



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:18 pm BST

PDB ID : 5TVX  
Title : Crystal structure of mitochondrial Hsp90 (TRAP1) with ATP in absence of Mg, fully hydrolyzed  
Authors : Elnatan, D.; Betegon, M.; Agard, D.A.  
Deposited on : 2016-11-10  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

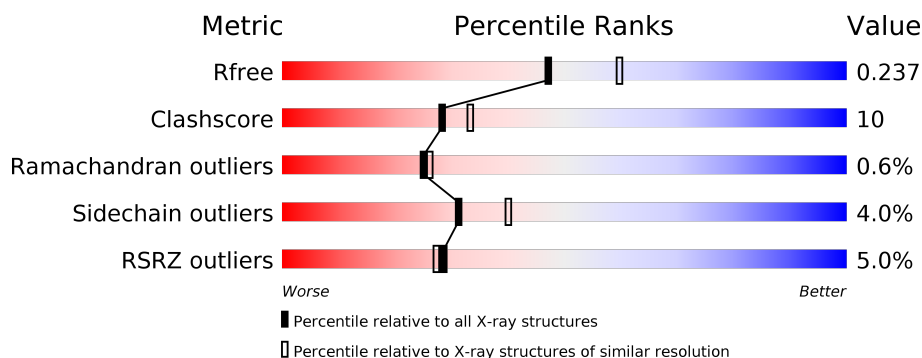
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	653	
1	B	653	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9998 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 TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	601	Total	C	N	O	S	1	0	0
			4853	3079	837	916	21			
1	A	588	Total	C	N	O	S	0	0	0
			4717	2989	816	891	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	GLY	-	expression tag	UNP A8WFFV1
B	68	ILE	-	expression tag	UNP A8WFFV1
B	69	ASP	-	expression tag	UNP A8WFFV1
B	70	PRO	-	expression tag	UNP A8WFFV1
B	71	PHE	-	expression tag	UNP A8WFFV1
B	72	THR	-	expression tag	UNP A8WFFV1
A	67	GLY	-	expression tag	UNP A8WFFV1
A	68	ILE	-	expression tag	UNP A8WFFV1
A	69	ASP	-	expression tag	UNP A8WFFV1
A	70	PRO	-	expression tag	UNP A8WFFV1
A	71	PHE	-	expression tag	UNP A8WFFV1
A	72	THR	-	expression tag	UNP A8WFFV1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

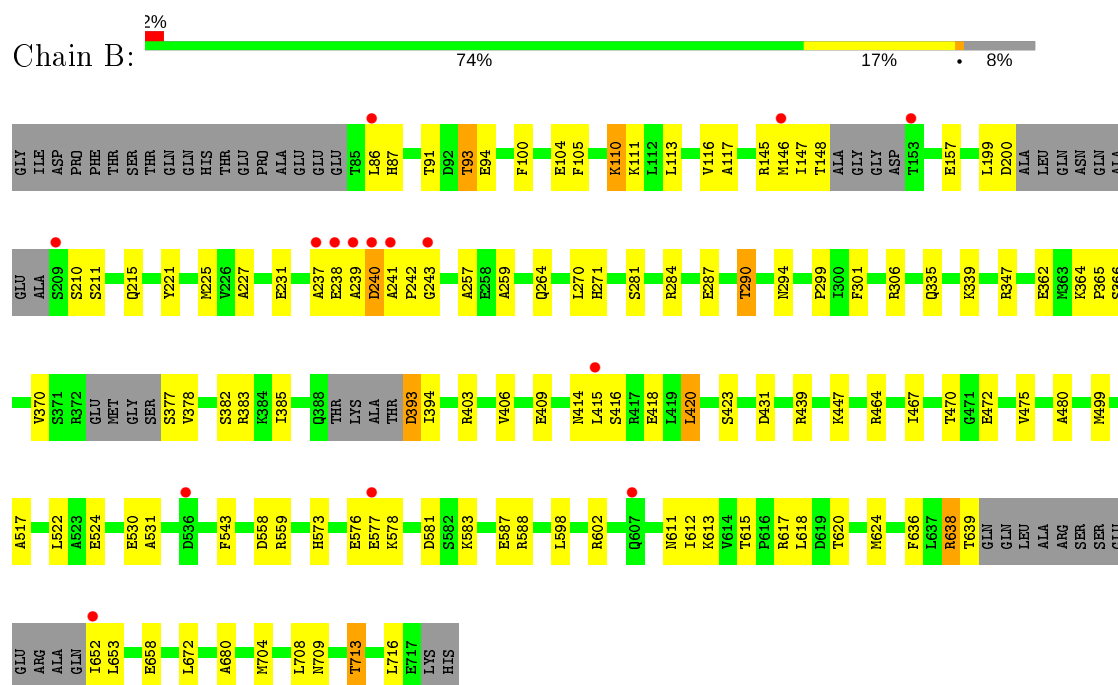
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	218	Total	O	0	0
			218	218		
3	A	156	Total	O	0	0
			156	156		

