



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID : 3H4M  
Title : AAA ATPase domain of the proteasome- activating nucleotidase  
Authors : Jeffrey, P.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.  
Deposited on : 2009-04-20  
Resolution : 3.11 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

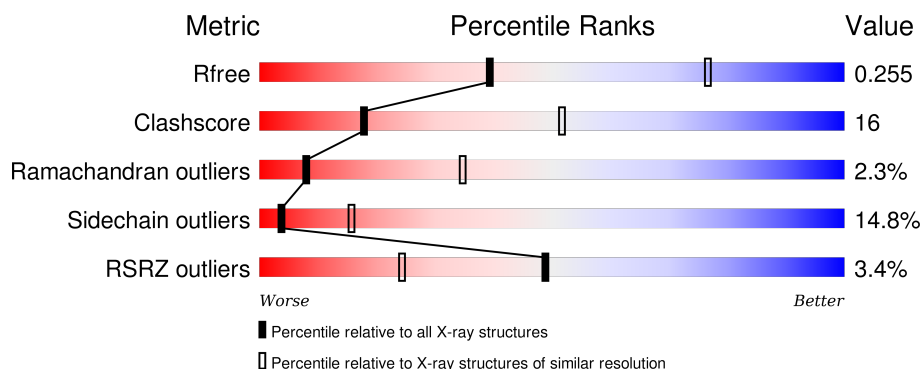
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	285	<div> <div>6%</div> <div>58% 27% 5% 8%</div> </div>
1	B	285	<div> <div>2%</div> <div>59% 24% 8% 8%</div> </div>
1	C	285	<div> <div>6%</div> <div>60% 26% 6% 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	C	439	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6162 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 Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2027	1282	350	384	11			
1	B	261	Total	C	N	O	S	0	0	0
			2027	1282	350	384	11			
1	C	261	Total	C	N	O	S	0	0	0
			2027	1282	350	384	11			

There are 27 discrepancies between the modelled and reference sequences:

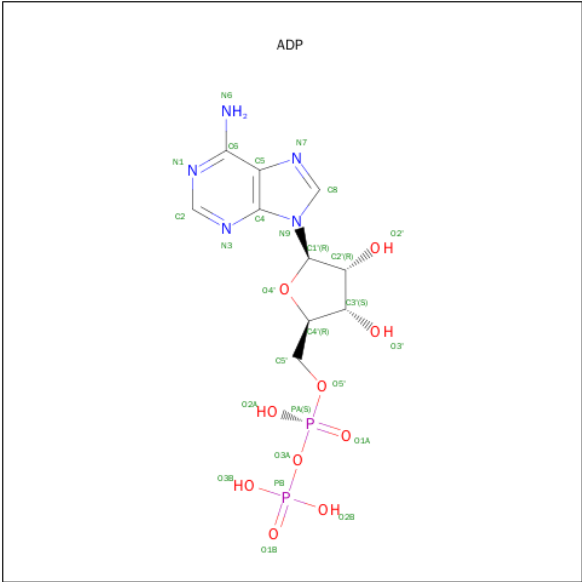
Chain	Residue	Modelled	Actual	Comment	Reference
A	154	MET	-	EXPRESSION TAG	UNP Q58576
A	431	LEU	-	EXPRESSION TAG	UNP Q58576
A	432	GLU	-	EXPRESSION TAG	UNP Q58576
A	433	HIS	-	EXPRESSION TAG	UNP Q58576
A	434	HIS	-	EXPRESSION TAG	UNP Q58576
A	435	HIS	-	EXPRESSION TAG	UNP Q58576
A	436	HIS	-	EXPRESSION TAG	UNP Q58576
A	437	HIS	-	EXPRESSION TAG	UNP Q58576
A	438	HIS	-	EXPRESSION TAG	UNP Q58576
B	154	MET	-	EXPRESSION TAG	UNP Q58576
B	431	LEU	-	EXPRESSION TAG	UNP Q58576
B	432	GLU	-	EXPRESSION TAG	UNP Q58576
B	433	HIS	-	EXPRESSION TAG	UNP Q58576
B	434	HIS	-	EXPRESSION TAG	UNP Q58576
B	435	HIS	-	EXPRESSION TAG	UNP Q58576
B	436	HIS	-	EXPRESSION TAG	UNP Q58576
B	437	HIS	-	EXPRESSION TAG	UNP Q58576
B	438	HIS	-	EXPRESSION TAG	UNP Q58576
C	154	MET	-	EXPRESSION TAG	UNP Q58576
C	431	LEU	-	EXPRESSION TAG	UNP Q58576
C	432	GLU	-	EXPRESSION TAG	UNP Q58576
C	433	HIS	-	EXPRESSION TAG	UNP Q58576
C	434	HIS	-	EXPRESSION TAG	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
C	435	HIS	-	EXPRESSION TAG	UNP Q58576
C	436	HIS	-	EXPRESSION TAG	UNP Q58576
C	437	HIS	-	EXPRESSION TAG	UNP Q58576
C	438	HIS	-	EXPRESSION TAG	UNP Q58576

- Molecule 2 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>).

