



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:50 PM UTC

PDB ID : 1ATN / pdb_00001atn
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

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

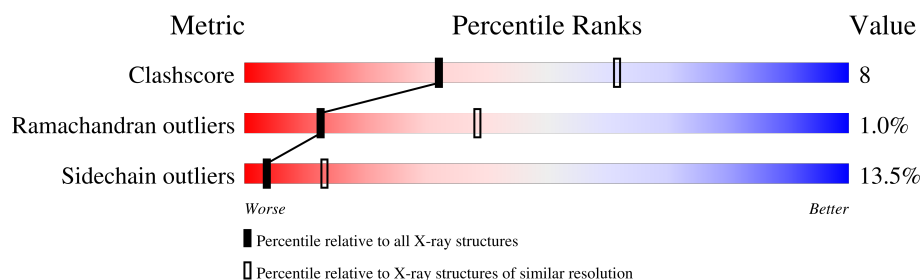
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 ≥ 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			

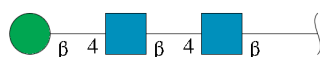
- Molecule 2 is a protein called DEOXYRIBONUCLEASE I.

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 (CCD ID: CA) (formula: Ca).

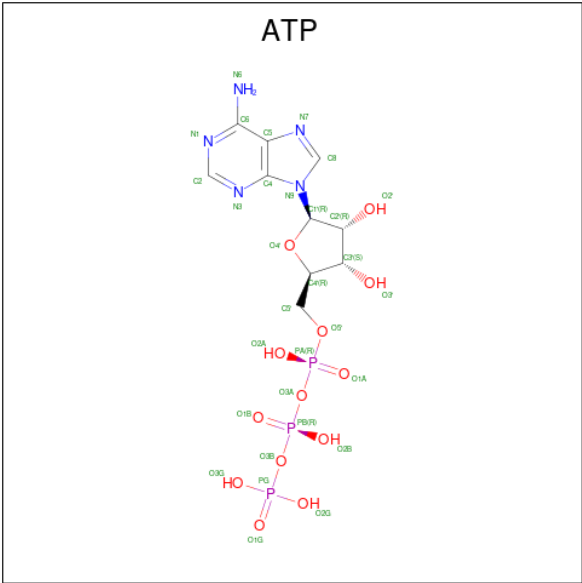
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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

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



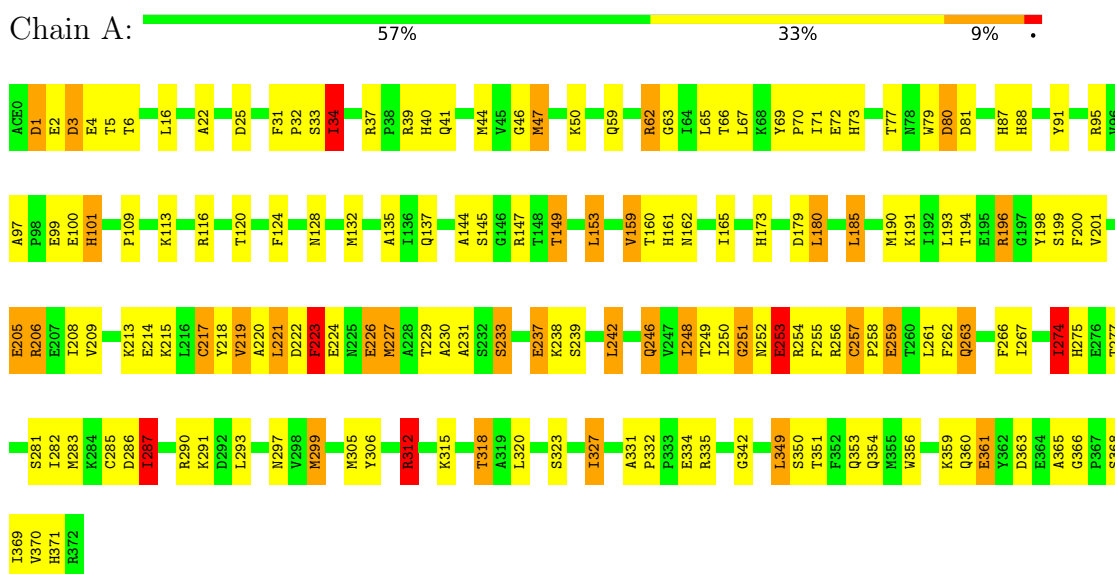
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots [i](#)

