



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 04:01 PM EDT

PDB ID : 1ATN  
Title : Atomic structure of the actin:DNASE I complex  
Authors : Kabsch, W.; Mannherz, H.G.; Suck, D.; Pai, E.; Holmes, K.C.  
Deposited on : 1991-03-08  
Resolution : 2.80 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](mailto: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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

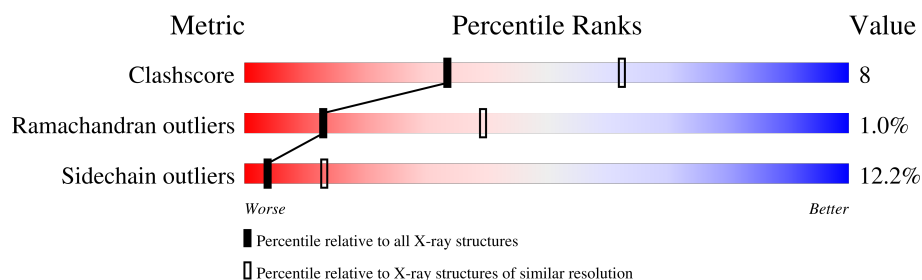
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)

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  $\geq 3$ , 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	373	
2	D	260	
3	B	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	1	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5019 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2911	1839	489	563	20			

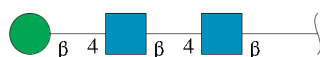
- Molecule 2 is a protein called DEOXYRIBONUCLEASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	258	Total	C	N	O	S	0	0	0
			2034	1290	339	397	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	102	GLY	GLU	conflict	UNP P00639
D	103	ASN	SER	conflict	UNP P00639

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O		0	0	0
			39	22	2	15				

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

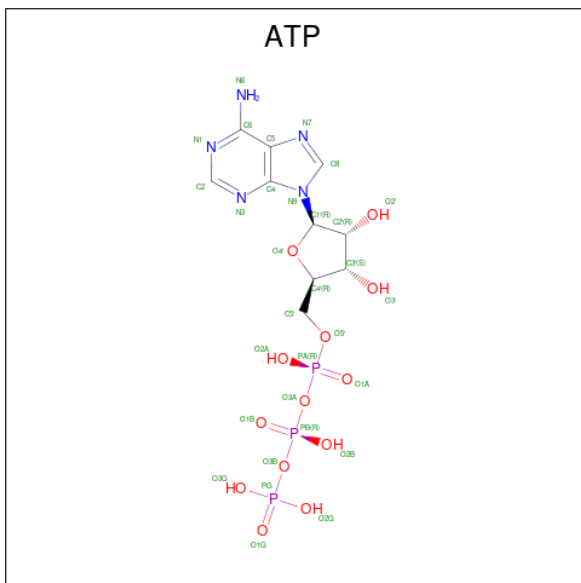
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Ca	0	0
			3	3		

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



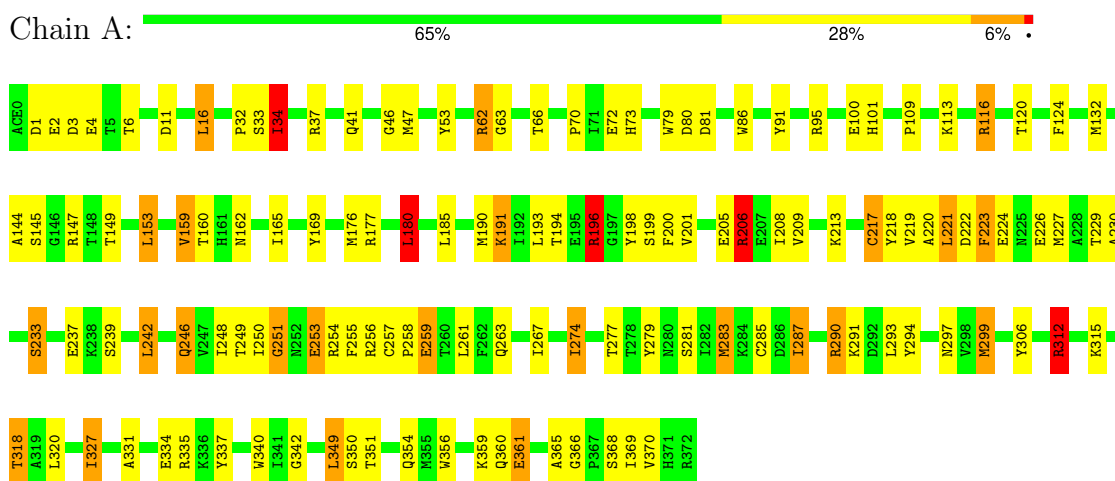
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

