
1:A:62:ARG:HB3	1:A:62:ARG:CZ	2.48	0.44
1:A:298:VAL:HG12	1:A:299:LEU:N	2.32	0.44
1:A:353:GLN:OE1	1:A:353:GLN:O	2.36	0.44
1:A:133:TYR:CE2	1:A:135:ALA:HB2	2.51	0.44
1:A:303:THR:O	1:A:303:THR:HG22	2.18	0.44
2:P:50:LEU:HD23	2:P:63:LEU:HD22	1.99	0.44
2:P:65:LEU:HA	2:P:65:LEU:HD12	1.73	0.44
2:P:82:GLU:O	2:P:128:TYR:HE1	2.01	0.44
1:A:100:GLU:O	1:A:100:GLU:HG2	2.18	0.44
1:A:180:LEU:HA	1:A:184:ASP:OD2	2.17	0.43
1:A:274:ILE:HA	1:A:274:ILE:HD12	1.77	0.43
1:A:86:TRP:O	1:A:87:HIS:C	2.61	0.43
1:A:160:THR:OG1	1:A:178:LEU:HB3	2.17	0.43
1:A:352:PHE:CE2	1:A:356:TRP:HZ3	2.36	0.43
1:A:155:SER:OG	1:A:160:THR:HG22	2.17	0.43
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.72	0.43
1:A:203:THR:O	1:A:204:ALA:HB3	2.17	0.43
1:A:227:MET:O	1:A:230:ALA:HB3	2.18	0.43
1:A:4:ASP:OD1	1:A:5:ILE:HD12	2.19	0.43
1:A:79:TRP:HZ3	1:A:86:TRP:CZ3	2.36	0.43
2:P:63:LEU:HD12	2:P:63:LEU:C	2.44	0.43
1:A:8:LEU:HB2	1:A:103:VAL:HG23	2.00	0.43
1:A:334:GLU:O	1:A:336:LYS:N	2.51	0.43
1:A:116:ARG:HD3	1:A:371:HIS:HE1	1.84	0.43
1:A:304:THR:O	1:A:309:ILE:HG21	2.19	0.43
1:A:304:THR:C	1:A:335:ARG:HH12	2.26	0.43
2:P:55:ARG:HD3	2:P:78:LEU:HD11	2.01	0.43
1:A:14:SER:HB2	4:A:1:ATP:PG	2.59	0.42
1:A:332:PRO:HA	1:A:333:PRO:HD2	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE3	1:A:355:MET:HB2	1.86	0.42
2:P:55:ARG:HD3	2:P:78:LEU:CD1	2.49	0.42
1:A:18:LYS:HG2	1:A:27:PRO:HG3	2.00	0.42
1:A:53:TYR:C	1:A:58:ALA:HB2	2.44	0.42
1:A:17:CYS:SG	1:A:31:PHE:CE1	3.12	0.42
2:P:91:SER:CB	2:P:95:ALA:HB3	2.41	0.42
1:A:118:LYS:HD2	1:A:118:LYS:HA	1.86	0.42
2:P:19:ALA:O	2:P:20:ALA:HB2	2.19	0.42
1:A:11:ASP:HA	1:A:106:THR:HB	2.01	0.41
2:P:69:LYS:HE2	2:P:69:LYS:HB2	1.88	0.41
1:A:240:TYR:HB3	1:A:248:ILE:CG1	2.50	0.41
1:A:20:GLY:HA3	1:A:340:TRP:HZ2	1.84	0.41
1:A:105:LEU:HD11	1:A:123:MET:CG	2.50	0.41
1:A:54:VAL:CG2	1:A:55:GLY:N	2.84	0.41
1:A:62:ARG:NH1	1:A:62:ARG:CB	2.84	0.41
1:A:39:ARG:HG3	1:A:40:HIS:N	2.35	0.41
1:A:50:LYS:C	1:A:52:SER:N	2.79	0.41
1:A:61:LYS:HB3	1:A:65:LEU:HD13	2.03	0.41
1:A:198:TYR:HB3	1:A:200:PHE:HE1	1.84	0.41
1:A:340:TRP:CZ3	1:A:344:SER:HB2	2.55	0.41
2:P:114:GLY:HA3	2:P:123:ILE:CD1	2.48	0.41
2:P:43:THR:OG1	2:P:46:GLU:HG3	2.21	0.41
1:A:352:PHE:CD2	1:A:356:TRP:CZ3	3.09	0.40
1:A:20:GLY:HA3	1:A:340:TRP:CZ2	2.56	0.40
2:P:13:ASP:HB3	2:P:15:THR:OG1	2.20	0.40
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.87	0.40
2:P:50:LEU:CD2	2:P:63:LEU:HD22	2.51	0.40
2:P:112:LEU:HD21	2:P:126:LYS:HE3	2.04	0.40
2:P:58:PHE:CZ	2:P:75:ASP:OD2	2.74	0.40
2:P:84:THR:HG21	2:P:124:ASN:HD21	1.85	0.40
1:A:286:ASP:OD1	1:A:288:ASP:HB2	2.22	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	372/375 (99%)	311 (84%)	41 (11%)	20 (5%)	1	2
2	P	138/140 (99%)	120 (87%)	14 (10%)	4 (3%)	3	5
All	All	510/515 (99%)	431 (84%)	55 (11%)	24 (5%)	2	2