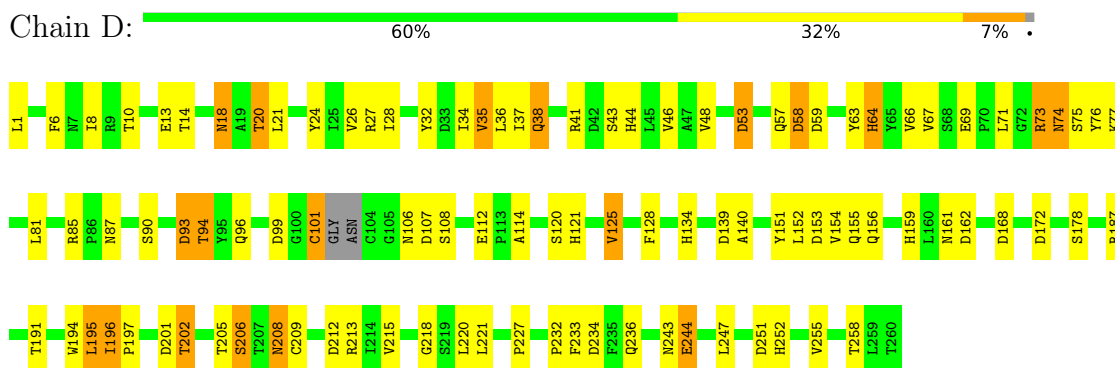
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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, α , β , γ	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 ²)	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: HIC, NAG, BMA, ACE, CA, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.16	13/2958 (0.4%)	2.00	98/4007 (2.4%)
2	D	1.34	8/2079 (0.4%)	2.09	83/2830 (2.9%)
All	All	1.24	21/5037 (0.4%)	2.04	181/6837 (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	1
2	D	0	3
All	All	0	4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	HIS	CD2-NE2	-7.36	1.29	1.37
1	A	88	HIS	CD2-NE2	-7.31	1.29	1.37
1	A	87	HIS	CD2-NE2	-7.19	1.29	1.37
1	A	275	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	40	HIS	CD2-NE2	-7.10	1.30	1.37
2	D	134	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	371	HIS	CD2-NE2	-6.60	1.30	1.37
2	D	252	HIS	CG-ND1	-6.56	1.31	1.38
1	A	88	HIS	CG-ND1	-6.42	1.31	1.38
1	A	101	HIS	CG-ND1	-6.36	1.31	1.38
2	D	64	HIS	CD2-NE2	-6.12	1.31	1.37
2	D	215	VAL	CA-CB	6.07	1.61	1.54
1	A	161	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	173	HIS	CD2-NE2	-5.90	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	244	GLU	CA-CB	5.87	1.62	1.53
2	D	159	HIS	CD2-NE2	-5.69	1.31	1.37
2	D	197	PRO	CA-CB	-5.58	1.45	1.53
1	A	275	HIS	CG-ND1	-5.48	1.32	1.38
2	D	44	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	259	GLU	CA-CB	5.15	1.62	1.53
1	A	214	GLU	CA-CB	5.02	1.61	1.53