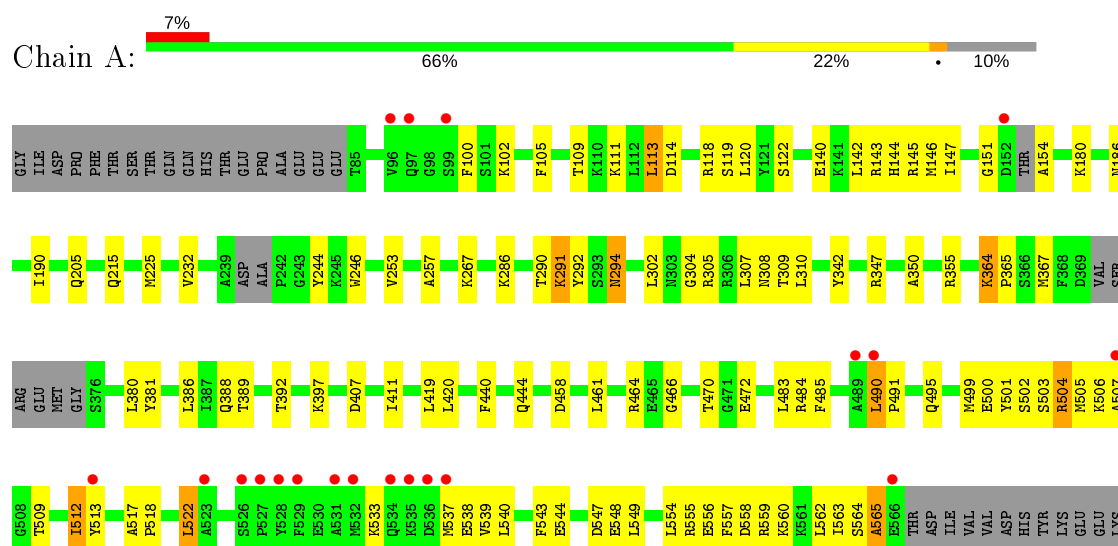
### 3 Residue-property plots

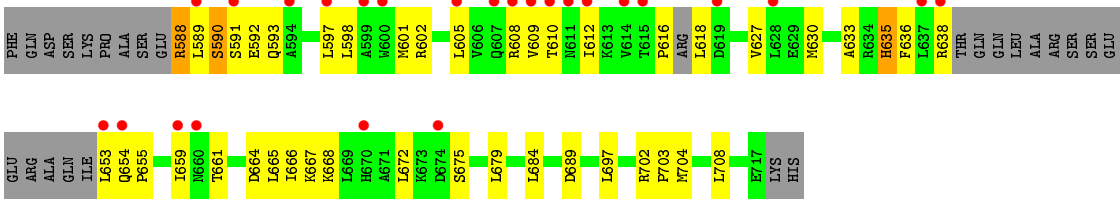
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: TNF receptor-associated protein 1



- Molecule 1: TNF receptor-associated protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.49 Å   96.82 Å   125.78 Å 90.00°   134.18°   90.00°	Depositor
Resolution (Å)	39.97 – 2.20 40.54 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.97-2.20) 99.5 (40.54-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.00 Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.189 , 0.236 0.189 , 0.237	Depositor DCC
$R_{free}$ test set	5440 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for h+2*l,k,-h-l 0.010 for h,-k,-h-l 0.018 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: 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	0.39	0/4800	0.56	0/6465
1	B	0.41	0/4942	0.57	0/6659
All	All	0.40	0/9742	0.57	0/13124

There are no bond length outliers.

There are no bond angle outliers.

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	4717	0	4717	114	0
1	B	4853	0	4852	86	0
2	A	27	0	12	3	0
2	B	27	0	12	0	0
3	A	156	0	0	8	0
3	B	218	0	0	16	1
All	All	9998	0	9593	189	1

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 10.

