



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:14 AM GMT

PDB ID : 3LDO  
Title : Crystal structure of human GRP78 (70kDa heat shock protein 5 / BIP) AT-Pase domain in complex with AMPPNP  
Authors : Dokurno, P.; Surgenor, A.E.; Shaw, T.; Macias, A.T.; Massey, A.J.; Williamson, D.S.  
Deposited on : 2010-01-13  
Resolution : 1.95 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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

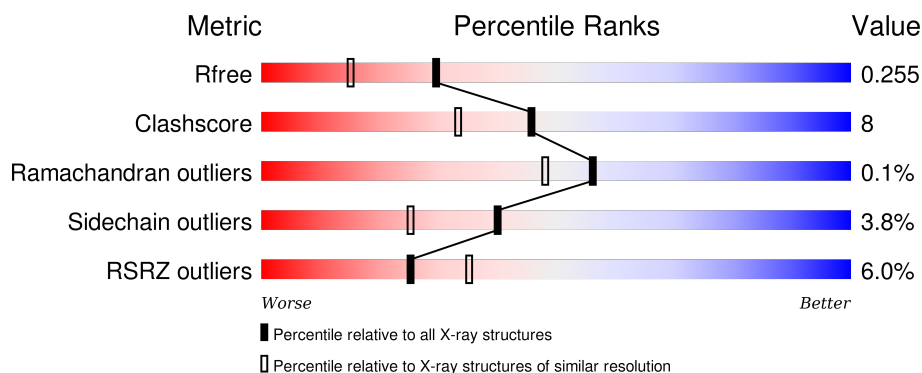
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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.

Mol	Chain	Length	Quality of chain
1	A	384	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>...</div> </div>
1	B	384	<div> <div>8%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6444 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.

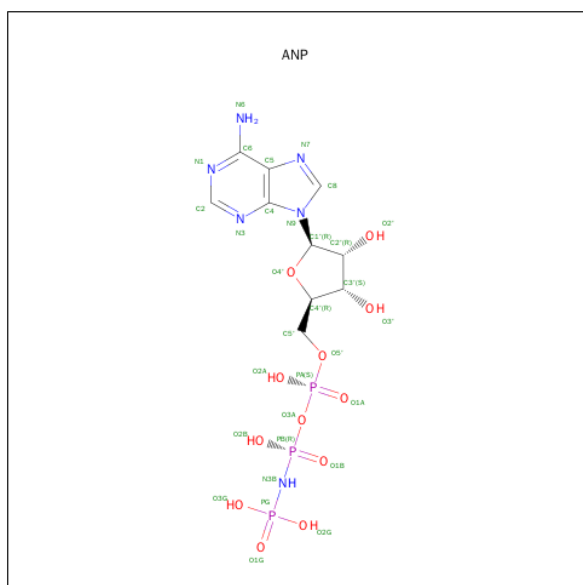
- Molecule 1 is a protein called 78 kDa glucose-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2940	1851	509	573	7			
1	B	381	Total	C	N	O	S	0	0	0
			2943	1854	507	575	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP P11021
A	25	SER	-	EXPRESSION TAG	UNP P11021
B	24	GLY	-	EXPRESSION TAG	UNP P11021
B	25	SER	-	EXPRESSION TAG	UNP P11021

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

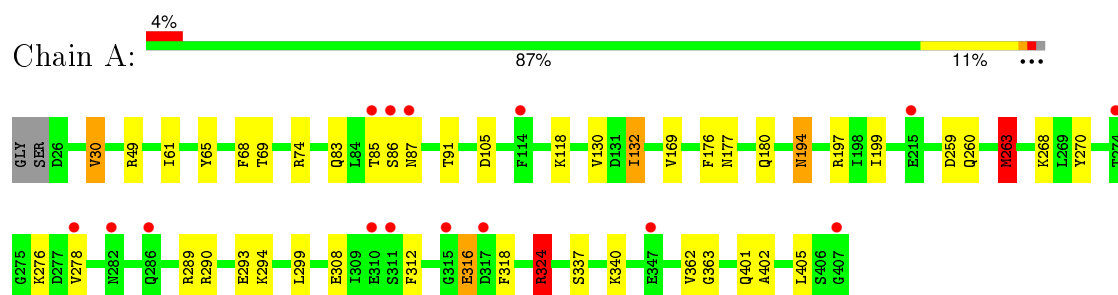
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	252	Total	O	0	0
			252	252		
3	B	247	Total	O	0	0
			247	247		

