



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:31 PM UTC

PDB ID : 2BTF / pdb_00002btf
Title : THE STRUCTURE OF CRYSTALLINE PROFILIN-BETA-ACTIN
Authors : Schutt, C.E.; Myslik, J.C.; Rozycki, M.D.; Goonesekere, N.C.W.
Deposited on : 1994-01-18
Resolution : 2.55 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

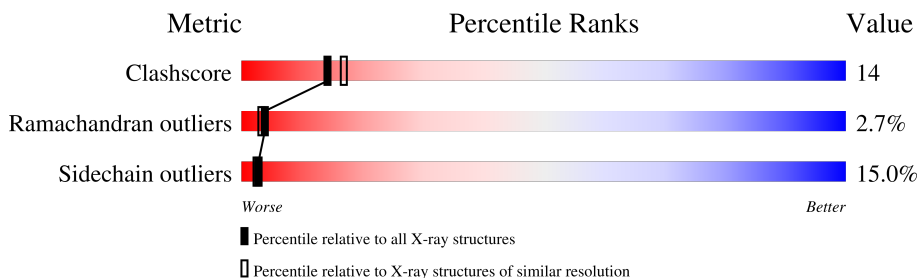
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4000 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 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			

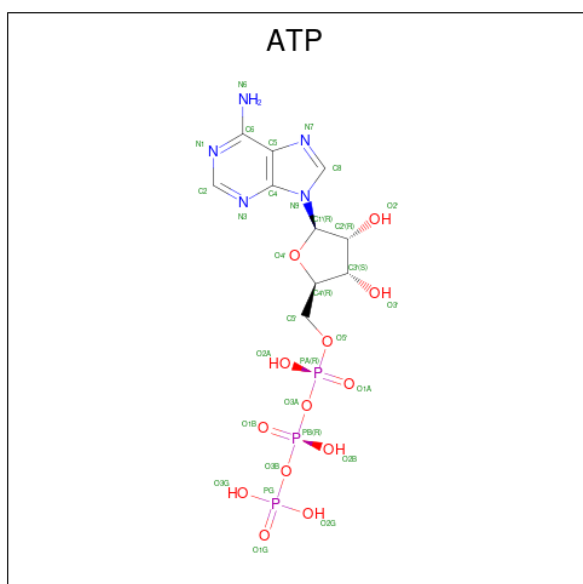
- Molecule 2 is a protein called PROFILIN.

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 STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

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



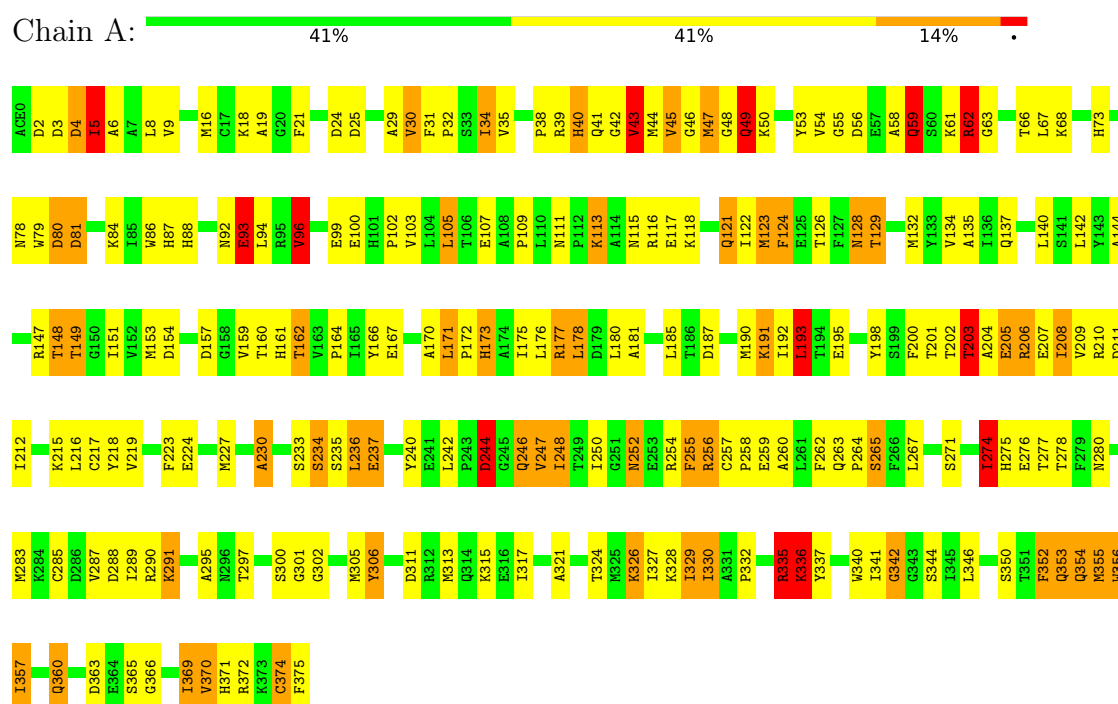
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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: 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	38.95Å 71.30Å 171.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.55	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4000	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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, ACE, SR, 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	1.28	14/2969 (0.5%)	2.29	169/4019 (4.2%)
2	P	1.36	9/1063 (0.8%)	2.34	65/1435 (4.5%)
All	All	1.30	23/4032 (0.6%)	2.30	234/5454 (4.3%)