All (189) 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:B:147:ILE:H	1:B:148:THR:HA	1.29	0.96
1:B:347:ARG:NH1	3:B:902:HOH:O	2.07	0.85
1:B:716:LEU:O	1:A:668:LYS:NZ	2.12	0.82
1:A:122:SER:OG	3:A:901:HOH:O	1.97	0.82
1:B:615:THR:O	3:B:901:HOH:O	2.00	0.79
1:A:386:LEU:HD21	1:A:389:THR:HG22	1.65	0.78
2:A:801:ADP:O1B	3:A:902:HOH:O	2.01	0.78
1:B:240:ASP:HB2	1:B:241:ALA:HA	1.67	0.77
1:A:588:ARG:NH1	3:A:904:HOH:O	2.13	0.76
1:B:147:ILE:N	1:B:148:THR:HA	2.01	0.76
1:A:490:LEU:HD22	1:A:491:PRO:HD3	1.70	0.74
1:A:672:LEU:HD22	1:A:679:LEU:HD12	1.71	0.73
1:B:239:ALA:H	1:B:241:ALA:HB2	1.52	0.72
1:A:590:SER:H	1:A:593:GLN:HE21	1.37	0.71
1:A:635:HIS:HB2	1:A:638:ARG:HD2	1.72	0.70
1:B:364:LYS:HG3	1:B:365:PRO:HD2	1.75	0.69
1:B:611:ASN:HA	3:B:921:HOH:O	1.93	0.68
1:B:104:GLU:HG2	1:A:253:VAL:HG12	1.74	0.68
1:B:237:ALA:HB2	1:B:264:GLN:HE22	1.57	0.68
1:B:414:ASN:ND2	3:B:910:HOH:O	2.23	0.67
1:A:627:VAL:HG11	1:A:633:ALA:HB2	1.74	0.67
1:B:470:THR:HG22	1:B:472:GLU:H	1.60	0.67
1:B:431:ASP:OD2	3:B:904:HOH:O	2.13	0.67
1:A:286:LYS:O	1:A:290:THR:HG23	1.95	0.67
1:B:393:ASP:OD1	3:B:903:HOH:O	2.12	0.67
1:A:512:ILE:HD11	1:A:540:LEU:HD12	1.77	0.65
1:A:114:ASP:OD1	1:A:118:ARG:NH2	2.29	0.65
1:B:652:ILE:N	3:B:916:HOH:O	2.29	0.65
1:B:231:GLU:OE2	1:B:271:HIS:NE2	2.21	0.64
1:A:350:ALA:O	3:A:906:HOH:O	2.14	0.64
1:A:616:PRO:O	1:A:618:LEU:N	2.30	0.64
1:A:154:ALA:N	3:A:909:HOH:O	2.30	0.64
1:B:638:ARG:HH12	1:B:639:THR:HG23	1.63	0.64
1:A:564:SER:OG	1:A:565:ALA:N	2.24	0.63
1:A:392:THR:O	1:A:397:LYS:NZ	2.32	0.62
1:A:589:LEU:HD13	1:A:667:LYS:HG2	1.82	0.61
1:B:709:ASN:O	1:B:713:THR:HG23	1.99	0.61
1:B:531:ALA:O	1:B:617:ARG:NH2	2.34	0.60
1:B:420:LEU:HD23	1:B:420:LEU:H	1.66	0.60
1:B:713:THR:HG22	1:A:665:LEU:HG	1.85	0.59
1:A:504:ARG:NH1	1:A:538:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:NZ	1:A:458:ASP:O	2.22	0.58
1:A:440:PHE:O	1:A:444:GLN:HG2	2.03	0.58
2:A:801:ADP:O1A	3:A:902:HOH:O	2.16	0.58
1:B:240:ASP:HB2	1:B:242:PRO:HD3	1.84	0.58
1:B:423:SER:OG	3:B:906:HOH:O	2.18	0.57
1:B:530:GLU:OE2	3:B:905:HOH:O	2.17	0.57
1:B:339:LYS:O	1:B:362:GLU:HB2	2.04	0.56
1:B:237:ALA:HB2	1:B:264:GLN:NE2	2.21	0.56
1:B:636:PHE:O	1:B:638:ARG:HD3	2.06	0.56
1:B:199:LEU:HD12	1:B:200:ASP:HA	1.87	0.56
1:A:518:PRO:HD2	1:A:630:MET:HE3	1.87	0.56
1:B:146:MET:HA	1:B:148:THR:HG22	1.89	0.55
1:B:414:ASN:ND2	1:B:416:SER:OG	2.39	0.55
1:A:558:ASP:O	1:A:560:LYS:HG3	2.08	0.54
1:A:598:LEU:O	1:A:602:ARG:NH1	2.40	0.54
1:B:116:VAL:O	3:B:907:HOH:O	2.18	0.54
1:B:439:ARG:NH1	3:B:909:HOH:O	2.22	0.54
1:B:110:LYS:HG2	1:B:111:LYS:N	2.23	0.53
1:A:605:LEU:HD11	1:A:684:LEU:HD11	1.90	0.53
1:B:243:GLY:O	1:B:259:ALA:N	2.37	0.53
1:A:518:PRO:HD2	1:A:630:MET:CE	2.40	0.52
1:A:500:GLU:HB3	1:A:504:ARG:NH2	2.23	0.52
1:A:659:ILE:HG23	1:A:666:ILE:HD12	1.91	0.52
