



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 12:20 am BST

PDB ID : 2P9N  
Title : Crystal Structure of bovine Arp2/3 complex co-crystallized with ADP  
Authors : Nolen, B.J.; Pollard, T.D.  
Deposited on : 2007-03-26  
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

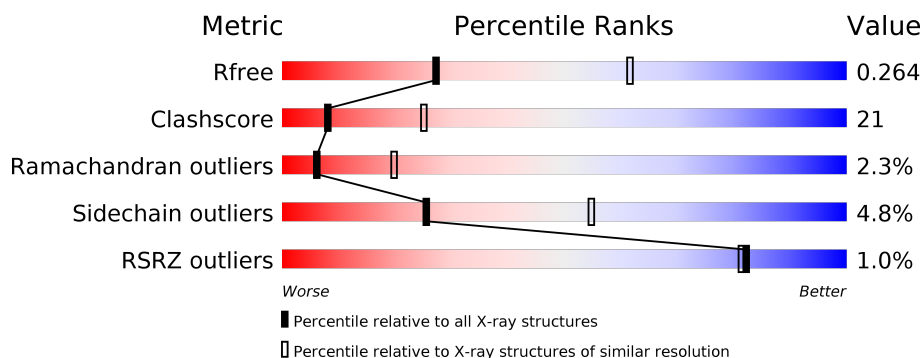
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>• 5%</div> </div> </div>
2	B	394	<div> <div>%</div> <div> <div></div> <div>29%</div> <div>18%</div> <div>•</div> <div>48%</div> </div> </div>
3	C	372	<div> <div></div> <div> <div>54%</div> <div>35%</div> <div>• 8%</div> </div> </div>
4	D	300	<div> <div></div> <div> <div>64%</div> <div>29%</div> <div>• 6%</div> </div> </div>
5	E	178	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>38%</div> <div>• • •</div> </div> </div>
6	F	168	<div> <div></div> <div> <div>74%</div> <div>23%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	151	<div><div><div>%</div><div><div></div><div>56%</div><div>30%</div><div>• • 11%</div></div></div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13541 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-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3177	2042	528	592	15			

- Molecule 2 is a protein called Actin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1572	1006	268	294	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	341	Total	C	N	O	S	0	0	0
			2648	1680	464	485	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	CONFLICT	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	283	Total	C	N	O	S	0	0	0
			2287	1453	396	430	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1408	904	235	260	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	134	Total	C	N	O	S	0	0	0
			1023	642	179	199	3			

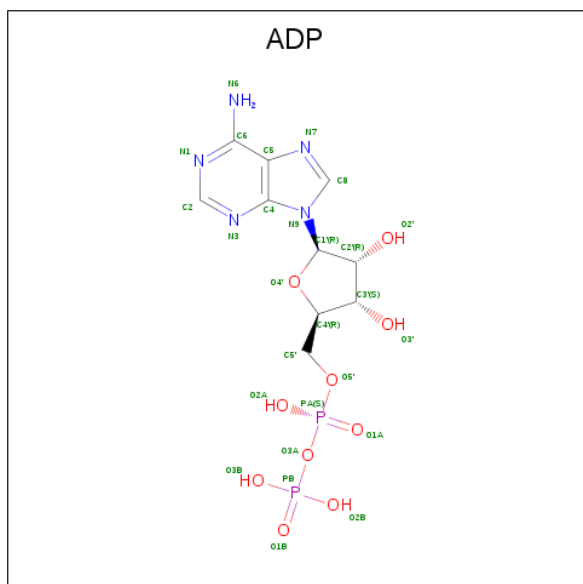
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	CONFLICT	UNP Q3SYX9
G	28	ASP	GLU	CONFLICT	UNP Q3SYX9