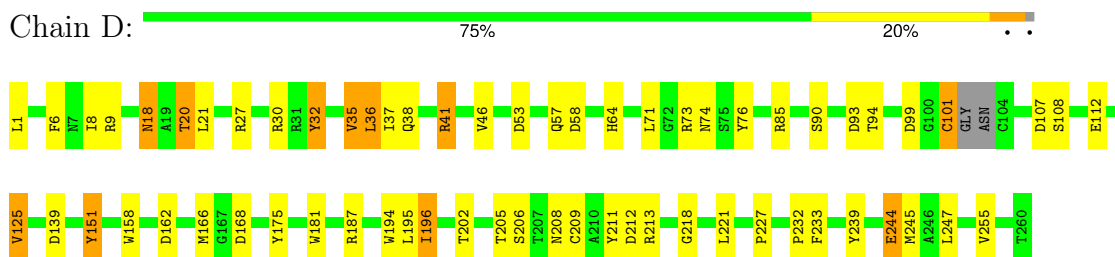
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



#### • Molecule 2: DEOXYRIBONUCLEASE I



#### • Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 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, $\alpha$ , $\beta$ , $\gamma$	132.90Å 56.30Å 109.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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: NAG, BMA, HIC, CA, ATP, ACE

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	0.89	2/2958 (0.1%)	1.64	52/4007 (1.3%)
2	D	1.04	1/2079 (0.0%)	1.77	36/2830 (1.3%)
All	All	0.96	3/5037 (0.1%)	1.70	88/6837 (1.3%)

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	1
2	D	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	GLU	CG-CD	6.22	1.61	1.51
2	D	244	GLU	CB-CG	5.63	1.62	1.52
1	A	259	GLU	CB-CG	5.04	1.61	1.52