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	29	ALA
1	A	62	ARG
1	A	64	ILE
1	A	203	THR
1	A	335	ARG
1	A	2	ASP
1	A	5	ILE
1	A	38	PRO
1	A	40	HIS
1	A	50	LYS
1	A	182	GLY
1	A	199	SER
1	A	201	THR
1	A	233	SER
2	P	52	GLY
1	A	43	VAL
1	A	251	GLY
1	A	324	THR
2	P	26	ASP
2	P	32	ALA
1	A	202	THR
1	A	243	PRO
2	P	12	ALA

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	316/316 (100%)	270 (85%)	46 (15%)	3	4
2	P	112/112 (100%)	92 (82%)	20 (18%)	2	2
All	All	428/428 (100%)	362 (85%)	66 (15%)	2	3

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	16	MET
1	A	18	LYS
1	A	25	ASP
1	A	31	PHE
1	A	34	ILE
1	A	38	PRO
1	A	43	VAL
1	A	45	VAL
1	A	47	MET
1	A	49	GLN
1	A	56	ASP
1	A	59	GLN
1	A	64	ILE
1	A	82	MET
1	A	104	LEU
1	A	106	THR
1	A	129	THR
1	A	148	THR
1	A	149	THR
1	A	180	LEU
1	A	193	LEU
1	A	194	THR
1	A	195	GLU
1	A	203	THR
1	A	205	GLU
1	A	233	SER
1	A	235	SER
1	A	238	LYS
1	A	239	SER
1	A	244	ASP
1	A	250	ILE
1	A	252	ASN
1	A	274	ILE
1	A	299	LEU

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Mol	Chain	Res	Type
1	A	314	GLN
1	A	322	PRO
1	A	324	THR
1	A	338	SER
1	A	341	ILE
1	A	346	LEU
1	A	348	SER
1	A	353	GLN
1	A	354	GLN
1	A	370	VAL
1	A	372	ARG
2	P	13	ASP
2	P	29	SER
2	P	49	ILE
2	P	56	SER
2	P	57	SER
2	P	58	PHE
2	P	61	ASN
2	P	65	LEU
2	P	77	LEU
2	P	84	THR
2	P	87	LEU
2	P	88	ARG
2	P	101	THR
2	P	102	VAL
2	P	103	THR
2	P	109	LEU
2	P	111	LEU
2	P	115	LYS
2	P	122	MET
2	P	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	128	ASN
1	A	137	GLN
1	A	173	HIS
1	A	263	GLN
1	A	280	ASN
1	A	360	GLN

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Mol	Chain	Res	Type
2	P	41	ASN
2	P	61	ASN
2	P	99	ASN

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	$\# Z > 2$
1	HIC	A	73	1	10,11,12	0.83	0	9,14,16	3.80	3 (33%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-10.73	108.56	112.66
1	A	73	HIC	CD2-NE2-CE1	2.58	107.73	106.71
1	A	73	HIC	CE1-ND1-CG	2.41	109.66	105.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 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
4	ATP	A	1	3	32,33,33	1.12	4 (12%)	48,52,52	0.79	2 (4%)

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	1	3	-	8/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	ATP	PA-O3A	3.41	1.63	1.59
4	A	1	ATP	PB-O3B	3.38	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	ATP	PB-O3A	2.33	1.62	1.59
4	A	1	ATP	PG-O3G	-2.16	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	ATP	O3G-PG-O1G	2.42	120.28	110.83
4	A	1	ATP	O2B-PB-O3A	2.03	112.75	107.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