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

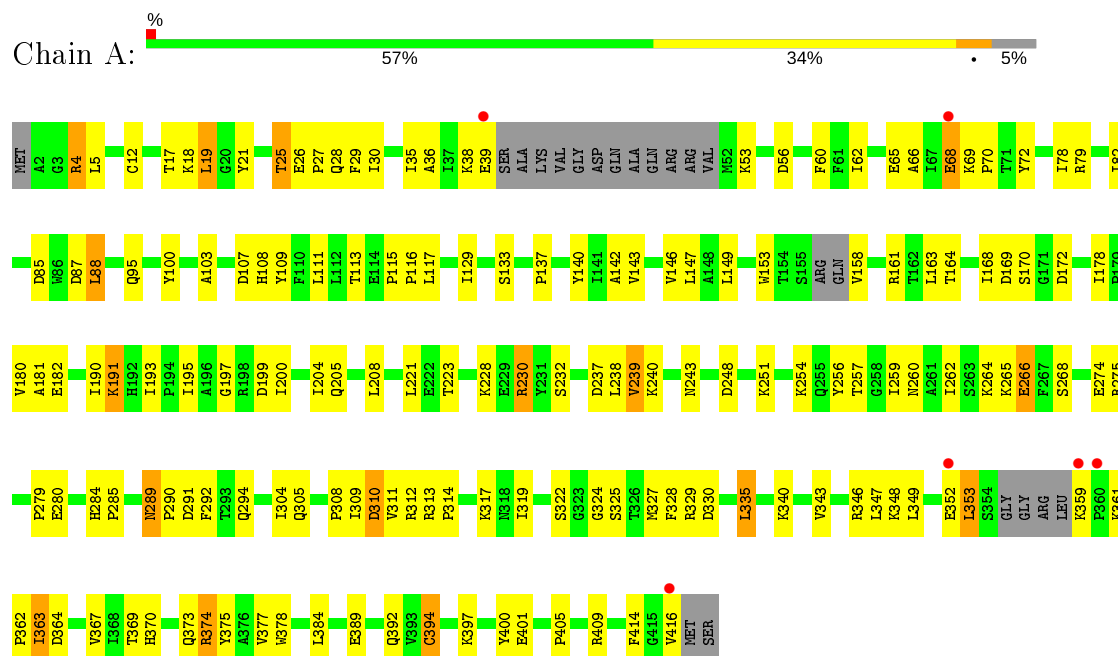


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

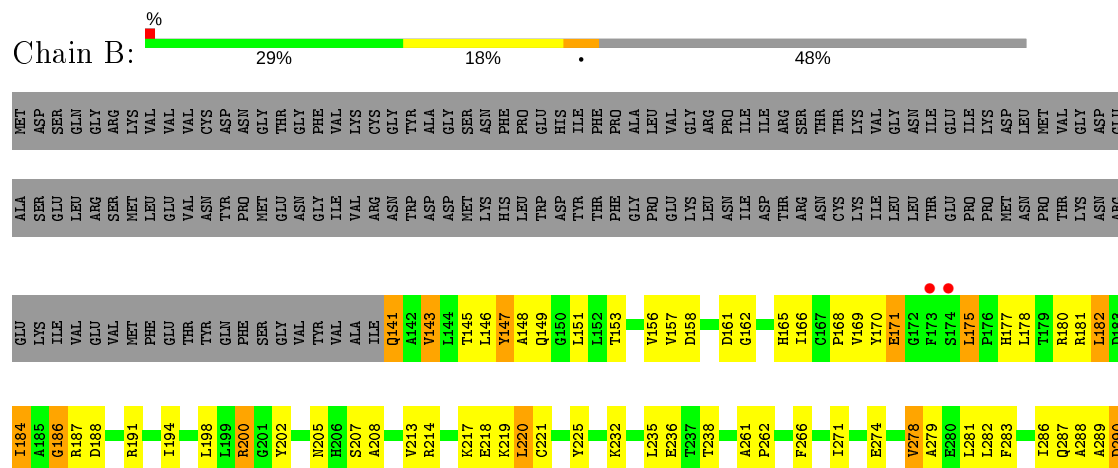
### 3 Residue-property plots [i](#)

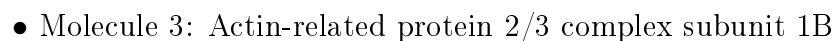
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Actin-like protein 3