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	P	0	2
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	7	ILE	CA-CB	7.43	1.63	1.54
1	A	192	ILE	CA-CB	7.03	1.64	1.54
1	A	88	HIS	CD2-NE2	-6.91	1.30	1.37
1	A	40	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	87	HIS	CD2-NE2	-6.54	1.30	1.37
2	P	119	HIS	CG-ND1	-6.46	1.31	1.38
2	P	119	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	371	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	161	HIS	CD2-NE2	-6.10	1.31	1.37
2	P	42	ILE	CA-CB	5.97	1.60	1.54
1	A	275	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	201	THR	CA-CB	5.78	1.63	1.53
2	P	31	TRP	CA-CB	-5.65	1.44	1.53
1	A	203	THR	CA-CB	5.63	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	133	HIS	CD2-NE2	-5.56	1.31	1.37
2	P	16	CYS	CA-CB	-5.55	1.44	1.53
1	A	122	ILE	CA-CB	5.52	1.60	1.54
1	A	129	THR	CA-CB	5.39	1.62	1.52
1	A	173	HIS	CD2-NE2	-5.34	1.31	1.37
2	P	22	VAL	CA-CB	5.13	1.61	1.54
2	P	105	THR	CA-CB	5.13	1.62	1.53
1	A	161	HIS	CG-ND1	-5.05	1.32	1.38
1	A	276	GLU	CA-CB	-5.03	1.45	1.53