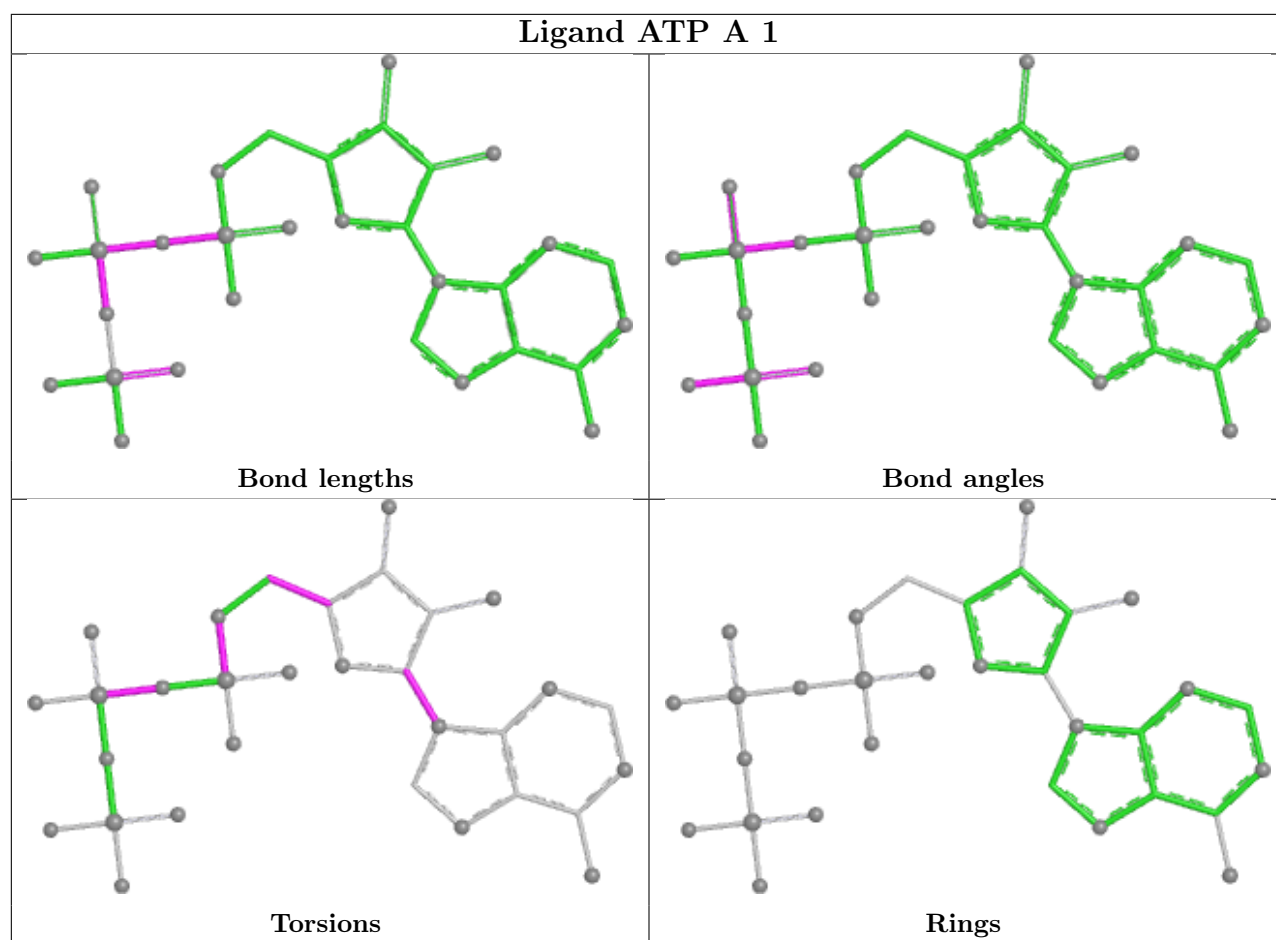
Mol	Chain	Res	Type	Atoms
4	A	1	ATP	C5'-O5'-PA-O1A
4	A	1	ATP	C5'-O5'-PA-O2A
4	A	1	ATP	C5'-O5'-PA-O3A
4	A	1	ATP	O4'-C4'-C5'-O5'
4	A	1	ATP	C3'-C4'-C5'-O5'
4	A	1	ATP	C2'-C1'-N9-C8
4	A	1	ATP	PA-O3A-PB-O2B
4	A	1	ATP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	ATP	3	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.