#### • Molecule 2: Actin-like protein 2





C346	V288	R179	I92	RET
D358	L269	P180	L93	A2
D351	F270	A181		F6
	A275	P182	I96	L7
		T183	R97	
		P184	A98	
		W185		P10
			V102	I11
		E193	R103	H14
		L194	W104	A15
		W195		W16
			I107	I17
		S201	E108	
		C202	K109	
		G203		Q22
			A112	I23
		V208		A24
		C209	G116	
		F210		P27
		S211	V119	I28
		A212	I120	I29
				H30
		R216	V124	E31
			F125	
		W219	E126	I34
			Q127	E36
		H222		
		D223	W131	
		ASN	W132	H46
		LEU	V133	E47
		ASP	C134	L48
		LYS	K135	K49
		LYS	H136	E50
		ALA	I137	H51
		SER		
		SER	P140	D59
		GLU	I141	
		GLY	R142	P62
		SER	S143	D63
		ALA	T144	
		ALA	V145	T69
		ALA	L146	
		L247		T72
		L248	H151	D73
		A249	P152	R74
				W75
			V155	A76
		T254		
		E255		
		S256	S161	W79
		S257	C162	T80
		L258	D163	L81
		V259	F164	
		A260		R84
		A261	Y172	T85
		G262	I173	H86
		H263	K174	K87
		D264	E175	P88
		C265	V176	T89
			E177	L90
		T267	E178	W91
		S343		

- Molecule 4: Actin-related protein 2/3 complex subunit 2

I238	E139	I1
I239	I140	I10
T240	R141	
I241		I15
I242	I144	
L243		F35
I244	R147	A36
H245		D37
T246	E150	
F247		Y43
R248	S156	H44
	K157	I45
A250	R158	
I251	D159	I49
I252		
H253	F169	T53
T254		K54
R255	V175	V55
R256		M56
R257	M182	
		I59
L274	R189	S60
	R190	L61
L277	A191	K62
M278	S192	F63
R281	Q197	L67
P282	V198	Q68
D283	L199	
ALA	F200	A72
GLU	S201	
LYS	H202	
LYS	R203	L75
GLU	E204	L76
MET	P205	K77
LYS	F206	
THR	L207	L84
ILE	E208	V85
THR	L209	
GLY	L210	Y91
LYS	D211	
THR	T212	S108
PHE	D213	L116
SER	A214	K117
SER		R118
ARG	I220	
	G221	F121
	Y222	A122
	I223	S123
	T224	V124
	F225	
	V226	Q130
	L227	F131
	F228	Q132
		E133
	H231	E134
		G135
	A234	K136
	P237	

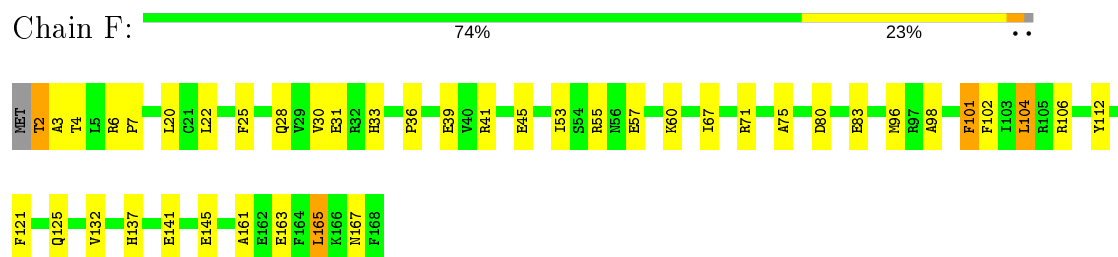
- Molecule 5: Actin-related protein 2/3 complex subunit 3