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	58	PHE	CA-CB-CG	12.76	126.56	113.80
1	A	375	PHE	CA-CB-CG	-11.87	101.93	113.80
1	A	244	ASP	CA-CB-CG	10.98	123.58	112.60
2	P	13	ASP	CA-CB-CG	10.89	123.49	112.60
2	P	47	VAL	N-CA-C	-9.80	100.82	110.72
2	P	51	VAL	N-CA-CB	-9.60	95.39	111.23
2	P	9	ASN	CB-CA-C	-9.42	96.45	110.96
1	A	288	ASP	CA-CB-CG	9.26	121.86	112.60
1	A	204	ALA	N-CA-C	-9.11	101.04	110.97
1	A	370	VAL	CB-CA-C	-9.09	98.07	112.16
1	A	237	GLU	CB-CG-CD	8.97	127.86	112.60
1	A	356	TRP	CB-CG-CD1	-8.48	114.17	126.90
1	A	4	ASP	N-CA-C	-8.47	92.00	107.75
1	A	5	ILE	O-C-N	8.45	133.13	122.57
1	A	5	ILE	CA-C-O	8.36	131.23	120.78
2	P	61	ASN	N-CA-C	8.36	121.51	111.82
2	P	13	ASP	N-CA-C	8.34	123.27	112.26
1	A	230	ALA	N-CA-C	-8.32	93.07	110.80
1	A	59	GLN	N-CA-C	-8.27	101.31	111.40
1	A	81	ASP	CA-CB-CG	-8.21	104.39	112.60
1	A	24	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	277	THR	CA-C-O	-8.13	112.33	120.70
1	A	353	GLN	OE1-CD-NE2	-8.11	114.49	122.60
1	A	335	ARG	N-CA-C	8.03	122.65	113.01
1	A	115	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	A	356	TRP	CG-CD2-CE3	7.99	141.89	133.90
1	A	374	CYS	CA-C-N	7.98	136.06	121.70
1	A	374	CYS	C-N-CA	7.98	136.06	121.70
2	P	135	ARG	CA-CB-CG	7.86	129.82	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	MET	CA-CB-CG	7.82	129.74	114.10
1	A	326	LYS	N-CA-C	-7.78	97.34	109.25
2	P	82	GLU	CA-CB-CG	-7.75	98.60	114.10
2	P	49	ILE	N-CA-C	-7.72	103.16	110.42
2	P	16	CYS	CA-CB-SG	-7.70	96.69	114.40
1	A	45	VAL	CA-C-O	7.68	130.38	120.78
1	A	353	GLN	CB-CG-CD	7.63	125.57	112.60
1	A	202	THR	N-CA-C	7.55	122.86	107.69
1	A	200	PHE	CA-CB-CG	-7.50	106.30	113.80
1	A	80	ASP	CA-CB-CG	7.48	120.08	112.60
1	A	99	GLU	N-CA-C	7.48	122.05	113.15
1	A	4	ASP	O-C-N	7.44	132.03	122.87
2	P	85	MET	N-CA-C	-7.42	96.85	109.24
1	A	375	PHE	N-CA-C	7.39	131.71	111.00
1	A	336	LYS	N-CA-C	-7.37	103.27	111.82
1	A	157	ASP	CA-CB-CG	7.29	119.89	112.60
2	P	86	ASP	CA-CB-CG	7.29	119.89	112.60
2	P	102	VAL	N-CA-C	-7.15	97.80	108.46
2	P	21	ILE	N-CA-C	-6.99	98.05	108.46
2	P	18	ASP	CA-CB-CG	6.95	119.55	112.60
1	A	56	ASP	N-CA-C	6.94	120.97	112.23
1	A	173	HIS	CB-CG-CD2	-6.92	122.20	131.20
1	A	161	HIS	CB-CG-CD2	-6.91	122.21	131.20
1	A	115	ASN	CB-CG-ND2	6.91	126.76	116.40
1	A	255	PHE	CA-CB-CG	6.88	120.69	113.80
2	P	88	ARG	CA-C-N	6.88	131.26	121.42
2	P	88	ARG	C-N-CA	6.88	131.26	121.42
1	A	356	TRP	CG-CD1-NE1	-6.87	101.27	110.20
2	P	134	LEU	N-CA-C	-6.76	103.69	112.68
1	A	262	PHE	CA-CB-CG	-6.76	107.04	113.80
1	A	356	TRP	CD1-CG-CD2	6.75	117.10	106.30
1	A	263	GLN	O-C-N	-6.72	115.20	121.32
1	A	277	THR	CA-CB-OG1	-6.69	99.57	109.60
2	P	27	SER	N-CA-C	-6.67	99.97	109.24
2	P	8	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	235	SER	N-CA-C	6.65	121.41	113.16
1	A	5	ILE	CA-CB-CG1	-6.64	99.11	110.40
1	A	117	GLU	CA-C-O	-6.63	113.87	120.70
1	A	49	GLN	CA-C-N	6.60	132.91	123.14
1	A	49	GLN	C-N-CA	6.60	132.91	123.14
2	P	9	ASN	N-CA-CB	6.54	119.46	109.91
2	P	133	HIS	CB-CG-CD2	-6.53	122.71	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ILE	N-CA-C	-6.52	98.35	107.80
2	P	51	VAL	CB-CA-C	6.49	121.93	111.29
1	A	147	ARG	CB-CG-CD	-6.46	96.43	111.30
1	A	62	ARG	CA-CB-CG	6.42	126.95	114.10
1	A	148	THR	N-CA-CB	-6.42	102.46	111.00
1	A	315	LYS	CA-CB-CG	6.40	126.90	114.10
1	A	111	ASN	OD1-CG-ND2	-6.40	116.20	122.60
2	P	104	MET	CA-CB-CG	6.40	126.89	114.10
1	A	24	ASP	CA-C-O	6.39	128.83	121.28
1	A	67	LEU	N-CA-C	6.38	119.12	108.73
