



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 04:13 AM EST

PDB ID : 2BTF  
Title : THE STRUCTURE OF CRYSTALLINE PROFILIN-BETA-ACTIN  
Authors : Schutt, C.E.; Myslik, J.C.; Rozycki, M.D.; Goonesekere, N.C.W.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

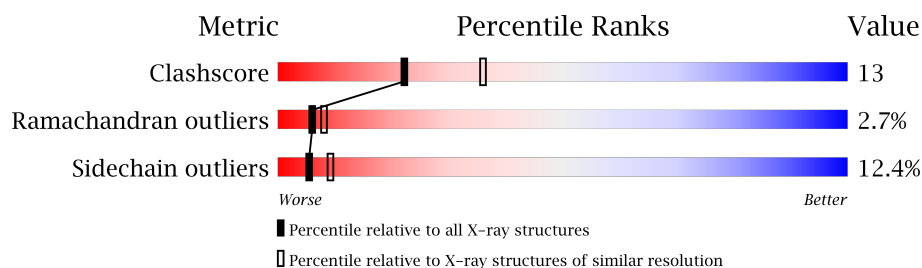
# 1 Overall quality at a glance

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	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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			

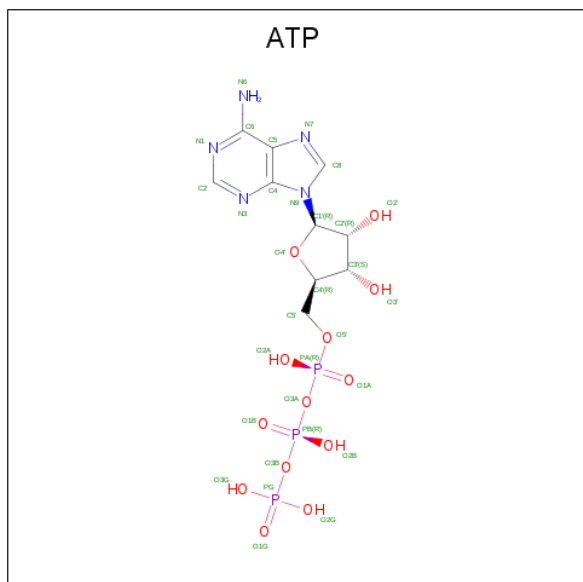
- Molecule 2 is a protein called PROFILIN.

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 (three-letter code: SR) (formula: Sr).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



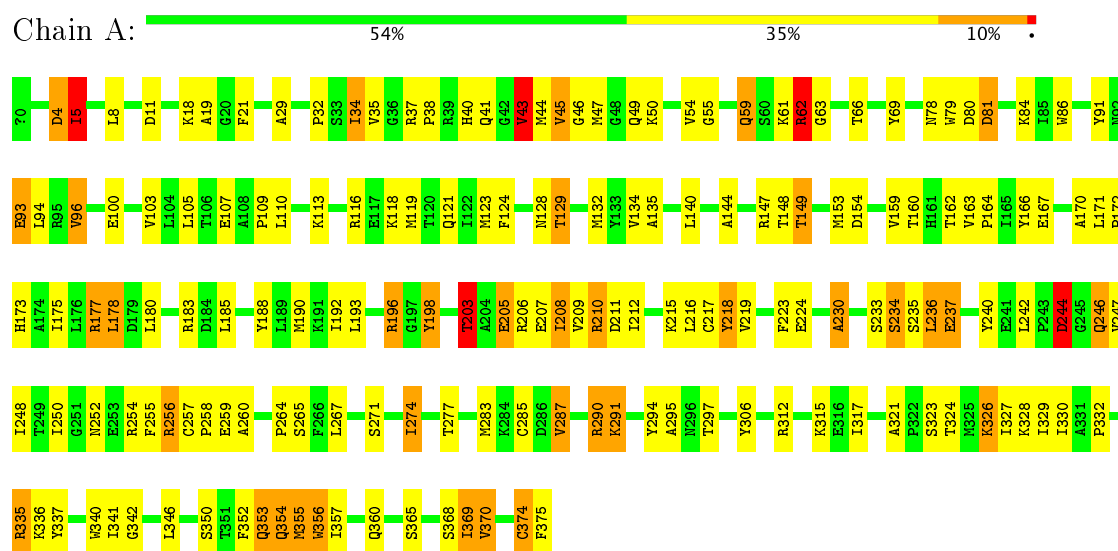
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