Q83	Q88	Q89	Q90	Q91	Q92	Q93	Q94	Q95	Q96	Q97	Q98	Q99	Q100	Q101	Q102	Q103	Q104	Q105	Q106	Q107	Q108	Q109	Q110	Q111	Q112	Q113	Q114	Q115	Q116	Q117	Q118	Q119	Q120	Q121	Q122	Q123	Q124	Q125	Q126	Q127	Q128	Q129	Q130	Q131	Q132	Q133	Q134	Q135	Q136	Q137	Q138	Q139	Q140	Q141	Q142	Q143	Q144	Q145	Q146	Q147	Q148	Q149	Q150	Q151	Q152	Q153	Q154	Q155	Q156	Q157	Q158	Q159	Q160	Q161	Q162	Q163	Q164	Q165	Q166	Q167	Q168	Q169	Q170	Q171	Q172	Q173	Q174	Q175	Q176	Q177	Q178	Q179	Q180	Q181	Q182	Q183	Q184	Q185	Q186	Q187	Q188	Q189	Q190	Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249	Q250	Q251	Q252	Q253	Q254	Q255	Q256	Q257	Q258	Q259	Q260	Q261	Q262	Q263	Q264	Q265	Q266	Q267	Q268	Q269	Q270	Q271	Q272	Q273	Q274	Q275	Q276	Q277	Q278	Q279	Q280	Q281	Q282	Q283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	Q292	Q293	Q294	Q295	Q296	Q297	Q298	Q299	Q300	Q301	Q302	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q310	Q311	Q312	Q313	Q314	Q315	Q316	Q317	Q318	Q319	Q320	Q321	Q322	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q332	Q333	Q334	Q335	Q336	Q337	Q338	Q339	Q340	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400	Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500	Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q54
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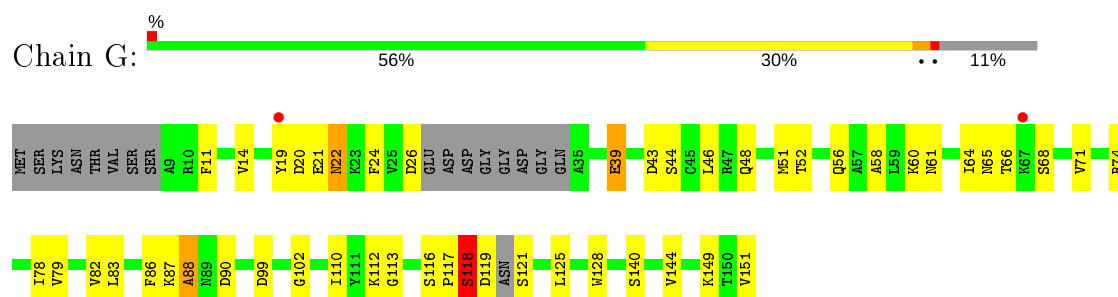


GLY  
GLN

- Molecule 6: Actin-related protein 2/3 complex subunit 4



- Molecule 7: Actin-related protein 2/3 complex subunit 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.13Å 129.27Å 203.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 46.83 – 2.84	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.85) 92.6 (46.83-2.84)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.272 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	3465 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ADP

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	0.41	0/3257	0.63	0/4418
2	B	0.36	0/1600	0.64	0/2167
3	C	0.40	0/2717	0.68	3/3688 (0.1%)
4	D	0.41	0/2336	0.64	1/3154 (0.0%)
5	E	0.36	0/1441	0.60	0/1941
6	F	0.43	0/1393	0.68	1/1868 (0.1%)
7	G	0.48	1/1034 (0.1%)	0.67	2/1389 (0.1%)
All	All	0.40	1/13778 (0.0%)	0.65	7/18625 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	118	SER	C-O	-5.56	1.12	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	116	SER	C-N-CD	7.62	144.41	128.40
4	D	204	GLU	N-CA-C	-7.43	90.94	111.00
6	F	101	PHE	N-CA-C	-5.40	96.42	111.00
3	C	137	ILE	N-CA-C	-5.32	96.64	111.00
3	C	283	GLY	N-CA-C	5.30	126.36	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3177	0	3123	146	0
2	B	1572	0	1559	91	0
3	C	2648	0	2602	134	0
4	D	2287	0	2252	72	0
5	E	1408	0	1408	74	0
6	F	1371	0	1410	37	0
7	G	1023	0	1041	45	0
8	A	1	0	0	0	0
9	A	27	0	12	2	0
9	B	27	0	12	8	0
All	All	13541	0	13419	575	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 21.

The worst 5 of 575 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)
3:C:256:SER:HB2	3:C:372:VAL:HG12	1.20	1.17
3:C:183:THR:HG22	3:C:185:TRP:H	1.08	1.09
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.34	1.08
5:E:88:LYS:H	5:E:153:ASN:ND2	1.52	1.07
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.23	0.99

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	389/418 (93%)	347 (89%)	36 (9%)	6 (2%)	10	30
2	B	201/394 (51%)	164 (82%)	24 (12%)	13 (6%)	1	3
3	C	337/372 (91%)	297 (88%)	34 (10%)	6 (2%)	8	25
4	D	281/300 (94%)	255 (91%)	24 (8%)	2 (1%)	22	50
5	E	169/178 (95%)	136 (80%)	25 (15%)	8 (5%)	2	7
6	F	165/168 (98%)	156 (94%)	8 (5%)	1 (1%)	25	53
7	G	128/151 (85%)	115 (90%)	10 (8%)	3 (2%)	6	20
All	All	1670/1981 (84%)	1470 (88%)	161 (10%)	39 (2%)	6	20