1	A	58	ALA	N-CA-C	-6.37	105.26	114.12
1	A	59	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	A	96	VAL	N-CA-CB	-6.37	104.39	112.60
1	A	181	ALA	CA-C-O	-6.36	114.38	121.05
1	A	275	HIS	CB-CG-CD2	-6.35	122.95	131.20
1	A	356	TRP	CE2-CD2-CG	-6.34	99.60	107.20
1	A	86	TRP	CG-CD2-CE3	6.28	140.18	133.90
1	A	252	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	190	MET	CA-CB-CG	6.25	126.60	114.10
1	A	217	CYS	CA-CB-SG	-6.22	100.10	114.40
1	A	265	SER	N-CA-C	-6.22	104.61	111.82
1	A	224	GLU	CA-CB-CG	6.20	126.49	114.10
1	A	311	ASP	CB-CA-C	-6.20	100.51	110.79
2	P	129	GLU	CB-CG-CD	6.18	123.11	112.60
1	A	2	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	301	GLY	CA-C-O	-6.16	116.47	121.77
2	P	89	THR	CA-C-O	-6.15	114.03	121.05
1	A	56	ASP	CA-CB-CG	6.14	118.75	112.60
1	A	280	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	87	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	206	ARG	CA-C-O	6.09	126.97	119.79
1	A	302	GLY	O-C-N	-6.09	116.35	122.19
2	P	101	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	142	LEU	N-CA-C	6.07	117.56	111.07
2	P	26	ASP	O-C-N	-6.07	114.52	122.59
2	P	89	THR	N-CA-CB	-6.05	100.93	110.06
1	A	202	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	340	TRP	CD2-CE2-CZ2	-6.03	116.37	122.40
1	A	337	TYR	N-CA-C	6.00	120.30	112.92
1	A	192	ILE	CA-CB-CG1	5.99	120.59	110.40
1	A	277	THR	CA-CB-CG2	5.96	120.62	110.50
2	P	42	ILE	CA-CB-CG1	-5.95	100.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	SER	CA-C-N	5.94	128.16	120.56
1	A	344	SER	C-N-CA	5.94	128.16	120.56
1	A	187	ASP	N-CA-C	5.93	117.74	111.28
2	P	124	ASN	OD1-CG-ND2	-5.92	116.67	122.60
1	A	25	ASP	O-C-N	-5.91	115.71	122.09
1	A	191	LYS	CA-C-O	-5.91	114.61	120.70
1	A	371	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	A	274	ILE	N-CA-CB	-5.89	101.51	111.23
1	A	363	ASP	O-C-N	5.89	128.14	122.07
2	P	105	THR	N-CA-C	-5.85	99.85	109.80
1	A	53	TYR	N-CA-C	-5.85	100.75	110.17
2	P	66	GLY	O-C-N	-5.84	116.07	122.90
1	A	247	VAL	N-CA-C	5.83	117.83	108.85
1	A	102	PRO	CB-CA-C	5.83	118.61	110.98
1	A	254	ARG	CB-CG-CD	-5.81	97.93	111.30
1	A	256	ARG	CA-CB-CG	5.81	125.72	114.10
2	P	61	ASN	CB-CG-ND2	-5.80	107.69	116.40
2	P	12	ALA	N-CA-C	5.80	118.34	111.33
1	A	274	ILE	CA-CB-CG1	-5.78	100.57	110.40
2	P	67	GLY	CA-C-N	5.78	129.57	121.02
2	P	67	GLY	C-N-CA	5.78	129.57	121.02
2	P	25	LYS	CA-C-O	-5.77	114.83	121.47
1	A	370	VAL	N-CA-CB	5.76	120.50	110.65
2	P	42	ILE	CA-CB-CG2	5.76	120.29	110.50
1	A	31	PHE	CA-C-N	5.76	126.09	119.93
1	A	31	PHE	C-N-CA	5.76	126.09	119.93
2	P	66	GLY	N-CA-C	-5.75	101.18	110.95
1	A	121	GLN	CG-CD-NE2	-5.74	107.79	116.40
1	A	235	SER	N-CA-CB	-5.73	101.68	110.44
1	A	248	ILE	N-CA-C	-5.71	100.06	108.85
1	A	129	THR	CA-CB-OG1	5.68	118.12	109.60
2	P	47	VAL	CA-C-N	5.67	126.28	119.98
2	P	47	VAL	C-N-CA	5.67	126.28	119.98
1	A	124	PHE	N-CA-C	5.67	118.32	111.40
2	P	79	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	352	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	171	LEU	CA-C-N	5.64	125.75	119.32
1	A	171	LEU	C-N-CA	5.64	125.75	119.32
1	A	30	VAL	O-C-N	-5.63	117.26	123.18
1	A	113	LYS	CB-CA-C	-5.63	101.50	110.84
1	A	192	ILE	CA-CB-CG2	-5.61	100.97	110.50
1	A	105	LEU	CA-C-O	-5.58	114.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	51	VAL	CA-C-N	5.57	125.63	120.34
2	P	51	VAL	C-N-CA	5.57	125.63	120.34
1	A	42	GLY	CA-C-N	5.56	131.98	121.97
1	A	42	GLY	C-N-CA	5.56	131.98	121.97
1	A	126	THR	CA-C-O	-5.56	114.07	120.24