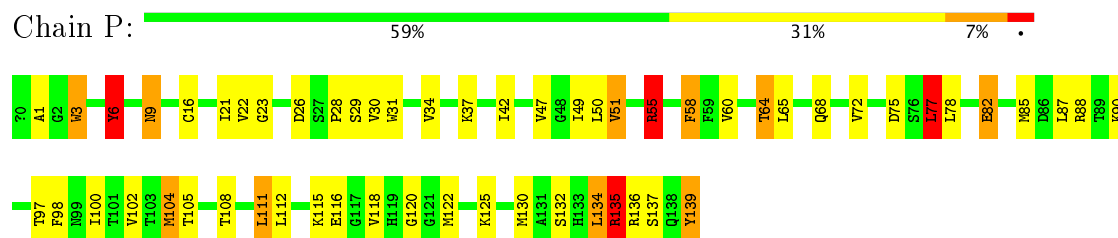
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: SR, HIC, 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	1.00	0/2969	1.94	88/4019 (2.2%)
2	P	1.01	0/1063	1.95	32/1435 (2.2%)
All	All	1.00	0/4032	1.94	120/5454 (2.2%)

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

There are no bond length outliers.

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	TRP	CD1-CG-CD2	13.50	117.10	106.30
1	A	5	ILE	CA-C-N	-11.78	91.29	117.20
1	A	210	ARG	NE-CZ-NH1	10.30	125.45	120.30
2	P	55	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	A	356	TRP	CB-CG-CD1	-9.87	114.17	127.00
1	A	290	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	132	MET	CA-CB-CG	9.67	129.74	113.30
1	A	356	TRP	CE2-CD2-CG	-9.63	99.60	107.30
2	P	16	CYS	CA-CB-SG	-9.62	96.69	114.00
2	P	55	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	62	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	79	TRP	CD1-CG-CD2	9.23	113.69	106.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	62	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	A	356	TRP	CG-CD2-CE3	8.88	141.89	133.90
1	A	356	TRP	CG-CD1-NE1	-8.83	101.27	110.10
1	A	196	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	A	4	ASP	CA-C-N	-8.68	98.10	117.20
2	P	31	TRP	CD1-CG-CD2	8.67	113.24	106.30
1	A	256	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	P	104	MET	CA-CB-CG	8.00	126.89	113.30
1	A	86	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	A	79	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	190	MET	CA-CB-CG	7.82	126.60	113.30
1	A	217	CYS	CA-CB-SG	-7.72	100.10	114.00
1	A	375	PHE	N-CA-C	7.67	131.71	111.00
1	A	340	TRP	CD1-CG-CD2	7.60	112.38	106.30
2	P	3	TRP	CD1-CG-CD2	7.55	112.34	106.30
2	P	6	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	69	TYR	CB-CG-CD2	-7.49	116.51	121.00
2	P	135	ARG	CA-CB-CG	7.46	129.82	113.40
1	A	183	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	86	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	188	TYR	CB-CG-CD2	-7.34	116.59	121.00
2	P	51	VAL	N-CA-CB	-7.32	95.39	111.50
2	P	3	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	37	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	P	31	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	4	ASP	N-CA-C	-7.04	92.00	111.00
1	A	370	VAL	CB-CA-C	-7.01	98.07	111.40
1	A	86	TRP	CG-CD2-CE3	6.98	140.18	133.90
2	P	9	ASN	CB-CA-C	-6.98	96.45	110.40
1	A	218	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	A	47	MET	CA-CB-CG	6.78	124.83	113.30
2	P	82	GLU	CA-CB-CG	-6.73	98.60	113.40
1	A	163	VAL	CG1-CB-CG2	-6.66	100.25	110.90
1	A	230	ALA	N-CA-C	-6.64	93.07	111.00
2	P	97	THR	CA-CB-CG2	-6.60	103.16	112.40
2	P	58	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	A	132	MET	CG-SD-CE	-6.56	89.70	100.20
1	A	5	ILE	O-C-N	6.52	133.13	122.70
1	A	91	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	A	5	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	A	62	ARG	CA-CB-CG	6.16	126.95	113.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	VAL	CA-CB-CG2	-6.16	101.66	110.90
1	A	315	LYS	CA-CB-CG	6.14	126.90	113.40
1	A	340	TRP	CE2-CD2-CG	-6.11	102.41	107.30