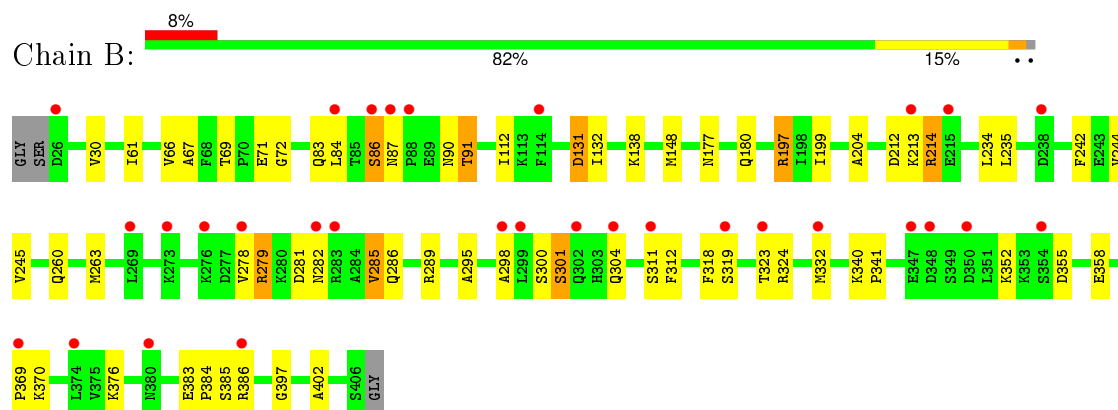
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 78 kDa glucose-regulated protein



- Molecule 1: 78 kDa glucose-regulated protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.62Å 74.56Å 89.95Å 90.00° 98.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 10.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (10.00-1.95) 99.2 (10.00-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.256 0.203 , 0.255	Depositor DCC
$R_{free}$ test set	3799 reflections (7.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 60.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 52273 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ANP

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	0.75	0/2985	0.75	4/4030 (0.1%)
1	B	0.72	0/2988	0.73	0/4034
All	All	0.73	0/5973	0.74	4/8064 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	105	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	324	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	324	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	263	MET	CG-SD-CE	-5.13	92.00	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	SER	Peptide