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	196	ILE	N-CA-C	-12.57	93.69	107.77
1	A	147	ARG	N-CA-C	9.40	123.32	110.35
1	A	3	ASP	CA-CB-CG	9.23	121.83	112.60
2	D	125	VAL	CB-CA-C	-9.09	96.78	111.59
1	A	179	ASP	CA-CB-CG	8.76	121.36	112.60
2	D	44	HIS	CA-CB-CG	-8.54	105.26	113.80
2	D	18	ASN	CA-CB-CG	8.37	120.97	112.60
1	A	363	ASP	CA-CB-CG	7.97	120.58	112.60
2	D	96	GLN	CG-CD-NE2	7.94	128.32	116.40
2	D	18	ASN	N-CA-CB	7.90	121.58	109.97
1	A	128	ASN	CA-CB-CG	7.85	120.45	112.60
2	D	125	VAL	N-CA-CB	7.84	120.63	110.13
1	A	286	ASP	CA-CB-CG	7.82	120.42	112.60
2	D	233	PHE	CA-C-O	7.73	128.67	120.33
2	D	128	PHE	CA-CB-CG	7.69	121.49	113.80
2	D	76	TYR	N-CA-C	-7.68	94.14	107.20
1	A	25	ASP	CA-CB-CG	7.64	120.24	112.60
2	D	96	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	A	360	GLN	N-CA-C	-7.58	102.71	110.97
1	A	223	PHE	CA-CB-CG	7.57	121.37	113.80
2	D	153	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	62	ARG	N-CA-C	7.50	120.33	111.71
1	A	252	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	A	215	LYS	N-CA-C	7.44	119.18	111.14
1	A	173	HIS	CA-CB-CG	-7.44	106.36	113.80
2	D	77	LYS	N-CA-C	7.43	121.66	110.14
2	D	106	ASN	CA-CB-CG	7.43	120.03	112.60
1	A	34	ILE	CA-CB-CG2	-7.33	98.03	110.50
1	A	159	VAL	CB-CA-C	-7.23	99.12	110.69
1	A	323	SER	N-CA-C	7.13	121.61	112.34
1	A	259	GLU	CB-CG-CD	7.13	124.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	244	GLU	CB-CG-CD	7.07	124.62	112.60
1	A	69	TYR	CA-C-N	7.01	126.71	119.56
1	A	69	TYR	C-N-CA	7.01	126.71	119.56
2	D	202	THR	N-CA-C	-6.99	102.79	112.30
1	A	287	ILE	CB-CA-C	-6.93	102.79	112.14
2	D	251	ASP	CA-CB-CG	6.88	119.47	112.60
1	A	287	ILE	N-CA-C	6.86	117.62	110.62
1	A	191	LYS	CA-C-O	-6.86	113.64	120.70
2	D	43	SER	N-CA-C	6.79	118.47	111.14
2	D	215	VAL	O-C-N	-6.78	115.94	123.26
1	A	259	GLU	N-CA-C	-6.74	104.16	112.38
1	A	214	GLU	CB-CG-CD	6.73	124.05	112.60
2	D	172	ASP	CA-CB-CG	6.63	119.23	112.60
2	D	67	VAL	O-C-N	-6.56	116.08	123.10
2	D	24	TYR	N-CA-C	-6.55	103.35	112.45
2	D	101	CYS	CA-CB-SG	6.49	129.33	114.40
2	D	48	VAL	N-CA-C	-6.46	104.20	110.72
1	A	371	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	286	ASP	CA-C-N	6.45	129.29	120.46
1	A	286	ASP	C-N-CA	6.45	129.29	120.46
2	D	59	ASP	N-CA-C	-6.42	99.12	109.40
2	D	34	ILE	O-C-N	-6.41	116.14	123.07
2	D	66	VAL	O-C-N	-6.41	116.28	123.20
2	D	244	GLU	CA-CB-CG	6.40	126.91	114.10
1	A	101	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	259	GLU	CA-CB-CG	6.39	126.88	114.10
1	A	47	MET	CA-CB-CG	-6.37	101.36	114.10
1	A	80	ASP	CA-CB-CG	6.37	118.97	112.60
2	D	227	PRO	O-C-N	6.35	129.91	122.98