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	41	ARG	NE-CZ-NH2	-11.05	114.78	120.30
2	D	213	ARG	NE-CZ-NH2	-10.11	115.25	120.30
2	D	175	TYR	CB-CG-CD2	-9.61	115.23	121.00
2	D	194	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	356	TRP	CD1-CG-CD2	9.08	113.57	106.30
2	D	30	ARG	NE-CZ-NH1	8.97	124.79	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	CYS	CA-CB-SG	8.52	129.33	114.00
1	A	177	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	A	86	TRP	CD1-CG-CD2	8.44	113.05	106.30
2	D	181	TRP	CD1-CG-CD2	8.33	112.96	106.30
2	D	158	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	A	356	TRP	CE2-CD2-CG	-7.90	100.98	107.30
2	D	53	ASP	CB-CG-OD1	7.87	125.38	118.30
2	D	125	VAL	CB-CA-C	-7.70	96.78	111.40
1	A	312	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	A	86	TRP	CE2-CD2-CG	-7.53	101.28	107.30
2	D	194	TRP	CE2-CD2-CG	-7.37	101.40	107.30
1	A	233	SER	CA-C-N	-7.36	101.00	117.20
1	A	180	LEU	CA-CB-CG	7.34	132.17	115.30
2	D	181	TRP	CE2-CD2-CG	-7.31	101.45	107.30
2	D	175	TYR	CB-CG-CD1	7.23	125.34	121.00
1	A	254	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	79	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	A	340	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	206	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	47	MET	CA-CB-CG	-7.02	101.36	113.30
1	A	79	TRP	CE2-CD2-CG	-7.00	101.70	107.30
2	D	158	TRP	CE2-CD2-CG	-6.98	101.72	107.30
2	D	239	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	A	340	TRP	CD1-CG-CD2	6.91	111.83	106.30
2	D	211	TYR	CB-CG-CD2	-6.88	116.87	121.00
2	D	36	LEU	CA-CB-CG	6.74	130.79	115.30
2	D	41	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	D	194	TRP	CG-CD1-NE1	-6.63	103.47	110.10
1	A	283	MET	CG-SD-CE	6.53	110.64	100.20
1	A	159	VAL	CB-CA-C	-6.46	99.12	111.40
1	A	196	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	169	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	A	34	ILE	CA-CB-CG2	-6.43	98.03	110.90
2	D	196	ILE	N-CA-C	-6.41	93.69	111.00
1	A	217	CYS	CA-CB-SG	-6.29	102.68	114.00
2	D	76	TYR	N-CA-C	-6.24	94.14	111.00
2	D	244	GLU	CA-CB-CG	6.14	126.91	113.40
1	A	259	GLU	CA-CB-CG	6.13	126.88	113.40
2	D	32	TYR	CB-CG-CD2	-6.12	117.33	121.00
2	D	18	ASN	N-CA-CB	6.10	121.58	110.60
1	A	16	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	349	LEU	CA-C-N	-6.03	103.93	117.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	125	VAL	CG1-CB-CG2	6.00	120.50	110.90
1	A	116	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	79	TRP	CG-CD2-CE3	5.86	139.17	133.90
1	A	200	PHE	CA-C-N	-5.85	104.32	117.20
1	A	335	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	D	18	ASN	CB-CA-C	-5.80	98.81	110.40
1	A	95	ARG	CA-CB-CG	5.79	126.13	113.40
1	A	254	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	335	ARG	CA-CB-CG	5.70	125.93	113.40
2	D	227	PRO	CA-C-N	-5.68	104.85	116.20
1	A	113	LYS	CA-CB-CG	5.59	125.71	113.40
1	A	279	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	D	233	PHE	CA-C-N	-5.56	104.96	117.20
1	A	254	ARG	N-CA-CB	-5.51	100.68	110.60
1	A	294	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	356	TRP	CG-CD2-CE3	5.49	138.84	133.90
2	D	27	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	D	151	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	356	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	A	79	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	A	147	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	11	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	356	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	251	GLY	CA-C-N	-5.34	105.45	117.20
1	A	176	MET	CG-SD-CE	5.29	108.67	100.20
1	A	335	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	D	213	ARG	CG-CD-NE	-5.26	100.75	111.80
2	D	35	VAL	CB-CA-C	-5.25	101.43	111.40
1	A	62	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	D	9	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	91	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	290	ARG	CA-C-N	5.17	128.58	117.20
2	D	27	ARG	CA-CB-CG	5.15	124.72	113.40
2	D	181	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	53	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	62	ARG	CA-CB-CG	5.09	124.60	113.40
1	A	337	TYR	CB-CG-CD1	-5.09	117.95	121.00
2	D	166	MET	CA-CB-CG	5.06	121.90	113.30
1	A	191	LYS	CA-C-N	5.06	128.33	117.20
1	A	86	TRP	CG-CD1-NE1	-5.00	105.10	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	ARG	Sidechain
2	D	151	TYR	Sidechain
2	D	41	ARG	Sidechain
2	D	85	ARG	Sidechain