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	GLU
2	B	147	TYR
2	B	171	GLU
5	E	153	ASN
2	B	145	THR

### 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	347/363 (96%)	330 (95%)	17 (5%)	25	54
2	B	164/345 (48%)	155 (94%)	9 (6%)	21	49
3	C	290/313 (93%)	278 (96%)	12 (4%)	30	61
4	D	249/264 (94%)	239 (96%)	10 (4%)	31	62
5	E	155/159 (98%)	147 (95%)	8 (5%)	23	51
6	F	154/155 (99%)	148 (96%)	6 (4%)	32	63
7	G	110/124 (89%)	102 (93%)	8 (7%)	14	35
All	All	1469/1723 (85%)	1399 (95%)	70 (5%)	25	55

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	182	PRO
4	D	108	SER
7	G	26	ASP
3	C	210	PHE
3	C	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	46	HIS
4	D	132	GLN
7	G	61	ASN
3	C	107	ASN
3	C	331	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
9	ADP	B	395	-	24,29,29	1.37	3 (12%)	29,45,45	1.53	4 (13%)
9	ADP	A	501	-	24,29,29	1.37	3 (12%)	29,45,45	1.68	5 (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
9	ADP	B	395	-	-	1/12/32/32	0/3/3/3
9	ADP	A	501	-	-	6/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	501	ADP	C2-N1	3.70	1.40	1.33
9	B	395	ADP	C2-N1	3.67	1.40	1.33
9	A	501	ADP	PB-O1B	3.40	1.61	1.50
9	B	395	ADP	PB-O1B	3.39	1.61	1.50
9	B	395	ADP	O4'-C1'	2.21	1.44	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	395	ADP	N3-C2-N1	-5.44	120.17	128.68
9	A	501	ADP	N3-C2-N1	-5.38	120.27	128.68
9	A	501	ADP	O4'-C1'-C2'	-3.95	101.15	106.93
9	A	501	ADP	PA-O3A-PB	-3.37	121.28	132.83
9	B	395	ADP	PA-O3A-PB	-2.75	123.40	132.83

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

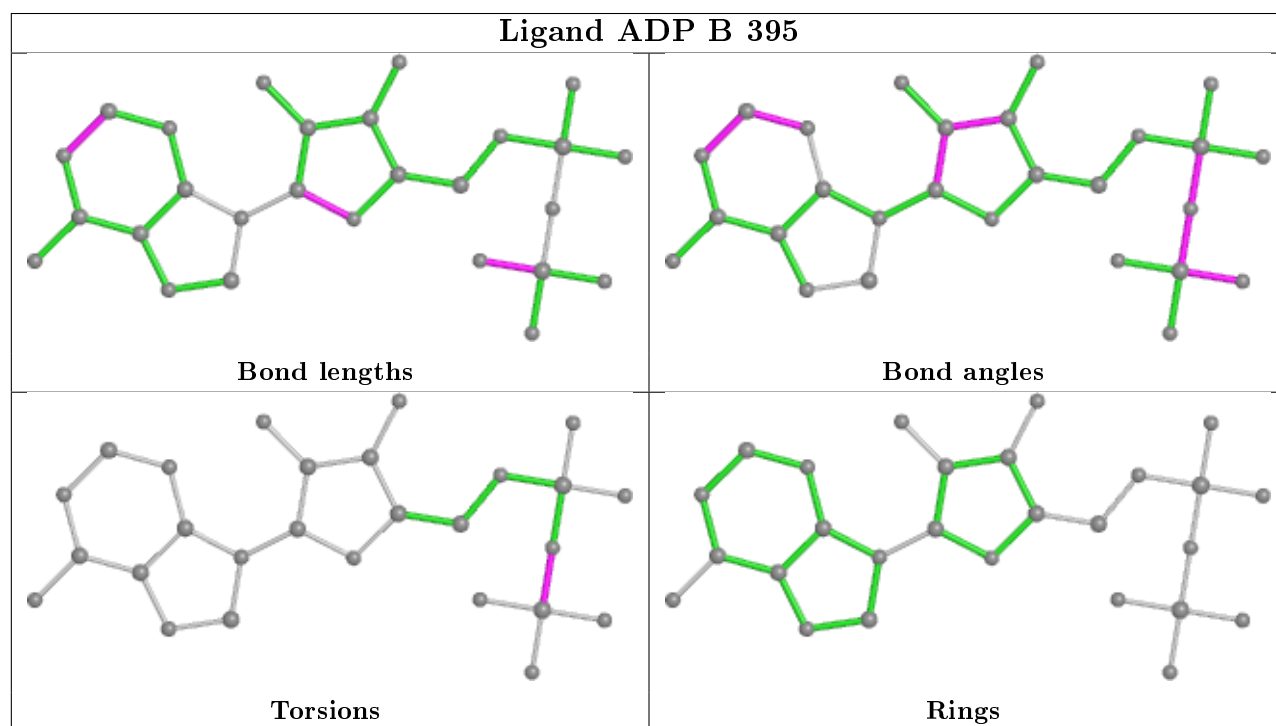
Mol	Chain	Res	Type	Atoms
9	A	501	ADP	C5'-O5'-PA-O2A
9	A	501	ADP	C5'-O5'-PA-O3A
9	A	501	ADP	PB-O3A-PA-O1A
9	A	501	ADP	C5'-O5'-PA-O1A
9	A	501	ADP	PB-O3A-PA-O2A