1	A	42	GLY	O-C-N	5.55	129.91	122.70
2	P	65	LEU	N-CA-C	-5.54	98.21	107.80
1	A	354	GLN	N-CA-C	-5.54	96.22	107.41
1	A	123	MET	CA-C-O	-5.54	114.97	120.90
1	A	278	THR	O-C-N	-5.50	116.37	122.09
2	P	49	ILE	O-C-N	-5.50	116.06	121.94
2	P	70	CYS	CA-C-O	-5.48	113.54	120.28
1	A	116	ARG	CG-CD-NE	5.44	123.97	112.00
1	A	147	ARG	N-CA-CB	-5.43	102.59	111.66
1	A	176	LEU	CD1-CG-CD2	-5.42	98.89	110.80
1	A	205	GLU	CA-CB-CG	5.41	124.92	114.10
2	P	89	THR	CA-CB-OG1	-5.41	101.49	109.60
1	A	147	ARG	CA-CB-CG	5.41	124.91	114.10
1	A	237	GLU	CA-CB-CG	5.40	124.89	114.10
2	P	95	ALA	O-C-N	-5.38	115.52	121.66
1	A	115	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	47	MET	CA-CB-CG	5.37	124.83	114.10
1	A	360	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	31	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	40	HIS	N-CA-CB	5.34	119.51	110.49
1	A	129	THR	CA-C-N	5.33	124.96	119.05
1	A	129	THR	C-N-CA	5.33	124.96	119.05
1	A	372	ARG	N-CA-C	-5.27	104.44	112.04
2	P	4	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	92	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	195	GLU	N-CA-C	-5.24	105.74	111.82
2	P	43	THR	CA-C-N	5.23	124.86	119.05
2	P	43	THR	C-N-CA	5.23	124.86	119.05
1	A	300	SER	CA-C-O	-5.23	115.49	121.40
1	A	39	ARG	CA-C-N	5.22	131.51	121.54
1	A	39	ARG	C-N-CA	5.22	131.51	121.54
1	A	137	GLN	N-CA-C	5.21	117.04	111.36
1	A	48	GLY	CA-C-O	-5.21	116.14	122.75
1	A	86	TRP	CE2-CD2-CG	-5.20	100.97	107.20
1	A	40	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	366	GLY	CA-C-N	5.19	124.80	119.56
1	A	366	GLY	C-N-CA	5.19	124.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	49	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	49	GLN	CG-CD-NE2	5.17	124.16	116.40
1	A	329	ILE	CA-C-O	-5.17	114.45	121.02
1	A	193	LEU	CA-C-N	5.15	128.14	120.31
1	A	193	LEU	C-N-CA	5.15	128.14	120.31
1	A	43	VAL	CA-CB-CG2	-5.14	101.66	110.40
1	A	274	ILE	CA-CB-CG2	5.13	119.22	110.50
1	A	128	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	88	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	111	ASN	CA-CB-CG	5.12	117.72	112.60
2	P	138	GLN	O-C-N	5.12	129.16	122.86
1	A	274	ILE	N-CA-C	5.11	119.98	109.34
1	A	6	ALA	N-CA-C	-5.11	99.92	110.80
1	A	53	TYR	CB-CA-C	5.10	118.12	109.50
1	A	329	ILE	N-CA-C	-5.10	101.12	108.87
1	A	132	MET	CG-SD-CE	-5.09	89.70	100.90
2	P	115	LYS	N-CA-C	-5.09	103.96	110.53
1	A	86	TRP	CB-CG-CD1	-5.09	119.27	126.90
1	A	306	TYR	CA-C-O	-5.08	114.97	119.75
2	P	38	THR	N-CA-C	5.08	117.60	111.40
1	A	162	THR	CB-CA-C	5.08	118.50	109.72
1	A	93	GLU	CB-CG-CD	5.06	121.20	112.60
2	P	101	THR	CA-CB-CG2	5.06	119.10	110.50
1	A	342	GLY	CA-C-N	5.06	125.45	119.94
1	A	342	GLY	C-N-CA	5.06	125.45	119.94
2	P	125	LYS	CA-C-O	-5.06	115.51	121.07
2	P	97	THR	CA-CB-OG1	5.05	117.17	109.60
2	P	23	GLY	O-C-N	-5.04	116.15	122.70
2	P	5	ALA	CA-C-N	5.04	127.29	120.44
2	P	5	ALA	C-N-CA	5.04	127.29	120.44
1	A	3	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	9	VAL	O-C-N	-5.02	117.23	122.95
1	A	30	VAL	CA-C-O	-5.01	115.17	120.48
1	A	337	TYR	N-CA-CB	-5.01	103.25	110.56
2	P	68	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	P	24	TYR	N-CA-C	-5.01	107.14	113.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ASP	Mainchain
2	P	139	TYR	Sidechain
2	P	6	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	92	0
2	P	1047	0	1050	24	0
3	A	1	0	0	0	0
4	A	31	0	12	1	0
All	All	4000	0	3946	113	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 14.