## 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	2940	0	2938	36	0
1	B	2943	0	2946	56	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
3	A	252	0	0	5	0
3	B	247	0	0	8	0
All	All	6444	0	5910	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (91) 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:131:ASP:HB3	3:B:606:HOH:O	1.49	1.09
1:A:85:THR:HB	3:A:479:HOH:O	1.58	1.00
1:B:260:GLN:HE22	1:B:289:ARG:HH21	1.16	0.90
1:B:263:MET:SD	3:B:595:HOH:O	2.31	0.89
1:A:130:VAL:HG23	1:A:132:ILE:HD11	1.60	0.83
1:A:130:VAL:HG23	1:A:132:ILE:CD1	2.09	0.82
1:B:214:ARG:CG	1:B:214:ARG:HH11	1.91	0.82
1:A:260:GLN:HA	1:A:263:MET:HG3	1.60	0.81
1:B:177:ASN:H	1:B:180:GLN:HE21	1.28	0.79
1:A:85:THR:HG22	1:A:87:ASN:H	1.49	0.78
1:B:263:MET:CE	1:B:289:ARG:HG3	2.14	0.77
1:B:260:GLN:HE22	1:B:289:ARG:NH2	1.85	0.74
1:A:169:VAL:CG1	1:A:199:ILE:HD12	2.18	0.74
1:B:263:MET:HE2	1:B:289:ARG:HA	1.69	0.73
1:B:260:GLN:NE2	1:B:289:ARG:HH21	1.89	0.71
1:A:177:ASN:H	1:A:180:GLN:HE21	1.39	0.70
1:B:263:MET:HE2	1:B:289:ARG:HG3	1.74	0.69
1:A:30:VAL:HG22	1:A:402:ALA:HB1	1.75	0.69
1:B:235:LEU:HD22	1:B:244:VAL:HG22	1.75	0.68
1:A:299:LEU:O	1:A:324:ARG:HD2	1.92	0.68
1:B:301:SER:O	1:B:324:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:CE2	1:A:74:ARG:HG3	2.32	0.65
1:A:197:ARG:HD2	1:A:405:LEU:HD11	1.77	0.65
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.62	0.64
1:B:263:MET:CG	3:B:595:HOH:O	2.44	0.63
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.62	0.63
1:B:87:ASN:O	3:B:524:HOH:O	2.15	0.63
1:B:263:MET:HG2	3:B:595:HOH:O	1.98	0.61
1:B:260:GLN:NE2	1:B:289:ARG:HE	2.00	0.59
1:B:197:ARG:HG2	1:B:199:ILE:HG23	1.84	0.58
1:A:263:MET:HE3	1:A:289:ARG:HA	1.86	0.57
1:B:212:ASP:HB3	1:B:242:PHE:CE1	2.40	0.57
1:A:259:ASP:O	1:A:263:MET:HG2	2.06	0.56
1:A:199:ILE:HD11	1:A:401:GLN:OE1	2.06	0.55
1:A:85:THR:HG22	1:A:87:ASN:N	2.20	0.55
1:B:84:LEU:HA	1:B:286:GLN:NE2	2.22	0.55
1:A:340:LYS:HG3	3:A:455:HOH:O	2.07	0.55
1:B:304:GLN:HG3	1:B:323:THR:HG22	1.89	0.55
1:B:278:VAL:HG21	1:B:312:PHE:CE2	2.41	0.55
1:A:30:VAL:HG22	1:A:402:ALA:CB	2.36	0.54
1:A:270:TYR:CE2	1:A:276:LYS:HE3	2.43	0.54
1:B:69:THR:HG22	1:B:83:GLN:HE22	1.73	0.52
1:B:204:ALA:O	1:B:397:GLY:HA3	2.09	0.52
1:B:67:ALA:HB2	1:B:91:THR:HB	1.92	0.52