There are no ring outliers.

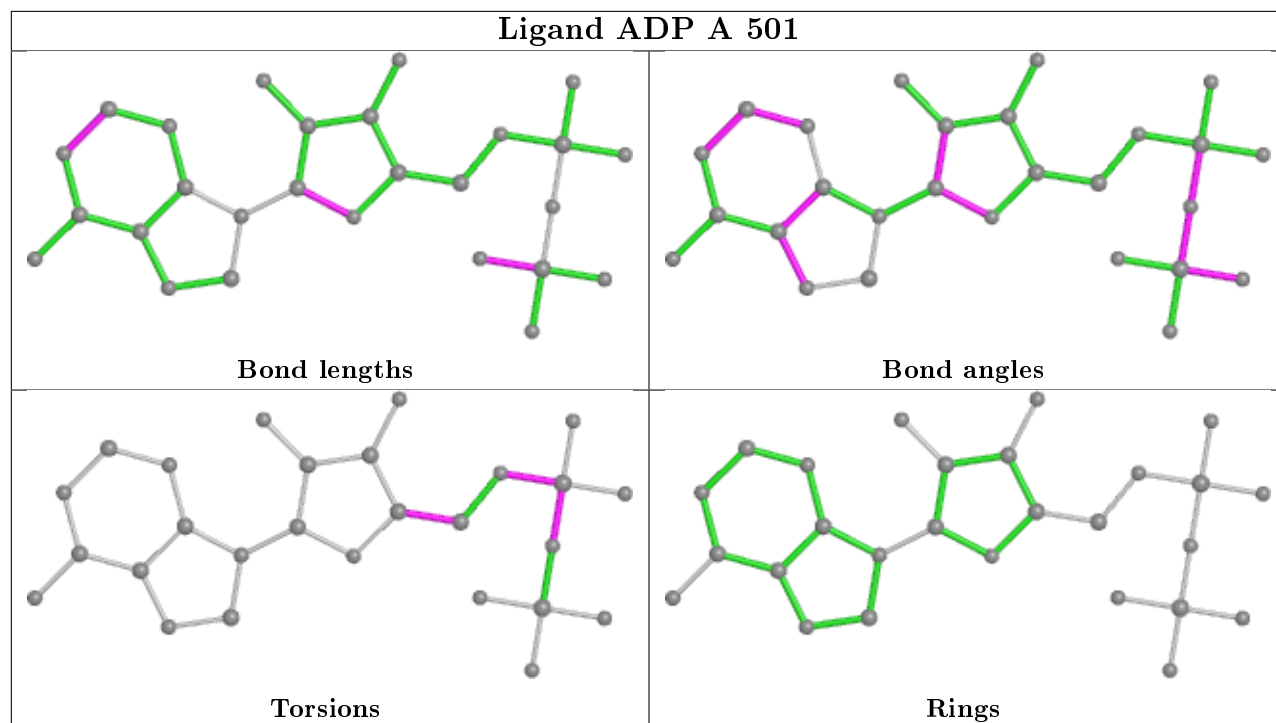
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	395	ADP	8	0
9	A	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	397/418 (94%)	-0.25	6 (1%) 73 72	21, 48, 87, 109	0
2	B	203/394 (51%)	-0.07	4 (1%) 65 62	29, 62, 101, 113	0
3	C	341/372 (91%)	-0.31	1 (0%) 94 94	27, 44, 71, 92	0
4	D	283/300 (94%)	-0.35	1 (0%) 92 92	25, 42, 66, 92	0
5	E	173/178 (97%)	-0.12	3 (1%) 70 68	44, 60, 86, 99	0
6	F	167/168 (99%)	-0.50	0 100 100	25, 36, 48, 75	0
7	G	134/151 (88%)	0.06	2 (1%) 73 72	36, 67, 86, 94	0
All	All	1698/1981 (85%)	-0.25	17 (1%) 82 81	21, 47, 87, 113	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	211	ASP	5.0
2	B	174	SER	4.4
2	B	337	LEU	3.8
7	G	67	LYS	3.6
1	A	359	LYS	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