1:B:239:ALA:H	1:B:241:ALA:CB	2.19	0.52
1:A:589:LEU:HB3	1:A:661:THR:HB	1.91	0.52
1:B:558:ASP:OD1	1:B:559:ARG:NH2	2.43	0.52
1:B:638:ARG:NH1	1:B:639:THR:HG23	2.25	0.52
1:A:342:TYR:OH	3:A:903:HOH:O	2.04	0.51
1:A:672:LEU:HA	1:A:675:SER:HB2	1.91	0.51
1:A:411:ILE:HG12	1:A:420:LEU:HD22	1.92	0.51
1:A:513:TYR:HB3	1:A:539:VAL:HG22	1.92	0.51
1:A:602:ARG:HG2	1:A:612:ILE:HD13	1.93	0.51
1:B:94:GLU:OE2	1:A:267:LYS:HE3	2.11	0.51
1:A:347:ARG:HB3	1:A:355:ARG:HE	1.76	0.50
1:B:638:ARG:HH11	1:B:638:ARG:H	1.58	0.50
1:A:485:PHE:HB2	1:A:540:LEU:HD22	1.94	0.50
1:A:564:SER:HG	1:A:565:ALA:H	1.57	0.50
1:B:576:GLU:O	1:B:578:LYS:N	2.45	0.50
1:B:284:ARG:NH1	1:B:287:GLU:OE2	2.45	0.50
1:A:659:ILE:HG23	1:A:666:ILE:CD1	2.42	0.50
1:B:470:THR:HG21	1:B:475:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ARG:NH1	3:B:928:HOH:O	2.43	0.50
1:A:505:MET:SD	1:A:560:LYS:HE2	2.53	0.49
1:B:618:LEU:HD11	1:B:624:MET:HG2	1.95	0.49
1:A:554:LEU:HD22	1:A:562:LEU:HD11	1.95	0.49
1:B:290:THR:O	1:B:294:ASN:HB2	2.12	0.49
1:A:500:GLU:O	1:A:504:ARG:NE	2.46	0.49
1:A:598:LEU:HD23	1:A:602:ARG:HH22	1.78	0.49
1:B:403:ARG:NH1	3:B:930:HOH:O	2.46	0.48
1:A:180:LYS:HB2	1:A:244:TYR:CE2	2.49	0.48
1:A:548:GLU:CD	1:A:548:GLU:H	2.16	0.48
1:A:597:LEU:O	1:A:601:MET:HG3	2.14	0.48
1:A:143:ARG:HA	1:A:146:MET:HE2	1.95	0.48
1:A:180:LYS:HB2	1:A:244:TYR:CZ	2.49	0.47
1:A:590:SER:H	1:A:593:GLN:NE2	2.08	0.47
1:A:635:HIS:HB2	1:A:638:ARG:HH11	1.80	0.47
1:B:383:ARG:CZ	1:B:409:GLU:HG2	2.45	0.47
1:A:364:LYS:NZ	1:A:365:PRO:HD2	2.31	0.46
1:A:502:SER:HA	1:A:505:MET:SD	2.55	0.46
1:A:549:LEU:HD23	1:A:549:LEU:H	1.80	0.46
1:A:364:LYS:HB2	1:A:364:LYS:HE2	1.57	0.46
1:A:554:LEU:O	1:A:555:ARG:HB3	2.14	0.46
1:B:157:GLU:HB3	1:B:299:PRO:HG2	1.97	0.46
1:A:608:ARG:HD3	1:A:608:ARG:H	1.80	0.46
1:A:689:ASP:HB3	1:A:704:MET:HE2	1.98	0.46
1:B:598:LEU:HD23	1:B:612:ILE:HG22	1.97	0.46
1:A:635:HIS:ND1	1:A:635:HIS:O	2.49	0.45
1:A:590:SER:HB3	1:A:593:GLN:NE2	2.32	0.45
1:B:100:PHE:HB3	1:A:257:ALA:HB2	1.99	0.45
1:B:227:ALA:HB2	1:B:270:LEU:HB3	1.98	0.45
1:A:548:GLU:HG2	1:A:549:LEU:H	1.82	0.45
1:A:610:THR:OG1	1:A:654:GLN:OE1	2.19	0.45
1:A:499:MET:HG3	1:A:557:PHE:HZ	1.82	0.45
1:A:302:LEU:HB2	1:A:307:LEU:HD11	1.99	0.44
1:A:517:ALA:HB1	1:A:630:MET:HE2	1.99	0.44
1:A:113:LEU:CD2	1:A:190:ILE:HD11	2.47	0.44
1:A:113:LEU:HD21	1:A:190:ILE:HD11	1.99	0.44
1:A:667:LYS:HE3	1:A:667:LYS:HB2	1.82	0.44
1:A:664:ASP:O	1:A:668:LYS:HB2	2.17	0.44
1:B:393:ASP:HB3	1:B:394:ILE:H	1.52	0.44
1:B:415:LEU:N	1:A:119:SER:O	2.47	0.44
1:A:397:LYS:HA	1:A:397:LYS:HD3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:O	1:A:407:ASP:HA	2.18	0.44
1:A:380:LEU:HD21	1:A:420:LEU:HD21	1.99	0.44
1:A:512:ILE:HG23	1:A:562:LEU:HA	2.00	0.44
1:B:517:ALA:O	1:B:543:PHE:HA	2.17	0.44