1:B:263:MET:HE1	1:B:289:ARG:HG3	1.92	0.52
1:A:270:TYR:HE2	1:A:276:LYS:HE3	1.75	0.51
1:A:91:THR:HB	3:A:495:HOH:O	2.10	0.50
1:B:340:LYS:HB2	1:B:341:PRO:HD3	1.93	0.50
1:B:214:ARG:NE	1:B:358:GLU:OE2	2.37	0.49
1:B:197:ARG:HG2	1:B:199:ILE:CG2	2.43	0.49
1:A:69:THR:HG22	1:A:83:GLN:HE22	1.77	0.49
1:A:312:PHE:N	1:A:316:GLU:O	2.45	0.49
1:A:169:VAL:HG11	1:A:199:ILE:HD12	1.92	0.49
1:A:194:ASN:C	1:A:194:ASN:HD22	2.16	0.49
1:A:259:ASP:O	1:A:263:MET:CG	2.61	0.49
1:A:293:GLU:CD	3:A:483:HOH:O	2.50	0.49
1:B:384:PRO:HG3	3:B:487:HOH:O	2.14	0.48
1:B:234:LEU:HD23	1:B:245:VAL:HB	1.96	0.48
1:B:132:ILE:HG12	1:B:138:LYS:HG3	1.96	0.47
1:B:282:ASN:HA	1:B:285:VAL:HG23	1.97	0.46
1:B:385:SER:O	1:B:386:ARG:HG2	2.15	0.46
1:B:352:LYS:O	1:B:355:ASP:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLN:HE22	1:B:289:ARG:HE	1.63	0.46
1:A:177:ASN:H	1:A:180:GLN:NE2	2.13	0.45
1:B:281:ASP:OD2	1:B:282:ASN:N	2.50	0.44
1:B:383:GLU:HA	1:B:383:GLU:OE2	2.19	0.43
1:B:260:GLN:HE22	1:B:289:ARG:CZ	2.31	0.43
1:A:130:VAL:CG2	1:A:132:ILE:HD11	2.41	0.43
1:B:30:VAL:HG22	1:B:402:ALA:HB1	2.01	0.42
1:B:300:SER:OG	2:B:501:ANP:N1	2.39	0.42
1:B:281:ASP:C	1:B:281:ASP:OD2	2.58	0.42
1:A:49:ARG:HG3	1:B:213:LYS:HE2	2.01	0.42
1:B:66:VAL:HG11	1:B:148:MET:SD	2.60	0.42
1:B:279:ARG:HG3	3:B:507:HOH:O	2.19	0.42
1:A:85:THR:HG22	1:A:86:SER:N	2.35	0.42
1:A:268:LYS:HE3	1:A:268:LYS:HB2	1.79	0.42
1:B:332:MET:SD	1:B:370:LYS:HE2	2.60	0.42
1:B:312:PHE:CD2	1:B:318:PHE:HB2	2.55	0.42
1:B:84:LEU:HA	1:B:286:GLN:HE22	1.85	0.42
1:B:295:ALA:O	1:B:298:ALA:HB3	2.19	0.42
1:B:112:ILE:HG23	3:B:431:HOH:O	2.20	0.42
1:B:90:ASN:ND2	1:B:131:ASP:H	2.18	0.41
1:B:260:GLN:HE22	1:B:289:ARG:NE	2.19	0.41
1:A:308:GLU:HA	1:A:318:PHE:O	2.20	0.41
1:A:362:VAL:HG12	1:A:363:GLY:N	2.35	0.41
1:B:72:GLY:HA2	1:B:132:ILE:O	2.20	0.41
1:A:176:PHE:CD2	1:A:180:GLN:HB3	2.55	0.41
1:B:177:ASN:H	1:B:180:GLN:NE2	2.05	0.41
1:A:289:ARG:HG2	3:A:476:HOH:O	2.22	0.40
1:B:376:LYS:HD2	1:B:383:GLU:OE2	2.21	0.40
1:A:118:LYS:HB2	1:A:118:LYS:HE3	1.78	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	380/384 (99%)	375 (99%)	4 (1%)	1 (0%)	46	35
1	B	379/384 (99%)	367 (97%)	12 (3%)	0	100	100
All	All	759/768 (99%)	742 (98%)	16 (2%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	VAL