## 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	2911	0	2869	57	0
2	D	2034	0	1969	23	0
3	B	39	0	34	1	0
4	A	1	0	0	0	0
4	D	3	0	0	0	0
5	A	31	0	12	1	0
All	All	5019	0	4884	75	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 (75) 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:3:ASP:HA	1:A:6:THR:HB	1.36	1.07
1:A:237:GLU:HA	1:A:251:GLY:HA2	1.60	0.82
1:A:223:PHE:HE1	1:A:255:PHE:HB2	1.46	0.78
1:A:223:PHE:HD2	1:A:312:ARG:HH21	1.33	0.76
1:A:253:GLU:HA	1:A:256:ARG:HG3	1.69	0.72
1:A:3:ASP:HA	1:A:6:THR:CB	2.18	0.72
1:A:46:GLY:H	2:D:94:THR:HG22	1.55	0.70
2:D:101:CYS:HB2	2:D:107:ASP:HB3	1.75	0.68
1:A:1:ASP:HA	1:A:4:GLU:HB3	1.74	0.68
1:A:41:GLN:HB2	2:D:64:HIS:CD2	2.29	0.68
1:A:160:THR:HG21	1:A:274:ILE:HD11	1.76	0.67
1:A:153:LEU:HD11	1:A:274:ILE:HG13	1.76	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:GLN:HE22	2:D:168:ASP:H	1.42	0.65
1:A:190:MET:SD	1:A:209:VAL:HG11	2.38	0.63
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.81	0.62
1:A:361:GLU:HB3	1:A:369:ILE:HG12	1.82	0.61
1:A:287:ILE:HD12	1:A:287:ILE:H	1.67	0.60
2:D:99:ASP:O	2:D:107:ASP:HA	2.02	0.60
1:A:223:PHE:HD2	1:A:312:ARG:NH2	1.99	0.59
2:D:38:GLN:HE22	2:D:168:ASP:N	2.02	0.57
2:D:205:THR:HG22	2:D:247:LEU:HD21	1.87	0.56
1:A:365:ALA:HB3	1:A:369:ILE:HB	1.88	0.55
1:A:46:GLY:N	2:D:94:THR:HG22	2.19	0.55
3:B:2:NAG:H61	3:B:3:BMA:H2	1.90	0.54
1:A:46:GLY:H	2:D:94:THR:CG2	2.21	0.53
1:A:185:LEU:HD23	1:A:306:TYR:OH	2.09	0.52
1:A:180:LEU:HD22	1:A:267:ILE:HD11	1.92	0.51
2:D:162:ASP:HA	2:D:218:GLY:HA3	1.91	0.51
1:A:285:CYS:O	1:A:290:ARG:NH1	2.43	0.51
1:A:41:GLN:HB2	2:D:64:HIS:NE2	2.26	0.50
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.94	0.50
1:A:124:PHE:CZ	1:A:132:MET:HG3	2.48	0.49
2:D:32:TYR:HB2	2:D:35:VAL:HG22	1.93	0.49
1:A:198:TYR:CZ	1:A:248:ILE:HG13	2.48	0.48
1:A:120:THR:HG21	1:A:370:VAL:HG11	1.95	0.48
1:A:250:ILE:HG23	1:A:253:GLU:HG2	1.96	0.48
1:A:253:GLU:HA	1:A:256:ARG:CG	2.42	0.48