1:A:636:PHE:CD1	1:A:653:LEU:HB2	2.52	0.43
1:A:636:PHE:CD2	1:A:653:LEU:HD22	2.53	0.43
1:A:501:TYR:CE2	1:A:538:GLU:HG2	2.54	0.43
1:A:563:ILE:HA	1:A:563:ILE:HD12	1.82	0.43
1:B:414:ASN:HD21	1:B:416:SER:HG	1.63	0.43
1:B:91:THR:O	1:B:93:THR:HG22	2.18	0.43
1:A:554:LEU:HD23	1:A:556:GLU:H	1.82	0.43
1:A:591:SER:HB2	1:A:592:GLU:OE1	2.18	0.43
1:A:609:VAL:HA	1:A:655:PRO:HD2	1.98	0.43
1:B:583:LYS:HB3	1:B:587:GLU:HB2	2.01	0.43
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.73	0.43
1:B:284:ARG:O	1:B:287:GLU:HG2	2.18	0.43
1:B:301:PHE:CE2	1:B:306:ARG:HB2	2.53	0.43
1:B:467:ILE:HD11	1:B:480:ALA:HA	2.01	0.43
1:A:388:GLN:HE21	1:A:419:LEU:HD23	1.83	0.43
1:A:547:ASP:OD2	3:A:907:HOH:O	2.21	0.43
1:A:232:VAL:HB	1:A:246:TRP:HB3	2.01	0.43
1:A:483:LEU:O	1:A:484:ARG:NH1	2.51	0.43
1:A:668:LYS:O	1:A:672:LEU:HD12	2.19	0.43
1:B:383:ARG:O	1:B:385:ILE:HD12	2.18	0.42
1:B:378:VAL:HG11	1:B:406:VAL:HG23	2.00	0.42
1:B:573:HIS:HE1	1:B:658:GLU:OE2	2.03	0.42
1:A:466:GLY:O	1:A:470:THR:HG23	2.19	0.42
1:A:522:LEU:HD21	1:A:697:LEU:HD21	2.01	0.42
1:B:672:LEU:HB3	1:B:680:ALA:HB2	2.01	0.42
1:A:144:HIS:HA	1:A:147:ILE:HD12	2.02	0.42
1:B:237:ALA:HA	1:B:238:GLU:C	2.39	0.42
1:B:240:ASP:CB	1:B:241:ALA:HA	2.42	0.42
1:B:613:LYS:O	1:B:658:GLU:HA	2.20	0.42
1:A:464:ARG:NH1	1:A:544:GLU:HG3	2.34	0.42
1:B:335:GLN:NE2	3:B:942:HOH:O	2.52	0.42
1:B:583:LYS:O	1:B:588:ARG:NH1	2.53	0.42
1:A:290:THR:O	1:A:294:ASN:HB2	2.20	0.41
1:A:533:LYS:HD2	1:A:533:LYS:HA	1.98	0.41
1:B:708:LEU:HD11	1:A:708:LEU:HD11	2.01	0.41
1:A:186:ASN:HB3	2:A:801:ADP:O4'	2.20	0.41
1:B:522:LEU:HD21	1:A:703:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:GLU:OE2	1:B:620:THR:HB	2.20	0.41
1:A:702:ARG:N	1:A:703:PRO:HD2	2.34	0.41
1:B:257:ALA:HB2	1:A:100:PHE:HD1	1.84	0.41
1:B:87:HIS:O	1:A:304:GLY:HA2	2.20	0.41
1:B:366:SER:O	1:B:370:VAL:HG23	2.20	0.41
1:A:140:GLU:OE2	1:A:143:ARG:NH1	2.53	0.41
1:A:364:LYS:HZ2	1:A:365:PRO:HG2	1.85	0.41
1:A:506:LYS:HA	1:A:506:LYS:HD3	1.84	0.41
1:B:105:PHE:O	1:A:109:THR:HG21	2.21	0.41
1:A:142:LEU:O	1:A:146:MET:HG3	2.21	0.41
1:A:291:LYS:HG2	1:A:292:TYR:CE2	2.56	0.41
1:A:500:GLU:HB3	1:A:504:ARG:HH21	1.85	0.41
1:B:499:MET:HG3	3:B:1038:HOH:O	2.19	0.41
1:B:602:ARG:NE	3:B:934:HOH:O	2.48	0.41
1:A:102:LYS:H	1:A:102:LYS:HG2	1.61	0.40
1:B:377:SER:HA	1:B:403:ARG:HH12	1.86	0.40
1:A:506:LYS:O	1:A:509:THR:OG1	2.28	0.40
1:B:117:ALA:O	1:B:225:MET:HG2	2.21	0.40
1:B:470:THR:HG22	1:B:472:GLU:N	2.32	0.40
1:B:86:LEU:HD22	1:A:305:ARG:HG2	2.04	0.40
1:B:113:LEU:HD11	1:A:105:PHE:CD2	2.56	0.40
1:B:116:VAL:HG11	1:B:221:TYR:HB2	2.03	0.40
1:A:517:ALA:O	1:A:543:PHE:HA	2.21	0.40
1:A:608:ARG:HD3	1:A:608:ARG:N	2.37	0.40
1:B:447:LYS:HE3	1:B:447:LYS:HB3	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1100:HOH:O	3:B:1101:HOH:O[2_757]	2.10	0.10