All (113) 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:43:VAL:HG21	1:A:49:GLN:HA	1.46	0.95
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.68	0.75
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.69	0.74
1:A:160:THR:HG21	1:A:274:ILE:HD11	1.70	0.73
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.72	0.72
1:A:205:GLU:HA	1:A:208:ILE:HB	1.72	0.71
1:A:240:TYR:HB3	1:A:248:ILE:HD12	1.74	0.68
1:A:242:LEU:HD23	1:A:246:GLN:HB3	1.80	0.64
1:A:227:MET:HE1	1:A:252:ASN:HD22	1.63	0.63
1:A:290:ARG:NH2	2:P:60:VAL:HG13	2.15	0.61
1:A:107:GLU:HG2	1:A:134:VAL:HG12	1.83	0.61
1:A:5:ILE:HD11	1:A:100:GLU:O	2.01	0.61
2:P:132:SER:HA	2:P:135:ARG:HG2	1.81	0.60
1:A:59:GLN:O	1:A:62:ARG:HB3	2.02	0.60
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.83	0.60
1:A:63:GLY:HA2	1:A:203:THR:HG21	1.84	0.59
1:A:81:ASP:HA	1:A:84:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HA	1:A:250:ILE:O	2.02	0.59
1:A:357:ILE:HG23	1:A:369:ILE:HD13	1.83	0.59
1:A:16:MET:HE3	1:A:30:VAL:HG12	1.85	0.58
1:A:218:TYR:O	1:A:255:PHE:HA	2.04	0.58
1:A:78:ASN:OD1	1:A:81:ASP:HB2	2.05	0.57
1:A:260:ALA:HB1	1:A:267:LEU:HG	1.88	0.56
1:A:8:LEU:HD22	1:A:21:PHE:HE1	1.74	0.53
1:A:153:MET:HG2	1:A:162:THR:HG22	1.91	0.53
1:A:35:VAL:HG22	1:A:54:VAL:HG22	1.92	0.52
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.92	0.52
1:A:352:PHE:HE2	1:A:356:TRP:CZ3	2.29	0.51
2:P:65:LEU:O	2:P:68:GLN:HB3	2.09	0.51
2:P:9:ASN:HD22	2:P:130:MET:HE1	1.74	0.51
1:A:178:LEU:HD13	1:A:274:ILE:HD12	1.91	0.51
1:A:185:LEU:HD23	1:A:306:TYR:OH	2.11	0.51
1:A:178:LEU:HD13	1:A:274:ILE:CD1	2.41	0.50
1:A:252:ASN:O	1:A:256:ARG:HG3	2.12	0.50
2:P:87:LEU:HB2	2:P:100:ILE:HB	1.93	0.50
2:P:102:VAL:HG13	2:P:111:LEU:HG	1.94	0.50
2:P:21:ILE:HG23	2:P:108:THR:HG23	1.94	0.50
1:A:144:ALA:HB2	1:A:342:GLY:CA	2.42	0.50
1:A:8:LEU:HD11	1:A:96:VAL:HG11	1.93	0.49
1:A:352:PHE:CD1	1:A:355:MET:SD	3.06	0.49
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.95	0.49
1:A:44:MET:HB3	1:A:47:MET:HE3	1.95	0.48
1:A:357:ILE:HD11	1:A:374:CYS:SG	2.54	0.48
1:A:290:ARG:HH22	2:P:60:VAL:HG13	1.79	0.47
1:A:230:ALA:HA	1:A:236:LEU:HG	1.97	0.47
1:A:227:MET:HE1	1:A:252:ASN:ND2	2.30	0.47
1:A:32:PRO:O	1:A:55:GLY:HA2	2.15	0.47
1:A:244:ASP:OD1	1:A:246:GLN:HB2	2.14	0.47
1:A:8:LEU:HD22	1:A:21:PHE:CE1	2.49	0.47
1:A:171:LEU:HB3	1:A:173:HIS:CE1	2.50	0.47
1:A:306:TYR:CE1	4:A:377:ATP:H2	2.33	0.47
1:A:59:GLN:HA	1:A:59:GLN:HE21	1.80	0.46
1:A:211:ASP:O	1:A:215:LYS:HD3	2.15	0.46
1:A:332:PRO:O	1:A:335:ARG:HB3	2.15	0.46
2:P:28:PRO:HB3	2:P:47:VAL:HG11	1.98	0.46
1:A:295:ALA:O	1:A:328:LYS:HB3	2.16	0.46
1:A:321:ALA:CB	1:A:327:ILE:HD11	2.46	0.46
1:A:8:LEU:CD1	1:A:96:VAL:HG11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:O	1:A:160:THR:HA	2.16	0.45
1:A:326:LYS:NZ	1:A:328:LYS:HD2	2.31	0.45
1:A:352:PHE:HE2	1:A:356:TRP:CH2	2.34	0.45
1:A:19:ALA:HB1	1:A:94:LEU:HD11	1.99	0.45
1:A:219:VAL:HG23	1:A:306:TYR:HB3	1.99	0.45
1:A:305:MET:HE2	1:A:336:LYS:HB2	1.98	0.44
1:A:5:ILE:HD13	1:A:5:ILE:HA	1.57	0.44
1:A:283:MET:HB3	1:A:283:MET:HE3	1.75	0.44
2:P:23:GLY:O	2:P:28:PRO:HA	2.16	0.44
1:A:43:VAL:HG21	1:A:50:LYS:H	1.82	0.44
1:A:118:LYS:O	1:A:121:GLN:HB3	2.18	0.44
1:A:144:ALA:HB2	1:A:342:GLY:HA2	1.99	0.44
2:P:6:TYR:HD2	2:P:130:MET:SD	2.40	0.44
1:A:59:GLN:HE22	1:A:62:ARG:NH1	2.16	0.43
1:A:29:ALA:HB1	1:A:93:GLU:HG2	2.01	0.43
1:A:32:PRO:HB3	1:A:34:ILE:HD11	1.99	0.43
1:A:149:THR:HG23	1:A:166:TYR:HA	1.99	0.43
1:A:135:ALA:CB	1:A:140:LEU:HD11	2.49	0.43
2:P:132:SER:HA	2:P:135:ARG:CG	2.49	0.43
1:A:159:VAL:HG21	1:A:177:ARG:HD2	2.01	0.43
1:A:354:GLN:O	1:A:355:MET:HB2	2.18	0.42
2:P:64:THR:HA	2:P:68:GLN:O	2.18	0.42
1:A:59:GLN:HE22	1:A:62:ARG:HH11	1.67	0.42
1:A:109:PRO:HB3	1:A:175:ILE:HD13	2.00	0.42
2:P:3:TRP:HZ3	2:P:134:LEU:HD11	1.84	0.42
1:A:47:MET:HE2	1:A:47:MET:HB3	1.85	0.42
1:A:170:ALA:O	1:A:172:PRO:HD3	2.19	0.42
1:A:103:VAL:HG22	1:A:129:THR:HG21	2.02	0.42
1:A:124:PHE:O	1:A:128:ASN:HA	2.18	0.42
2:P:6:TYR:CD1	2:P:6:TYR:N	2.88	0.42
1:A:264:PRO:HD2	1:A:271:SER:O	2.20	0.42
2:P:6:TYR:O	2:P:9:ASN:HB2	2.20	0.42
1:A:113:LYS:HE3	2:P:82:GLU:OE2	2.20	0.41
1:A:287:VAL:O	1:A:291:LYS:NZ	2.53	0.41
1:A:166:TYR:CE1	1:A:167:GLU:HG2	2.55	0.41
1:A:193:LEU:O	1:A:198:TYR:CD2	2.74	0.41
2:P:22:VAL:HG22	2:P:30:VAL:HG22	2.02	0.41
1:A:45:VAL:O	1:A:45:VAL:HG12	2.19	0.41
1:A:105:LEU:HD11	1:A:123:MET:HG3	2.02	0.41
1:A:193:LEU:O	1:A:198:TYR:HD2	2.03	0.41
1:A:223:PHE:CD1	1:A:259:GLU:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:O	1:A:342:GLY:HA3	2.21	0.41
1:A:274:ILE:HD12	1:A:274:ILE:HA	1.85	0.41
2:P:105:THR:HA	2:P:135:ARG:HH21	1.85	0.41
1:A:43:VAL:HG21	1:A:49:GLN:CA	2.32	0.41
1:A:164:PRO:HG2	1:A:285:CYS:SG	2.61	0.40
1:A:297:THR:O	1:A:330:ILE:N	2.52	0.40
2:P:98:PHE:CE1	2:P:116:GLU:HB2	2.56	0.40
2:P:98:PHE:HE1	2:P:116:GLU:HB2	1.85	0.40
1:A:211:ASP:O	1:A:215:LYS:HB2	2.21	0.40
1:A:341:ILE:O	1:A:341:ILE:HG22	2.21	0.40
2:P:34:VAL:HG12	2:P:37:LYS:HG3	2.04	0.40
1:A:353:GLN:NE2	1:A:356:TRP:HE1	2.19	0.40
2:P:50:LEU:O	2:P:77:LEU:HD12	2.21	0.40
2:P:55:ARG:NE	2:P:78:LEU:HD22	2.35	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%)	328 (88%)	33 (9%)	11 (3%)	3	2
2	P	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	5	5
All	All	510/515 (99%)	454 (89%)	42 (8%)	14 (3%)	4	3