### 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	313/320 (98%)	302 (96%)	11 (4%)	43	29
1	B	315/320 (98%)	302 (96%)	13 (4%)	37	22
All	All	628/640 (98%)	604 (96%)	24 (4%)	40	25

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	61	ILE
1	A	65	TYR
1	A	132	ILE
1	A	194	ASN
1	A	263	MET
1	A	290	ARG
1	A	294	LYS
1	A	316	GLU
1	A	324	ARG
1	A	337	SER
1	B	61	ILE
1	B	71	GLU
1	B	86	SER
1	B	91	THR

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Mol	Chain	Res	Type
1	B	131	ASP
1	B	197	ARG
1	B	214	ARG
1	B	279	ARG
1	B	285	VAL
1	B	301	SER
1	B	311	SER
1	B	319	SER
1	B	369	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	83	GLN
1	A	180	GLN
1	A	194	ASN
1	A	302	GLN
1	A	380	ASN
1	B	83	GLN
1	B	87	ASN
1	B	90	ASN
1	B	136	GLN
1	B	180	GLN
1	B	260	GLN
1	B	265	HIS
1	B	286	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	ANP	A	408	-	27,33,33	1.89	7 (25%)	30,52,52	2.80	6 (20%)
2	ANP	B	501	-	27,33,33	3.07	9 (33%)	30,52,52	2.76	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	ANP	A	408	-	-	0/12/38/38	0/3/3/3
2	ANP	B	501	-	-	0/12/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ANP	PB-O2B	-2.50	1.49	1.56
2	B	501	ANP	PG-O3G	-2.18	1.50	1.56
2	A	408	ANP	PG-O3G	-2.04	1.51	1.56
2	B	501	ANP	PA-O2A	-2.01	1.46	1.54
2	A	408	ANP	PG-O1G	2.33	1.48	1.46
2	A	408	ANP	PG-O2G	2.54	1.63	1.56
2	A	408	ANP	PB-N3B	2.71	1.70	1.63
2	A	408	ANP	O4'-C4'	2.75	1.51	1.45
2	B	501	ANP	PG-N3B	2.98	1.71	1.63
2	B	501	ANP	C2-N1	3.45	1.40	1.33
2	A	408	ANP	C2-N1	4.02	1.41	1.33
2	A	408	ANP	PB-O1B	4.72	1.51	1.46
2	B	501	ANP	O4'-C1'	5.07	1.47	1.41
2	B	501	ANP	PB-O3A	5.40	1.65	1.59
2	B	501	ANP	PB-O1B	5.52	1.52	1.46
2	B	501	ANP	PG-O1G	10.75	1.58	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	408	ANP	N3-C2-N1	-11.39	120.18	128.89
2	B	501	ANP	N3-C2-N1	-11.28	120.26	128.89
2	A	408	ANP	O1G-PG-N3B	-5.51	103.44	111.90
2	B	501	ANP	O1G-PG-N3B	-5.27	103.81	111.90
2	A	408	ANP	C4'-O4'-C1'	-4.27	105.03	109.72
2	B	501	ANP	C4'-O4'-C1'	-3.96	105.37	109.72
2	A	408	ANP	O2G-PG-O1G	-3.32	104.67	113.49
2	B	501	ANP	O2G-PG-O1G	-3.14	105.15	113.49
2	A	408	ANP	O1B-PB-N3B	-2.09	108.69	111.90
2	B	501	ANP	O1B-PB-N3B	-2.01	108.82	111.90
2	A	408	ANP	O2B-PB-O1B	4.25	118.87	110.00
2	B	501	ANP	O2B-PB-O1B	4.33	119.03	110.00

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
2	B	501	ANP	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 ⓘ

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	382/384 (99%)	0.12	15 (3%) 43 54	7, 17, 35, 43	20 (5%)
1	B	381/384 (99%)	0.46	31 (8%) 15 23	8, 21, 39, 48	20 (5%)
All	All	763/768 (99%)	0.29	46 (6%) 25 35	7, 19, 38, 48	40 (5%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	SER	9.5
1	B	87	ASN	5.1
1	A	86	SER	4.7
1	B	26	ASP	3.5
1	B	114	PHE	3.5
1	A	274	THR	3.4
1	A	407	GLY	3.2
1	B	88	PRO	3.1
1	B	283	ARG	2.9
1	B	269	LEU	2.9
1	B	302	GLN	2.9
1	A	311	SER	2.9
1	B	319	SER	2.8
1	B	84	LEU	2.8
1	B	304	GLN	2.8
1	A	317	ASP	2.7
1	A	286	GLN	2.7
1	B	299	LEU	2.7
1	A	87	ASN	2.6
1	A	215	GLU	2.6
1	A	85	THR	2.5
1	A	310	GLU	2.5
1	B	369	PRO	2.4
1	B	350	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	276	LYS	2.4
1	B	374	LEU	2.3
1	B	380	ASN	2.3
1	A	114	PHE	2.3
1	B	298	ALA	2.3
1	A	315	GLY	2.3
1	B	354	SER	2.3
1	B	332	MET	2.3
1	B	278	VAL	2.3
1	B	348	ASP	2.3
1	B	273	LYS	2.2
1	B	323	THR	2.2
1	B	347	GLU	2.1
1	A	278	VAL	2.1
1	A	282	ASN	2.1
1	B	215	GLU	2.1
1	B	311	SER	2.1
1	A	347	GLU	2.1
1	B	386	ARG	2.0
1	B	282	ASN	2.0
1	B	213	LYS	2.0
1	B	238	ASP	2.0

## 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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	A	408	31/31	0.98	0.07	-0.56	6,10,13,16	0
2	ANP	B	501	31/31	0.98	0.08	-0.93	7,13,18,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.