## 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	574/653 (88%)	547 (95%)	22 (4%)	5 (1%)	17	16
1	B	589/653 (90%)	567 (96%)	20 (3%)	2 (0%)	41	46
All	All	1163/1306 (89%)	1114 (96%)	42 (4%)	7 (1%)	25	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	577	GLU
1	A	565	ALA
1	A	151	GLY
1	B	215	GLN
1	A	215	GLN
1	A	308	ASN
1	A	507	ALA

### 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	515/574 (90%)	491 (95%)	24 (5%)	26	33
1	B	534/574 (93%)	516 (97%)	18 (3%)	37	47
All	All	1049/1148 (91%)	1007 (96%)	42 (4%)	31	40

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	THR
1	B	110	LYS
1	B	145	ARG
1	B	210	SER
1	B	211	SER
1	B	240	ASP

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Mol	Chain	Res	Type
1	B	281	SER
1	B	290	THR
1	B	382	SER
1	B	393	ASP
1	B	418	GLU
1	B	420	LEU
1	B	524	GLU
1	B	581	ASP
1	B	638	ARG
1	B	653	LEU
1	B	704	MET
1	B	713	THR
1	A	111	LYS
1	A	113	LEU
1	A	120	LEU
1	A	145	ARG
1	A	205	GLN
1	A	225	MET
1	A	291	LYS
1	A	294	ASN
1	A	309	THR
1	A	364	LYS
1	A	367	MET
1	A	461	LEU
1	A	472	GLU
1	A	490	LEU
1	A	495	GLN
1	A	503	SER
1	A	504	ARG
1	A	512	ILE
1	A	522	LEU
1	A	537	MET
1	A	559	ARG
1	A	588	ARG
1	A	590	SER
1	A	635	HIS

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

Mol	Chain	Res	Type
1	B	264	GLN
1	B	603	ASN

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Mol	Chain	Res	Type
1	A	294	ASN
1	A	593	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 ⓘ

2 ligands 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$
2	ADP	B	801	-	24,29,29	0.87	1 (4%)	29,45,45	1.25	4 (13%)
2	ADP	A	801	-	24,29,29	0.95	1 (4%)	29,45,45	1.26	6 (20%)

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
2	ADP	B	801	-	-	2/12/32/32	0/3/3/3
2	ADP	A	801	-	-	1/12/32/32	0/3/3/3



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ADP	C5-C4	2.51	1.47	1.40
2	B	801	ADP	C5-C4	2.44	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ADP	N3-C2-N1	-2.74	124.39	128.68
2	A	801	ADP	N3-C2-N1	-2.58	124.64	128.68
2	B	801	ADP	O3B-PB-O2B	2.56	117.41	107.64
2	B	801	ADP	C3'-C2'-C1'	2.22	104.31	100.98
2	B	801	ADP	C4-C5-N7	-2.18	107.13	109.40
2	A	801	ADP	C2-N1-C6	2.17	122.46	118.75
2	A	801	ADP	O2'-C2'-C1'	-2.13	102.99	110.85
2	A	801	ADP	O2A-PA-O1A	2.13	122.76	112.24
2	A	801	ADP	N6-C6-N1	2.10	122.93	118.57
2	A	801	ADP	C3'-C2'-C1'	2.04	104.05	100.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O2B
2	B	801	ADP	O4'-C4'-C5'-O5'
2	B	801	ADP	C3'-C4'-C5'-O5'