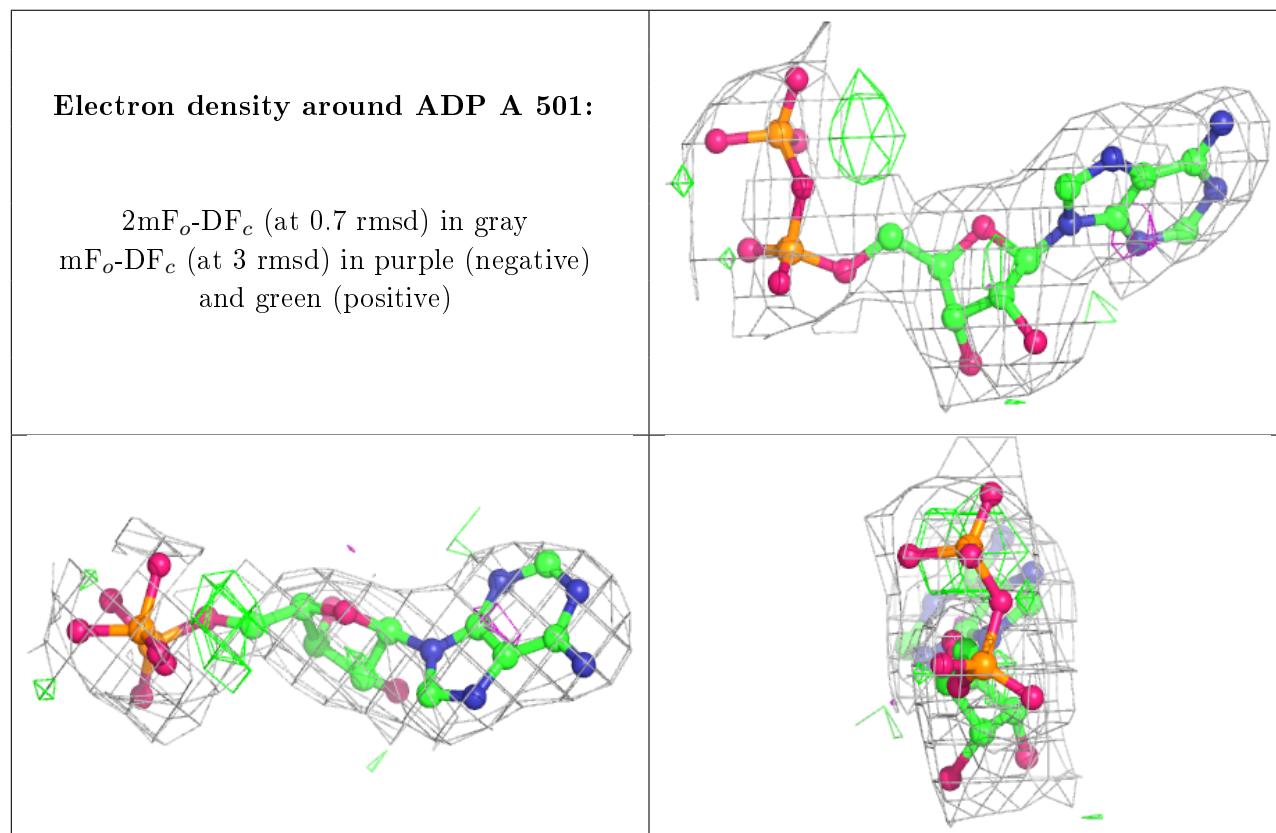
There are no carbohydrates in this entry.