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	203	THR
1	A	233	SER
1	A	355	MET

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Mol	Chain	Res	Type
1	A	5	ILE
1	A	40	HIS
1	A	234	SER
1	A	244	ASP
2	P	137	SER
1	A	369	ILE
2	P	1	ALA
1	A	46	GLY
1	A	61	LYS
2	P	120	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/316 (100%)	270 (85%)	46 (15%)	3	2
2	P	112/112 (100%)	94 (84%)	18 (16%)	2	2
All	All	428/428 (100%)	364 (85%)	64 (15%)	3	2

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	18	LYS
1	A	34	ILE
1	A	38	PRO
1	A	41	GLN
1	A	49	GLN
1	A	59	GLN
1	A	62	ARG
1	A	66	THR
1	A	68	LYS
1	A	80	ASP
1	A	93	GLU
1	A	96	VAL

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Mol	Chain	Res	Type
1	A	148	THR
1	A	149	THR
1	A	151	ILE
1	A	177	ARG
1	A	178	LEU
1	A	180	LEU
1	A	191	LYS
1	A	193	LEU
1	A	203	THR
1	A	206	ARG
1	A	207	GLU
1	A	208	ILE
1	A	210	ARG
1	A	234	SER
1	A	236	LEU
1	A	244	ASP
1	A	246	GLN
1	A	247	VAL
1	A	265	SER
1	A	274	ILE
1	A	289	ILE
1	A	291	LYS
1	A	313	MET
1	A	324	THR
1	A	329	ILE
1	A	330	ILE
1	A	335	ARG
1	A	336	LYS
1	A	346	LEU
1	A	350	SER
1	A	360	GLN
1	A	365	SER
1	A	370	VAL
2	P	29	SER
2	P	49	ILE
2	P	51	VAL
2	P	55	ARG
2	P	64	THR
2	P	65	LEU
2	P	72	VAL
2	P	75	ASP
2	P	77	LEU

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Mol	Chain	Res	Type
2	P	90	LYS
2	P	104	MET
2	P	111	LEU
2	P	115	LYS
2	P	116	GLU
2	P	125	LYS
2	P	134	LEU
2	P	135	ARG
2	P	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	87	HIS
1	A	353	GLN
2	P	9	ASN
2	P	119	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	HIC	A	73	1	10,11,12	1.46	1 (10%)	9,14,16	4.63	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	-	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	-3.40	1.32	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-10.44	108.67	112.66
1	A	73	HIC	CD2-NE2-CE1	7.87	109.82	106.71
1	A	73	HIC	CB-CG-ND1	2.55	129.35	121.74
1	A	73	HIC	CB-CG-CD2	-2.54	123.83	129.96

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](#)

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	377	3	32,33,33	1.73	6 (18%)	48,52,52	1.44	7 (14%)