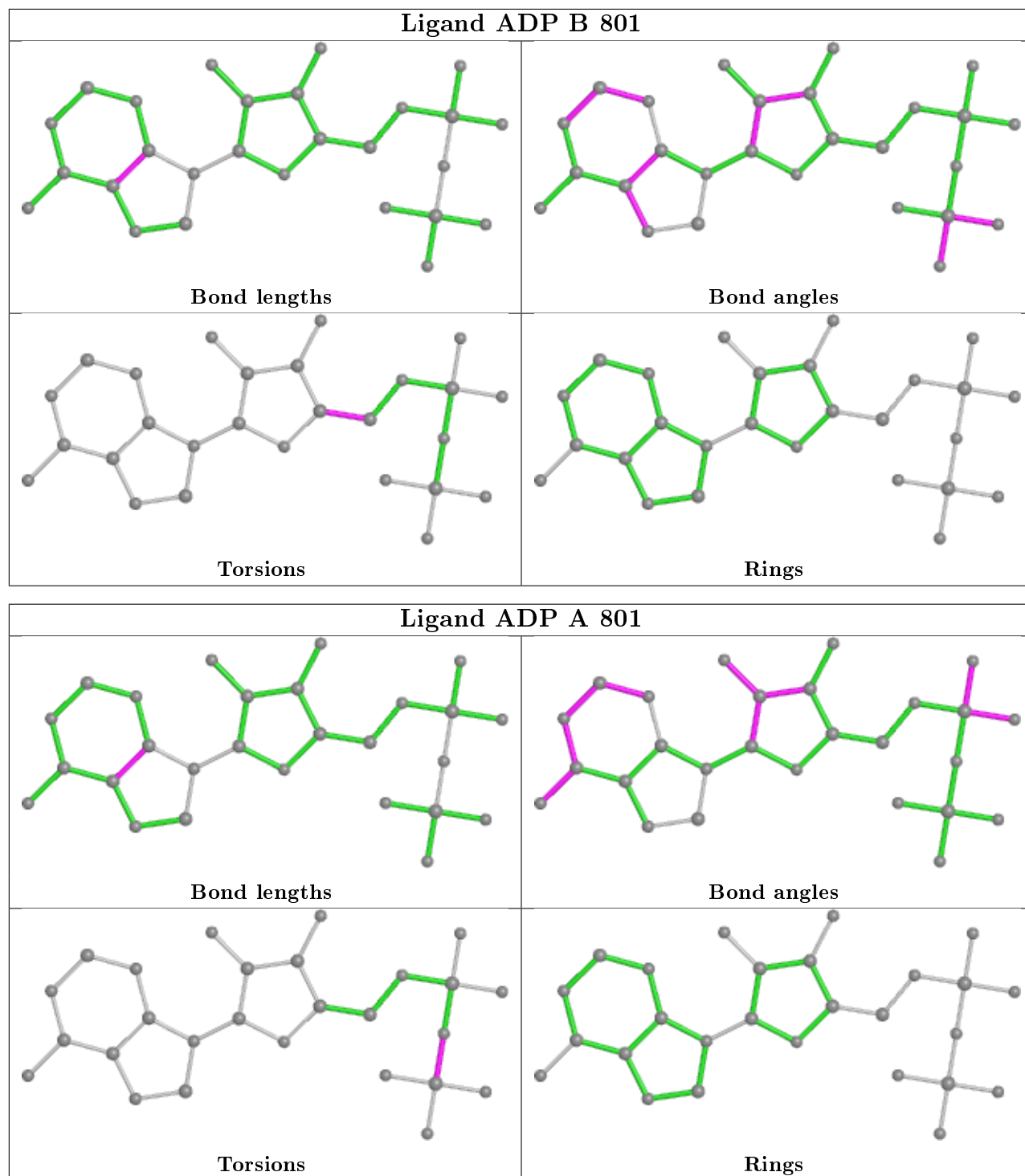
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	588/653 (90%)	0.08	45 (7%)	13 12	30, 69, 129, 157	0
1	B	601/653 (92%)	-0.38	15 (2%)	57 55	29, 59, 99, 137	1 (0%)
All	All	1189/1306 (91%)	-0.15	60 (5%)	28 27	29, 63, 119, 157	1 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	ASP	6.2
1	A	535	LYS	5.6
1	B	240	ASP	5.4
1	A	597	LEU	5.1
1	A	605	LEU	5.1
1	B	153	THR	5.0
1	A	659	ILE	4.3
1	A	628	LEU	4.2
1	A	527	PRO	4.2
1	A	537	MET	4.0
1	A	609	VAL	3.9
1	B	607	GLN	3.8
1	A	594	ALA	3.7
1	A	607	GLN	3.7
1	A	534	GLN	3.7
1	B	239	ALA	3.6
1	A	528	TYR	3.6
1	A	531	ALA	3.6
1	A	489	ALA	3.4
1	A	619	ASP	3.4
1	A	615	THR	3.2
1	A	507	ALA	3.2
1	A	532	MET	3.2
1	A	611	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	612	ILE	3.0
1	A	610	THR	3.0
1	A	600	TRP	2.9
1	B	146	MET	2.9
1	B	237	ALA	2.9
1	A	660	ASN	2.8
1	A	589	LEU	2.8
1	A	513	TYR	2.8
1	B	238	GLU	2.8
1	B	209	SER	2.8
1	A	591	SER	2.7
1	A	490	LEU	2.7
1	A	638	ARG	2.6
1	A	526	SER	2.6
1	A	637	LEU	2.6
1	A	566	GLU	2.5
1	A	599	ALA	2.5
1	A	152	ASP	2.5
1	A	670	HIS	2.5
1	B	86	LEU	2.4
1	B	243	GLY	2.4
1	A	654	GLN	2.4
1	A	608	ARG	2.3
1	A	96	VAL	2.3
1	B	536	ASP	2.3
1	B	241	ALA	2.3
1	A	97	GLN	2.2
1	A	529	PHE	2.2
1	A	653	LEU	2.2
1	B	415	LEU	2.2
1	A	523	ALA	2.1
1	B	652	ILE	2.1
1	A	99	SER	2.1
1	B	577	GLU	2.1
1	A	674	ASP	2.1
1	A	614	VAL	2.1

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

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

## 6.3 Carbohydrates [i](#)

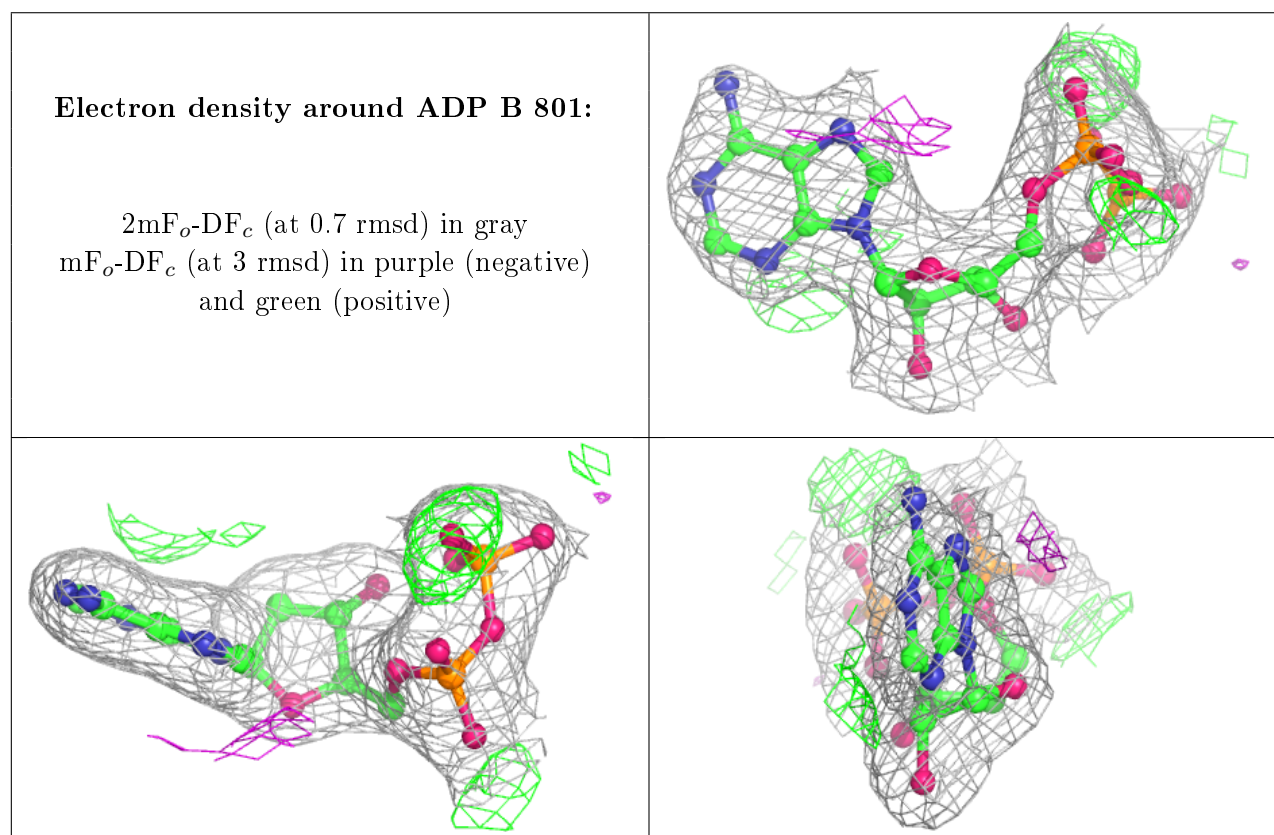
There are no carbohydrates in this entry.