1:A:318:THR:HA	1:A:327:ILE:HG12	1.94	0.48
1:A:213:LYS:O	1:A:217:CYS:HB2	2.13	0.47
2:D:202:THR:HG22	2:D:232:PRO:HG3	1.97	0.47
1:A:162:ASN:OD1	1:A:277:THR:HG22	2.15	0.47
1:A:6:THR:HG22	1:A:101:HIS:HA	1.97	0.46
2:D:38:GLN:NE2	2:D:168:ASP:H	2.11	0.46
1:A:299:MET:HE2	1:A:331:ALA:HB2	1.97	0.46
1:A:223:PHE:CD2	1:A:259:GLU:HG3	2.51	0.46
1:A:366:GLY:O	1:A:369:ILE:HG22	2.16	0.46
1:A:32:PRO:HB2	1:A:34:ILE:HD11	1.98	0.45
2:D:187:ARG:HA	2:D:187:ARG:HD2	1.74	0.45
1:A:190:MET:O	1:A:194:THR:HG23	2.16	0.44
2:D:196:ILE:HG21	2:D:212:ASP:O	2.17	0.44
1:A:193:LEU:O	1:A:198:TYR:HD2	2.01	0.43
1:A:220:ALA:HB3	1:A:223:PHE:CD1	2.53	0.43
2:D:6:PHE:O	2:D:37:ILE:HA	2.17	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:O	1:A:208:ILE:HG22	2.18	0.43
2:D:18:ASN:HD22	2:D:20:THR:HG23	1.84	0.43
1:A:223:PHE:HB3	1:A:259:GLU:OE2	2.18	0.43
1:A:149:THR:HA	1:A:165:ILE:O	2.19	0.43
1:A:217:CYS:C	1:A:218:TYR:HD1	2.22	0.42
1:A:222:ASP:OD1	1:A:224:GLU:HB3	2.19	0.42
2:D:208:ASN:C	2:D:209:CYS:SG	2.98	0.42
1:A:196:ARG:HH21	1:A:249:THR:HG23	1.85	0.42
2:D:73:ARG:NH1	2:D:107:ASP:O	2.53	0.42
1:A:206:ARG:O	1:A:209:VAL:HG12	2.20	0.41
1:A:221:LEU:HA	1:A:312:ARG:HG2	2.02	0.41
1:A:226:GLU:HG3	1:A:255:PHE:CE2	2.56	0.41
1:A:180:LEU:HD11	1:A:261:LEU:HD23	2.01	0.41
1:A:227:MET:O	1:A:230:ALA:HB3	2.21	0.41
1:A:369:ILE:HG23	1:A:370:VAL:N	2.35	0.41
2:D:18:ASN:HB2	2:D:21:LEU:HB2	2.03	0.41
1:A:144:ALA:HB2	1:A:342:GLY:CA	2.51	0.41
1:A:193:LEU:HD11	1:A:250:ILE:HG13	2.02	0.40
2:D:8:ILE:HD12	2:D:37:ILE:HG23	2.02	0.40
1:A:63:GLY:HA3	2:D:46:VAL:HA	2.03	0.40
1:A:219:VAL:HG22	1:A:258:PRO:CB	2.51	0.40
1:A:306:TYR:CE1	5:A:375:ATP:H2	2.40	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	370/373 (99%)	335 (90%)	29 (8%)	6 (2%)	8	27
2	D	254/260 (98%)	238 (94%)	16 (6%)	0	100	100
All	All	624/633 (99%)	573 (92%)	45 (7%)	6 (1%)	13	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	274	ILE
1	A	233	SER
1	A	2	GLU
1	A	253	GLU
1	A	242	LEU