2	D	18	ASN	CB-CA-C	-6.34	98.81	109.65
1	A	282	ILE	CA-C-O	-6.31	114.05	121.05
1	A	217	CYS	N-CA-C	6.25	119.53	110.28
1	A	1	ASP	CA-CB-CG	6.22	118.82	112.60
2	D	28	ILE	O-C-N	6.14	128.29	121.90
1	A	219	VAL	CB-CA-C	-6.14	103.01	110.99
2	D	236	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	205	GLU	N-CA-C	-6.12	104.55	112.68
1	A	128	ASN	N-CA-CB	-6.11	102.62	111.91
1	A	219	VAL	N-CA-CB	6.11	119.60	111.90
2	D	87	ASN	OD1-CG-ND2	-6.10	116.50	122.60
2	D	28	ILE	CA-C-N	6.09	128.81	120.46
2	D	28	ILE	C-N-CA	6.09	128.81	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74	ASN	CA-CB-CG	6.07	118.67	112.60
2	D	63	TYR	CA-C-O	6.04	127.97	120.54
1	A	95	ARG	CA-CB-CG	6.01	126.13	114.10
2	D	81	LEU	O-C-N	-5.98	116.21	123.27
1	A	59	GLN	OE1-CD-NE2	-5.96	116.64	122.60
2	D	201	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	231	ALA	N-CA-C	5.96	117.44	111.07
2	D	159	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	5	THR	CA-C-N	5.93	130.62	120.72
1	A	5	THR	C-N-CA	5.93	130.62	120.72
1	A	335	ARG	CA-CB-CG	5.92	125.93	114.10
1	A	252	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	34	ILE	CB-CA-C	-5.91	102.40	110.90
2	D	191	THR	N-CA-C	-5.90	104.93	111.36
1	A	97	ALA	N-CA-C	-5.89	102.35	109.72
2	D	35	VAL	CB-CA-C	-5.89	101.43	110.50
2	D	213	ARG	N-CA-C	5.88	119.15	109.85
2	D	208	ASN	CA-C-O	5.87	126.67	120.33
1	A	263	GLN	CA-C-N	5.87	125.49	119.56
1	A	263	GLN	C-N-CA	5.87	125.49	119.56
1	A	233	SER	CA-C-O	5.87	128.90	120.51
2	D	178	SER	N-CA-C	5.82	118.40	111.71
1	A	257	CYS	O-C-N	-5.82	116.25	120.27
1	A	254	ARG	N-CA-CB	-5.81	100.68	110.49
1	A	113	LYS	CA-CB-CG	5.80	125.71	114.10
2	D	236	GLN	N-CA-C	-5.79	104.88	111.07
1	A	161	HIS	CB-CG-CD2	-5.76	123.71	131.20
2	D	201	ASP	N-CA-C	-5.75	99.36	108.73
2	D	53	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	335	ARG	N-CA-C	5.73	123.00	110.80
1	A	135	ALA	O-C-N	-5.70	116.68	123.06
2	D	69	GLU	CB-CG-CD	5.69	122.27	112.60
2	D	14	THR	CA-C-O	-5.68	114.85	120.70
1	A	185	LEU	N-CA-C	5.68	118.41	111.82
1	A	263	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	D	87	ASN	CA-CB-CG	5.67	118.27	112.60
2	D	196	ILE	CA-C-N	5.66	125.64	120.21
2	D	196	ILE	C-N-CA	5.66	125.64	120.21
2	D	140	ALA	CA-C-O	-5.64	114.86	120.90
2	D	38	GLN	OE1-CD-NE2	-5.64	116.96	122.60
2	D	195	LEU	CD1-CG-CD2	-5.62	98.42	110.80
1	A	262	PHE	CA-CB-CG	-5.61	108.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	258	THR	CA-C-O	-5.61	114.27	120.38
2	D	161	ASN	CB-CG-ND2	5.52	124.68	116.40
1	A	275	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	44	MET	N-CA-C	-5.49	102.40	110.52
2	D	75	SER	CA-C-N	5.48	129.00	121.33