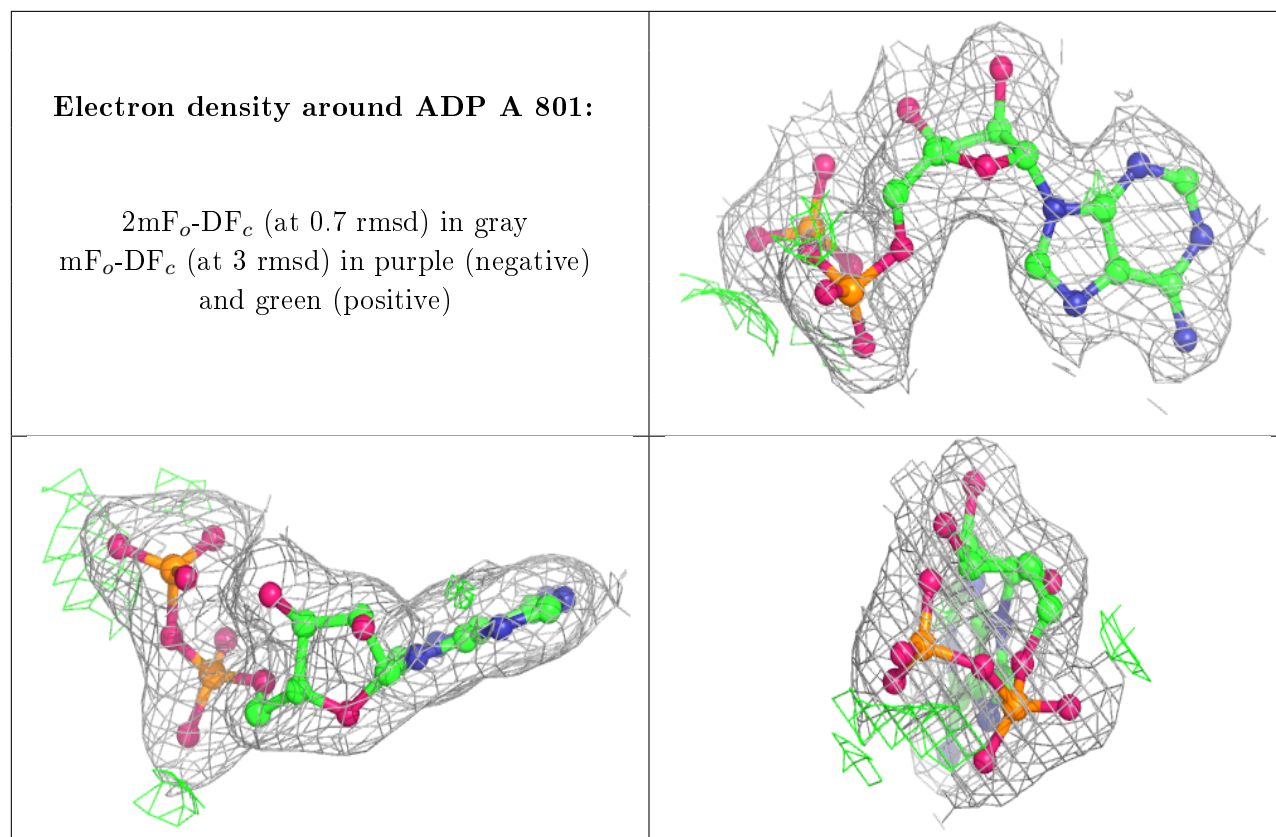
## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	801	27/27	0.97	0.12	44,56,69,82	0
2	ADP	A	801	27/27	0.99	0.14	27,36,46,51	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.