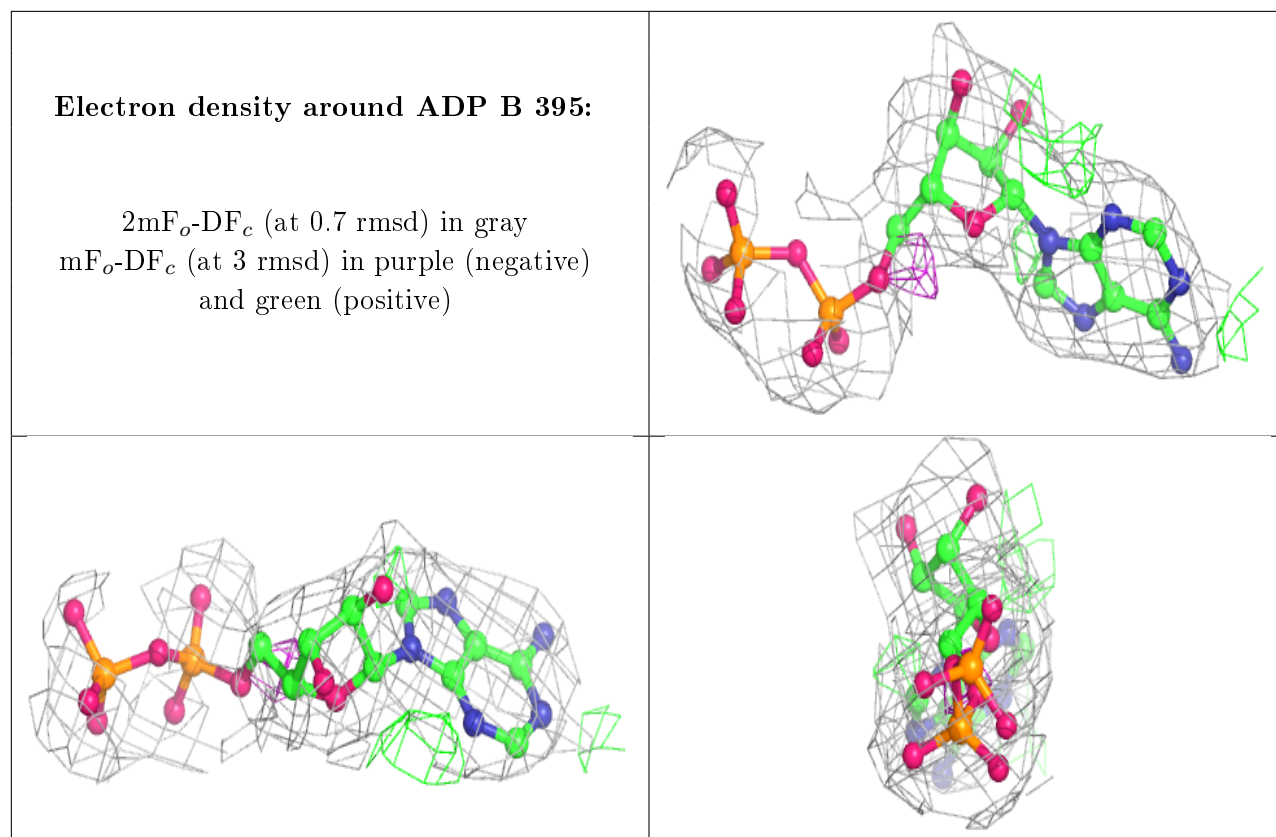
## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	ADP	A	501	27/27	0.87	0.17	55,64,95,96	0
9	ADP	B	395	27/27	0.93	0.15	54,60,74,76	0
8	CA	A	500	1/1	0.97	0.18	68,68,68,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.