2	D	75	SER	C-N-CA	5.48	129.00	121.33
1	A	349	LEU	CA-C-N	5.48	127.62	120.28
1	A	349	LEU	C-N-CA	5.48	127.62	120.28
1	A	137	GLN	CA-C-O	-5.47	115.26	121.00
1	A	31	PHE	CA-CB-CG	5.44	119.24	113.80
1	A	200	PHE	CA-C-O	5.44	127.80	121.11
1	A	312	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	A	226	GLU	N-CA-C	-5.42	107.31	114.04
2	D	114	ALA	N-CA-C	-5.42	102.46	110.48
1	A	116	ARG	N-CA-C	-5.41	105.38	111.28
2	D	195	LEU	N-CA-C	5.41	119.99	112.90
2	D	18	ASN	N-CA-C	-5.40	102.29	110.28
2	D	252	HIS	CA-C-O	-5.39	115.13	121.44
2	D	93	ASP	CA-CB-CG	-5.38	107.22	112.60
1	A	237	GLU	N-CA-C	5.38	117.23	110.24
2	D	155	GLN	CA-C-O	-5.37	114.86	120.55
1	A	257	CYS	N-CA-CB	-5.37	105.29	110.39
1	A	91	TYR	N-CA-C	5.33	118.94	112.23
1	A	77	THR	N-CA-CB	-5.32	102.70	110.47
1	A	349	LEU	O-C-N	5.32	129.41	122.87
2	D	27	ARG	CA-CB-CG	5.31	124.72	114.10
1	A	251	GLY	O-C-N	5.30	129.59	122.70
1	A	332	PRO	CA-C-N	5.28	124.60	118.85
1	A	332	PRO	C-N-CA	5.28	124.60	118.85
1	A	79	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	A	62	ARG	CA-CB-CG	5.25	124.60	114.10
2	D	120	SER	O-C-N	-5.22	116.44	123.23
1	A	274	ILE	N-CA-CB	-5.21	102.64	111.23
2	D	234	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	252	ASN	CB-CG-ND2	5.20	124.20	116.40
2	D	206	SER	N-CA-C	5.20	121.87	110.80
1	A	101	HIS	CA-C-O	-5.18	114.88	119.86
1	A	356	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	D	194	TRP	CG-CD1-NE1	-5.18	103.47	110.20
1	A	22	ALA	N-CA-C	-5.17	102.40	110.10
1	A	40	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	34	ILE	CA-CB-CG1	5.16	119.16	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	LYS	CB-CG-CD	-5.14	99.47	111.30
1	A	248	ILE	N-CA-CB	-5.14	103.46	110.56
1	A	360	GLN	CB-CG-CD	5.14	121.34	112.60
1	A	71	ILE	N-CA-CB	-5.12	105.95	112.15
2	D	10	THR	N-CA-CB	-5.12	104.13	111.91
2	D	154	VAL	N-CA-C	-5.12	105.40	110.62
2	D	213	ARG	CG-CD-NE	-5.11	100.75	112.00
1	A	233	SER	O-C-N	5.11	129.38	122.59
1	A	217	CYS	CA-CB-SG	-5.09	102.68	114.40
1	A	149	THR	CA-CB-OG1	-5.08	101.98	109.60
2	D	58	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	27	ARG	CB-CG-CD	-5.08	99.62	111.30
1	A	227	MET	N-CA-C	-5.05	105.69	111.14
2	D	73	ARG	CA-CB-CG	5.04	124.18	114.10
1	A	88	HIS	CB-CG-CD2	-5.03	124.67	131.20
2	D	243	ASN	N-CA-C	-5.03	105.88	111.36
2	D	220	LEU	N-CA-CB	-5.02	102.72	110.20
2	D	26	VAL	N-CA-C	5.02	115.74	110.62
1	A	371	HIS	CB-CG-CD2	-5.01	124.68	131.20
2	D	13	GLU	O-C-N	5.01	127.43	122.12
2	D	159	HIS	CB-CG-CD2	-5.01	124.69	131.20
1	A	359	LYS	CB-CG-CD	5.00	122.81	111.30
2	D	13	GLU	CB-CA-C	-5.00	102.48	110.79
1	A	266	PHE	CA-CB-CG	5.00	118.80	113.80