2	P	135	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	147	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	P	122	MET	CG-SD-CE	-5.96	90.66	100.20
1	A	224	GLU	CA-CB-CG	5.95	126.49	113.40
1	A	86	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	A	129	THR	CA-CB-CG2	-5.89	104.15	112.40
1	A	235	SER	N-CA-CB	-5.88	101.68	110.50
1	A	81	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	277	THR	CA-CB-CG2	5.88	120.62	112.40
1	A	147	ARG	CB-CG-CD	-5.83	96.43	111.60
1	A	4	ASP	O-C-N	5.83	132.03	122.70
1	A	116	ARG	CG-CD-NE	5.80	123.97	111.80
2	P	26	ASP	CA-C-N	5.79	129.94	117.20
1	A	374	CYS	C-N-CA	5.75	136.06	121.70
1	A	147	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	356	TRP	CD1-NE1-CE2	5.66	114.09	109.00
2	P	42	ILE	CA-CB-CG1	-5.64	100.29	111.00
1	A	218	TYR	CB-CG-CD1	5.63	124.38	121.00
1	A	256	ARG	CA-CB-CG	5.60	125.72	113.40
2	P	88	ARG	NE-CZ-NH2	5.57	123.08	120.30
2	P	51	VAL	CB-CA-C	5.54	121.93	111.40
2	P	118	VAL	CG1-CB-CG2	-5.51	102.09	110.90
1	A	274	ILE	CA-CB-CG1	-5.49	100.57	111.00
1	A	354	GLN	N-CA-C	-5.48	96.22	111.00
1	A	337	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	323	SER	N-CA-CB	-5.43	102.35	110.50
1	A	353	GLN	CB-CG-CD	5.37	125.57	111.60
1	A	254	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	356	TRP	CB-CA-C	-5.33	99.74	110.40
1	A	37	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	5	ILE	CA-C-O	5.30	131.23	120.10
2	P	77	LEU	CA-CB-CG	5.29	127.46	115.30
2	P	58	PHE	CA-CB-CG	5.28	126.56	113.90
1	A	44	MET	CG-SD-CE	-5.27	91.77	100.20
1	A	198	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	254	ARG	CB-CG-CD	-5.26	97.93	111.60
2	P	31	TRP	CG-CD1-NE1	-5.25	104.85	110.10
2	P	3	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	A	45	VAL	CA-C-N	-5.25	105.71	116.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	85	MET	N-CA-C	-5.24	96.85	111.00
1	A	205	GLU	CA-CB-CG	5.24	124.92	113.40
1	A	147	ARG	CA-CB-CG	5.23	124.91	113.40
1	A	237	GLU	CA-CB-CG	5.22	124.89	113.40
2	P	112	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	43	VAL	CA-CB-CG1	5.16	118.64	110.90
1	A	312	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	329	ILE	CG1-CB-CG2	-5.13	100.12	111.40
2	P	3	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	A	287	VAL	CG1-CB-CG2	-5.12	102.70	110.90
2	P	26	ASP	O-C-N	-5.11	114.52	122.70
1	A	119	MET	CA-CB-CG	5.10	121.97	113.30
1	A	79	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	11	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	237	GLU	CB-CG-CD	5.06	127.86	114.20
1	A	326	LYS	N-CA-C	-5.06	97.34	111.00
1	A	116	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	110	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	192	ILE	CA-CB-CG1	5.05	120.59	111.00
1	A	340	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	294	TYR	CB-CG-CD2	-5.04	117.97	121.00
2	P	72	VAL	CG1-CB-CG2	-5.03	102.86	110.90
2	P	139	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	283	MET	CA-CB-CG	-5.01	104.79	113.30

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 ⓘ

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	85	0
2	P	1047	0	1050	23	0
3	A	1	0	0	0	0
4	A	31	0	12	1	0
All	All	4000	0	3946	105	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 13.