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	377	3	-	3/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	377	ATP	PA-O3A	-4.56	1.54	1.59
4	A	377	ATP	PB-O3A	-4.27	1.54	1.59
4	A	377	ATP	C8-N7	2.79	1.37	1.31
4	A	377	ATP	PG-O1G	-2.66	1.42	1.50
4	A	377	ATP	C4-N9	-2.60	1.32	1.37
4	A	377	ATP	C2-N3	-2.13	1.30	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	377	ATP	O2G-PG-O3B	3.43	116.15	104.64
4	A	377	ATP	C6-C5-N7	3.12	138.11	132.09
4	A	377	ATP	N3-C4-N9	-2.94	122.16	127.17
4	A	377	ATP	N9-C8-N7	-2.80	109.96	113.94
4	A	377	ATP	C5-C4-N9	2.79	108.85	105.81
4	A	377	ATP	C6-C5-C4	-2.64	113.57	117.18
4	A	377	ATP	C2-N1-C6	2.08	122.15	118.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

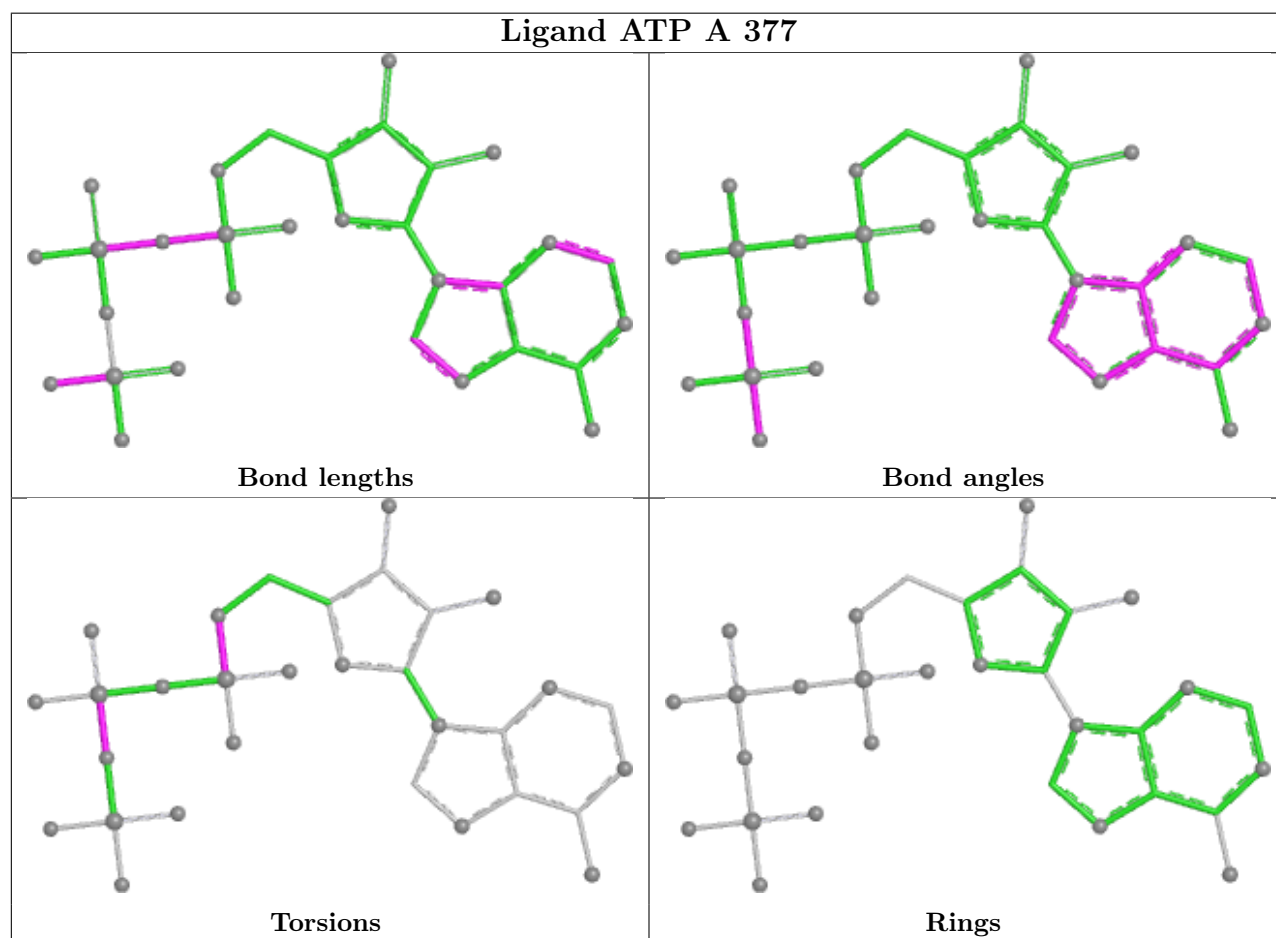
Mol	Chain	Res	Type	Atoms
4	A	377	ATP	C5'-O5'-PA-O1A
4	A	377	ATP	PG-O3B-PB-O2B
4	A	377	ATP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	377	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.