### 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	314/314 (100%)	267 (85%)	47 (15%)	2	8
2	D	227/228 (100%)	208 (92%)	19 (8%)	9	28
All	All	541/542 (100%)	475 (88%)	66 (12%)	4	13

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

Mol	Chain	Res	Type
1	A	16	LEU
1	A	33	SER
1	A	34	ILE
1	A	37	ARG
1	A	66	THR
1	A	72	GLU
1	A	80	ASP
1	A	100	GLU
1	A	109	PRO
1	A	116	ARG
1	A	145	SER
1	A	153	LEU
1	A	159	VAL
1	A	180	LEU
1	A	191	LYS
1	A	196	ARG
1	A	199	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	201	VAL
1	A	206	ARG
1	A	221	LEU
1	A	223	PHE
1	A	229	THR
1	A	239	SER
1	A	242	LEU
1	A	246	GLN
1	A	263	GLN
1	A	281	SER
1	A	283	MET
1	A	287	ILE
1	A	291	LYS
1	A	293	LEU
1	A	297	ASN
1	A	299	MET
1	A	312	ARG
1	A	315	LYS
1	A	318	THR
1	A	320	LEU
1	A	327	ILE
1	A	334	GLU
1	A	349	LEU
1	A	350	SER
1	A	351	THR
1	A	354	GLN
1	A	359	LYS
1	A	360	GLN
1	A	361	GLU
1	A	368	SER
2	D	1	LEU
2	D	20	THR
2	D	36	LEU
2	D	57	GLN
2	D	58	ASP
2	D	71	LEU
2	D	74	ASN
2	D	90	SER
2	D	93	ASP
2	D	108	SER
2	D	112	GLU
2	D	125	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	139	ASP
2	D	195	LEU
2	D	206	SER
2	D	221	LEU
2	D	244	GLU
2	D	245	MET
2	D	255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	41	GLN
1	A	92	ASN
1	A	137	GLN
1	A	252	ASN
1	A	263	GLN
1	A	354	GLN
2	D	38	GLN
2	D	61	ASN
2	D	155	GLN
2	D	161	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	8,11,12	1.57	1 (12%)	5,14,16	1.70	2 (40%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-3.38	1.33	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	CG-CD2-NE2	-2.71	104.84	107.78
1	A	73	HIC	CD2-NE2-CE1	2.05	111.25	107.96

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](#)

3 monosaccharides are 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
3	NAG	B	1	3,2	14,14,15	0.76	0	17,19,21	2.60	5 (29%)
3	NAG	B	2	3	14,14,15	1.12	1 (7%)	17,19,21	1.59	4 (23%)
3	BMA	B	3	3	11,11,12	2.42	5 (45%)	15,15,17	1.52	2 (13%)

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	NAG	B	1	3,2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3	BMA	C4-C3	3.90	1.62	1.52
3	B	3	BMA	C1-C2	3.40	1.60	1.52
3	B	3	BMA	C4-C5	3.20	1.59	1.53
3	B	3	BMA	C2-C3	3.08	1.57	1.52
3	B	3	BMA	O5-C1	2.52	1.47	1.43
3	B	2	NAG	C4-C5	2.31	1.57	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	C1-O5-C5	7.97	122.86	112.19
3	B	1	NAG	C1-C2-N2	4.36	117.31	110.43
3	B	3	BMA	C3-C4-C5	3.78	117.09	110.23
3	B	2	NAG	C1-O5-C5	3.17	116.43	112.19
3	B	1	NAG	C4-C3-C2	-3.13	106.44	111.02
3	B	2	NAG	O4-C4-C3	-3.02	103.25	110.38
3	B	1	NAG	C2-N2-C7	-2.87	119.06	122.90
3	B	1	NAG	O4-C4-C5	2.56	115.62	109.32
3	B	3	BMA	O2-C2-C1	2.53	115.01	109.22
3	B	2	NAG	C3-C4-C5	2.16	114.15	110.23
3	B	2	NAG	C2-N2-C7	-2.02	120.20	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1	NAG	C1

All (2) torsion outliers are listed below:

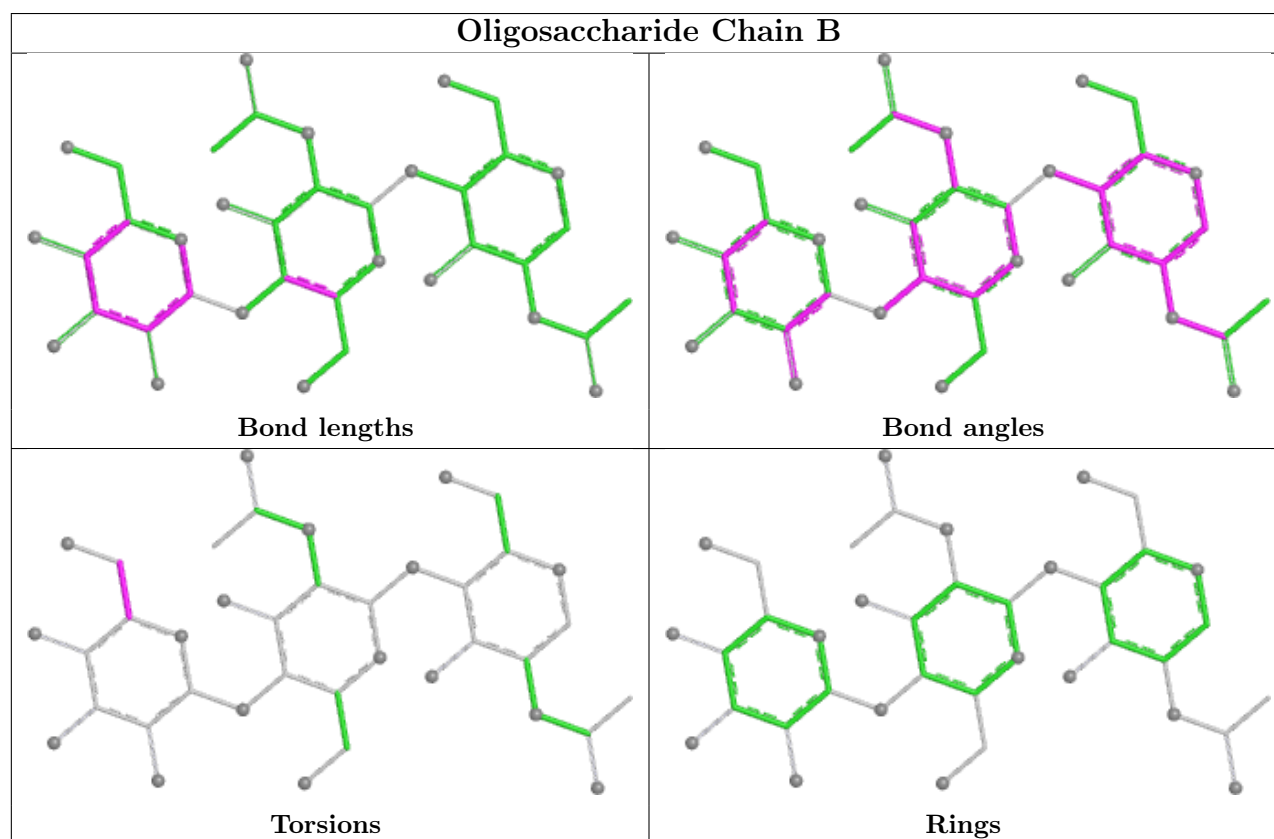
Mol	Chain	Res	Type	Atoms
3	B	3	BMA	C4-C5-C6-O6
3	B	3	BMA	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3	BMA	1	0
3	B	2	NAG	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 oligosaccharide.



## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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	$\# Z  > 2$
5	ATP	A	375	4	28,33,33	1.21	3 (10%)	34,52,52	1.37	6 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	A	375	4	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	375	ATP	C2-N1	2.89	1.39	1.33
5	A	375	ATP	PB-O3B	2.80	1.62	1.59
5	A	375	ATP	O4'-C1'	2.15	1.43	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	375	ATP	C5-C6-N6	3.54	125.71	120.31
5	A	375	ATP	O4'-C1'-N9	3.02	112.75	108.75
5	A	375	ATP	C5-C6-N1	-2.28	114.79	120.23
5	A	375	ATP	O4'-C4'-C5'	-2.11	102.56	109.33
5	A	375	ATP	O3'-C3'-C2'	-2.11	105.06	111.82
5	A	375	ATP	C2'-C3'-C4'	-2.04	98.66	102.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