All (105) 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: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:237:GLU:HA	1:A:250:ILE:O	2.02	0.59
1:A:81:ASP:HA	1:A:84:LYS:HG2	1.83	0.59
1:A:357:ILE:HG23	1:A:369:ILE:HD13	1.83	0.59
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:153:MET:HG2	1:A:162:THR:HG22	1.91	0.53
1:A:8:LEU:HD22	1:A:21:PHE:HE1	1.74	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:171:LEU:HB3	1:A:173:HIS:CE1	2.50	0.47
1:A:8:LEU:HD22	1:A:21:PHE:CE1	2.49	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
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:219:VAL:HG23	1:A:306:TYR:HB3	1.99	0.45
1:A:19:ALA:HB1	1:A:94:LEU:HD11	1.99	0.45
1:A:5:ILE:HA	1:A:5:ILE:HD13	1.57	0.44
2:P:23:GLY:O	2:P:28:PRO:HA	2.16	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
1:A:43:VAL:HG21	1:A:50:LYS:H	1.82	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:149:THR:HG23	1:A:166:TYR:HA	1.99	0.43
1:A:32:PRO:HB3	1:A:34:ILE:HD11	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:PRO:HB3	1:A:175:ILE:HD13	2.00	0.42
1:A:59:GLN:HE22	1:A:62:ARG:HH11	1.67	0.42
2:P:3:TRP:HZ3	2:P:134:LEU:HD11	1.84	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:287:VAL:O	1:A:291:LYS:NZ	2.53	0.41
1:A:113:LYS:HE3	2:P:82:GLU:OE2	2.20	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
1:A:140:LEU:O	1:A:342:GLY:HA3	2.21	0.41
1:A:274:ILE:HA	1:A:274:ILE:HD12	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:HG22	1:A:341:ILE:O	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 [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	372/375 (99%)	328 (88%)	33 (9%)	11 (3%)	5	6
2	P	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	8	11
All	All	510/515 (99%)	454 (89%)	42 (8%)	14 (3%)	6	8

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
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%)	279 (88%)	37 (12%)	6	11
2	P	112/112 (100%)	96 (86%)	16 (14%)	4	6
All	All	428/428 (100%)	375 (88%)	53 (12%)	5	9

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	34	ILE
1	A	38	PRO
1	A	41	GLN
1	A	59	GLN
1	A	62	ARG
1	A	66	THR
1	A	80	ASP
1	A	93	GLU
1	A	96	VAL
1	A	148	THR
1	A	149	THR
1	A	177	ARG
1	A	178	LEU
1	A	180	LEU
1	A	196	ARG
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	291	LYS
1	A	324	THR
1	A	335	ARG
1	A	336	LYS
1	A	346	LEU
1	A	350	SER
1	A	360	GLN
1	A	365	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	368	SER
1	A	370	VAL
2	P	29	SER
2	P	49	ILE
2	P	51	VAL
2	P	55	ARG
2	P	58	PHE
2	P	64	THR
2	P	75	ASP
2	P	77	LEU
2	P	90	LYS
2	P	104	MET
2	P	111	LEU
2	P	115	LYS
2	P	125	LYS
2	P	134	LEU
2	P	135	ARG
2	P	136	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	87	HIS
1	A	353	GLN
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	9,11,12	1.78	2 (22%)	7,14,16	0.94	0

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	-	0/4/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-4.09	1.32	1.38
1	A	73	HIC	CE1-ND1	-2.02	1.31	1.35

There are no bond angle outliers.

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 carbohydrates 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	27,33,33	1.16	1 (3%)	25,52,52	1.25	2 (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
4	ATP	A	377	3	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	377	ATP	PG-O1G	-2.51	1.42	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	377	ATP	N3-C2-N1	-3.48	125.82	128.86
4	A	377	ATP	C1'-N9-C4	-2.59	122.16	126.64

There are no chirality outliers.

There are no torsion outliers.

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.