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	61	0
2	D	2034	0	1969	24	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	79	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 (79) 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
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:190:MET:HE1	1:A:206:ARG:HA	1.83	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
1:A:299:MET:HE2	1:A:331:ALA:HB2	1.88	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:217:CYS:C	1:A:218:TYR:HD1	2.22	0.47
2:D:208:ASN:C	2:D:209:CYS:SG	2.98	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: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
1:A:253:GLU:H	1:A:253:GLU:CD	2.25	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
1:A:47:MET:HB2	1:A:47:MET:HE2	1.79	0.44
2:D:196:ILE:HG21	2:D:212:ASP:O	2.17	0.44
1:A:39:ARG:HH21	2:D:53:ASP:CG	2.26	0.43
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
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:222:ASP:OD1	1:A:224:GLU:HB3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

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	370/373 (99%)	335 (90%)	29 (8%)	6 (2%)	7	27
2	D	254/260 (98%)	238 (94%)	16 (6%)	0	100	100
All	All	624/633 (99%)	573 (92%)	45 (7%)	6 (1%)	12	38

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%)	263 (84%)	51 (16%)	2	8
2	D	227/228 (100%)	205 (90%)	22 (10%)	8	25
All	All	541/542 (100%)	468 (86%)	73 (14%)	4	13

All (73) 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	65	LEU
1	A	66	THR
1	A	67	LEU
1	A	72	GLU
1	A	80	ASP
1	A	99	GLU
1	A	100	GLU
1	A	109	PRO
1	A	145	SER
1	A	153	LEU
1	A	159	VAL
1	A	180	LEU
1	A	196	ARG
1	A	199	SER
1	A	201	VAL
1	A	206	ARG
1	A	221	LEU
1	A	223	PHE
1	A	229	THR
1	A	238	LYS
1	A	239	SER
1	A	242	LEU
1	A	246	GLN

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Mol	Chain	Res	Type
1	A	253	GLU
1	A	263	GLN
1	A	274	ILE
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	305	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	353	GLN
1	A	354	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	94	THR
2	D	108	SER
2	D	112	GLU
2	D	121	HIS
2	D	125	VAL
2	D	139	ASP
2	D	152	LEU
2	D	156	GLN
2	D	195	LEU

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Mol	Chain	Res	Type
2	D	206	SER
2	D	221	LEU
2	D	244	GLU
2	D	255	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	41	GLN
1	A	78	ASN
1	A	137	GLN
1	A	263	GLN
1	A	354	GLN
2	D	38	GLN
2	D	57	GLN
2	D	96	GLN
2	D	134	HIS
2	D	159	HIS
2	D	161	ASN
2	D	236	GLN

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	1.33	1 (10%)	9,14,16	6.01	5 (55%)

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	-2.70	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-12.84	107.75	112.66
1	A	73	HIC	CD2-NE2-CE1	11.49	111.25	106.71
1	A	73	HIC	CZ-NE2-CE1	-3.10	119.40	126.71
1	A	73	HIC	CA-CB-CG	-2.80	106.86	113.77
1	A	73	HIC	CZ-NE2-CD2	2.52	129.35	126.03

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 ⓘ

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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:

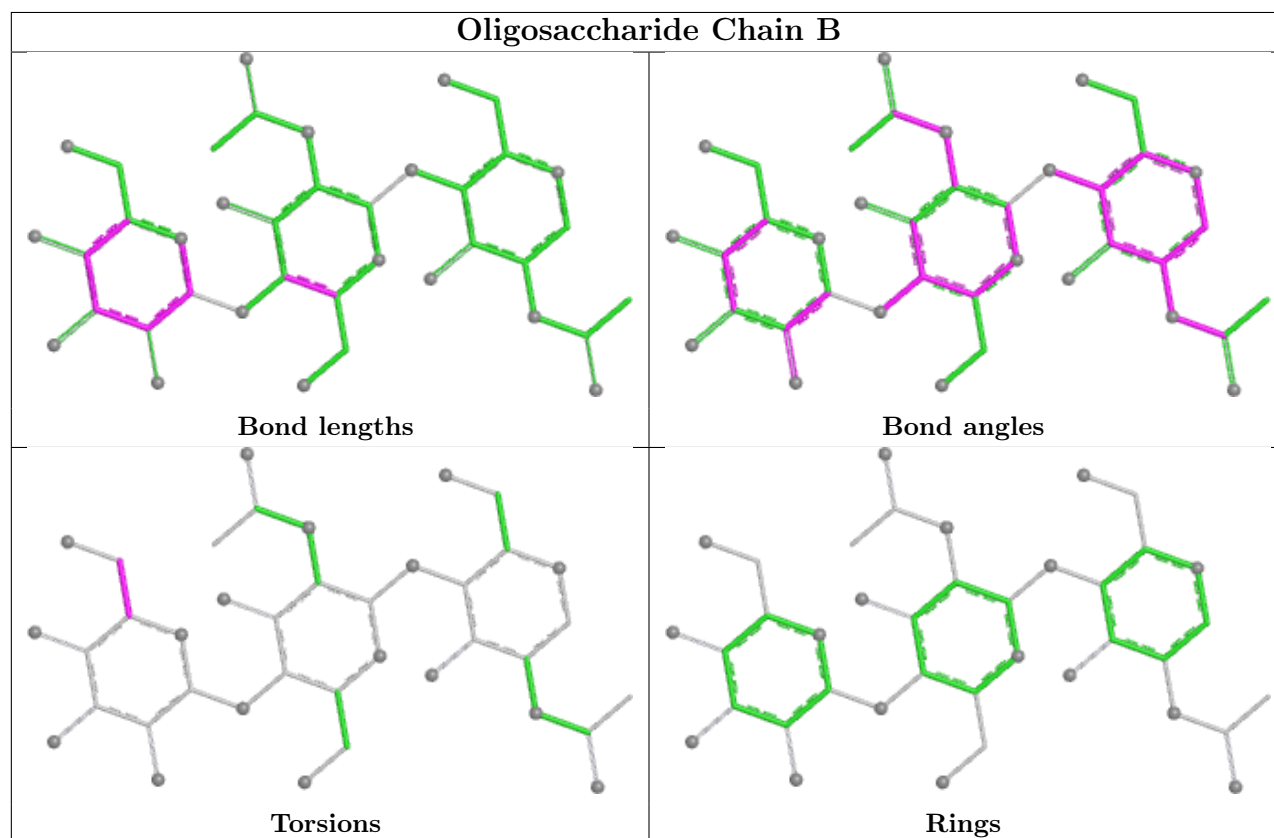
Mol	Chain	Res	Type	Atoms
3	B	3	BMA	C4-C5-C6-O6
3	B	3	BMA	O5-C5-C6-O6

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	32,33,33	1.15	2 (6%)	48,52,52	1.13	4 (8%)

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	-	2/22/38/38	0/3/3/3

All (2) 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

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	375	ATP	O4'-C1'-N9	2.43	112.75	108.09
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:

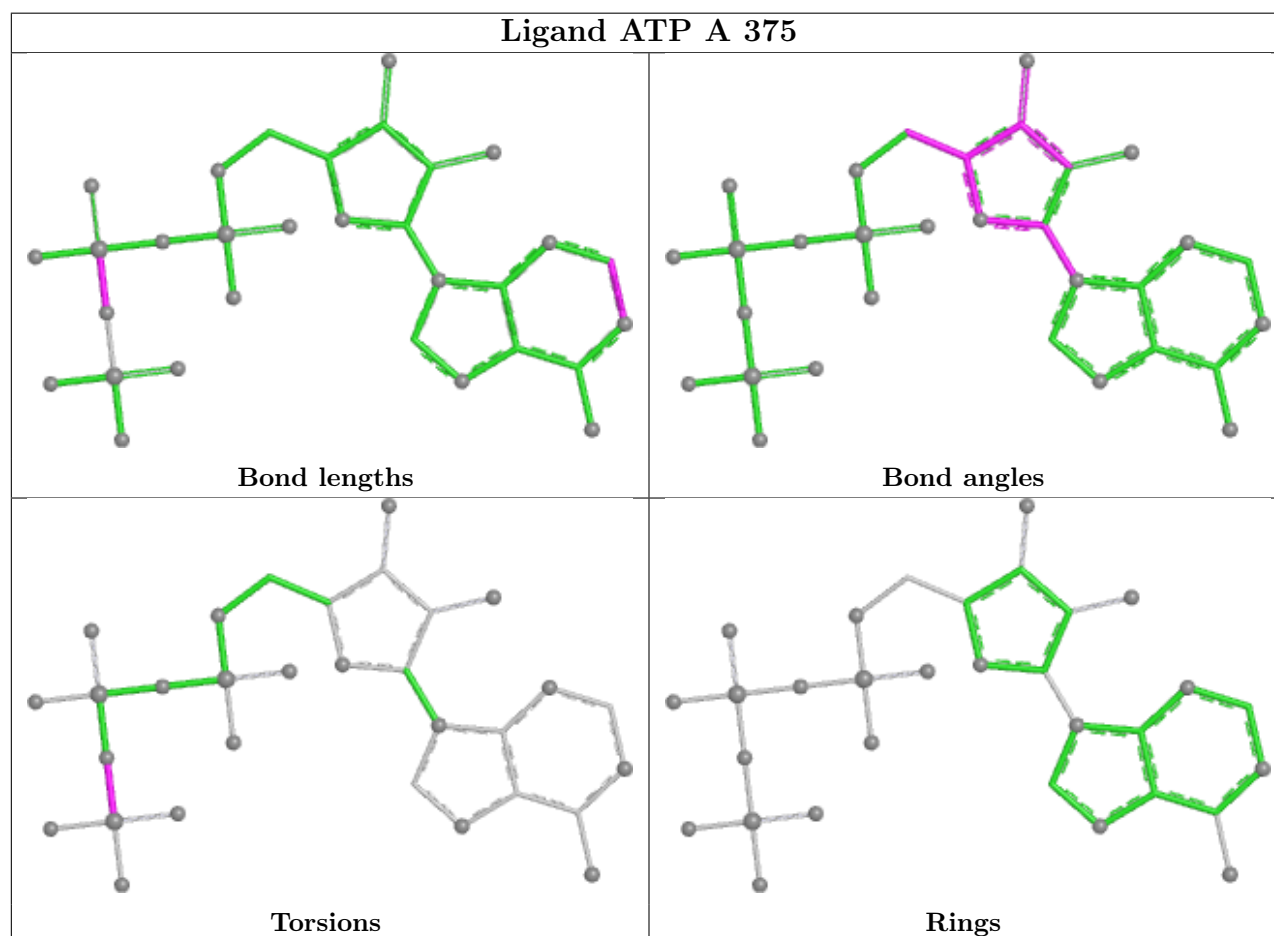
Mol	Chain	Res	Type	Atoms
5	A	375	ATP	PB-O3B-PG-O2G
5	A	375	ATP	PB-O3B-PG-O3G

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 [i](#)

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.