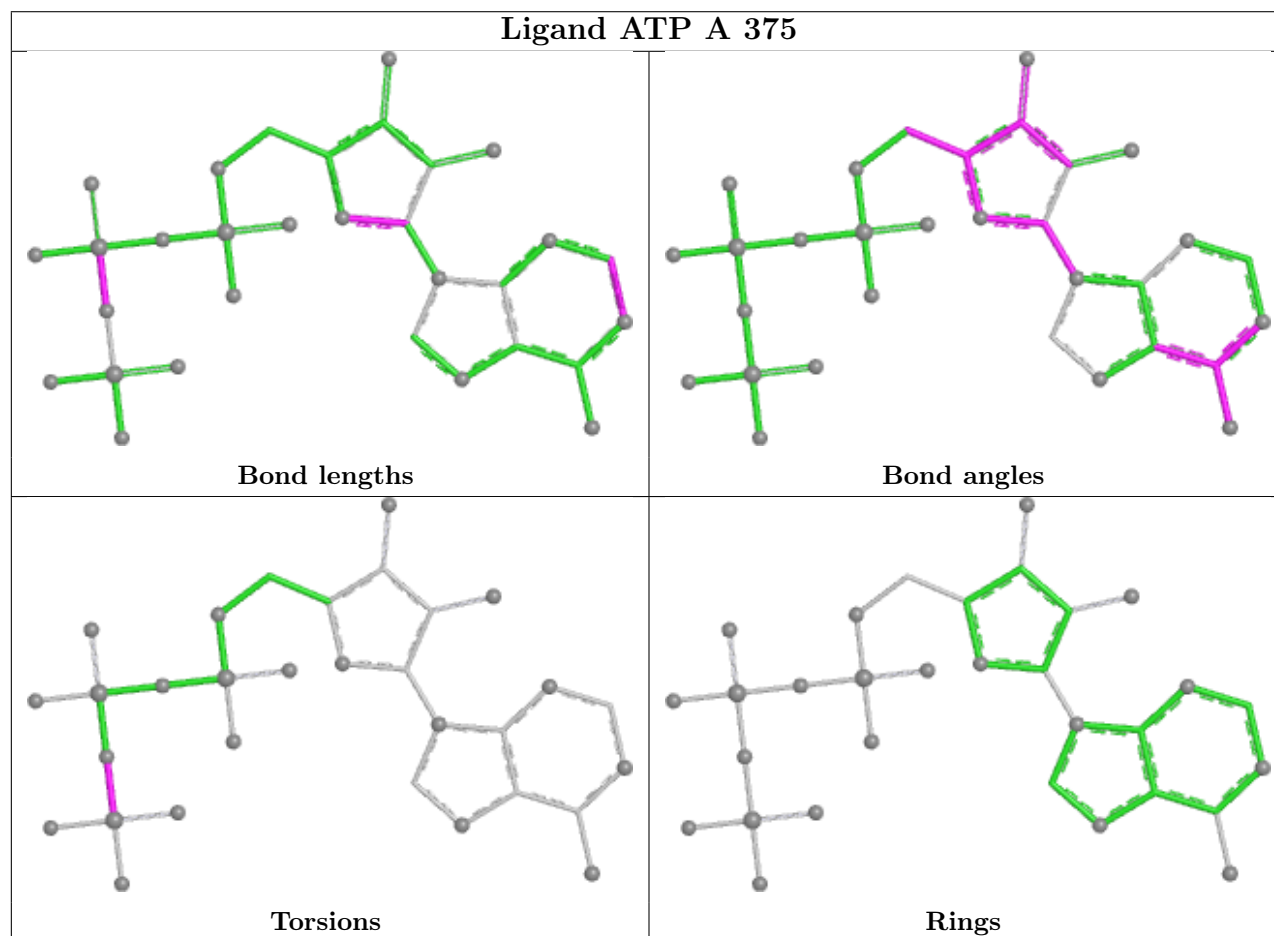
Mol	Chain	Res	Type	Atoms
5	A	375	ATP	PB-O3B-PG-O2G
5	A	375	ATP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	375	ATP	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.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.