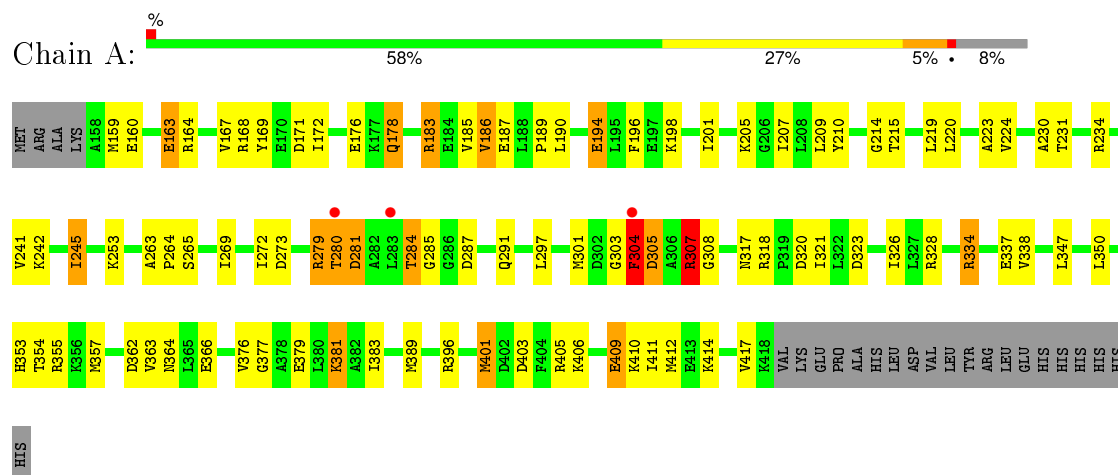


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	10	5	10	2	0	0
2	B	1	Total	10	5	10	2	0	0
2	C	1	Total	10	5	10	2	0	0

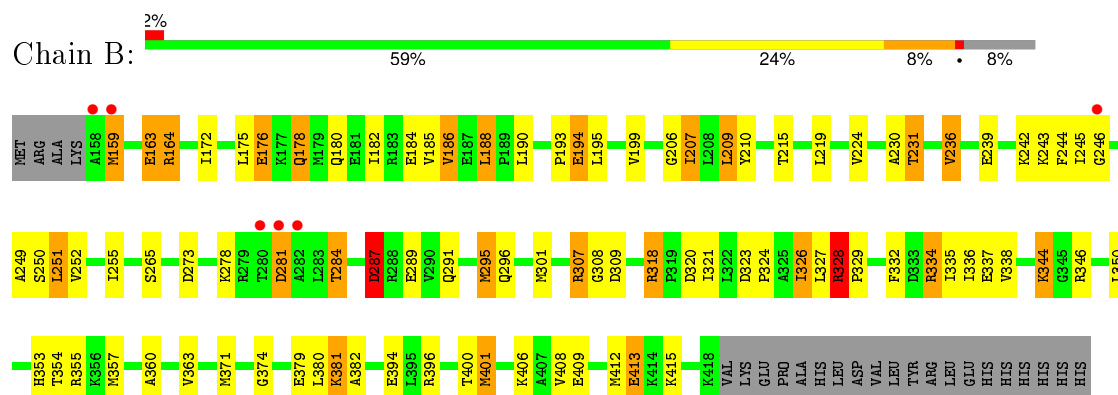
### 3 Residue-property plots

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.

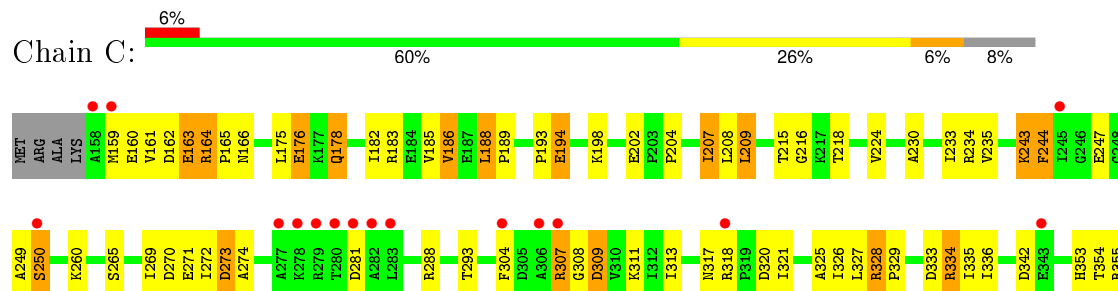
#### • Molecule 1: Proteasome-activating nucleotidase

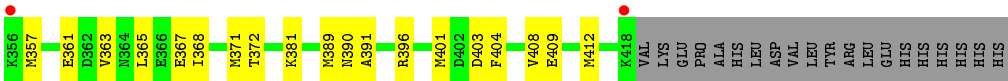


#### • Molecule 1: Proteasome-activating nucleotidase



#### • Molecule 1: Proteasome-activating nucleotidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.42Å 116.42Å 164.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.11 34.57 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-3.11) 95.8 (34.57-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.221 , 0.277 0.205 , 0.255	Depositor DCC
$R_{free}$ test set	1139 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.7	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 94.2	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 22731 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.55	0/2052	0.67	0/2759
1	B	0.61	0/2052	0.78	1/2759 (0.0%)
1	C	0.43	0/2052	0.62	1/2759 (0.0%)
All	All	0.54	0/6156	0.69	2/8277 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	GLY	N-CA-C	-6.10	97.85	113.10
1	C	288	ARG	NE-CZ-NH1	5.99	123.29	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	396	ARG	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	2027	0	2108	67	0
1	B	2027	0	2108	71	0
1	C	2027	0	2108	58	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
2	C	27	0	12	10	0
All	All	6162	0	6360	198	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 16.

All (198) 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:183:ARG:HG2	1:A:183:ARG:HH11	1.09	1.13
1:A:334:ARG:HG2	1:A:334:ARG:HH11	0.97	1.12
1:B:334:ARG:HH11	1:B:334:ARG:HG2	1.15	1.10
1:B:334:ARG:CG	1:B:334:ARG:HH11	1.69	1.03
1:A:334:ARG:HH11	1:A:334:ARG:CG	1.77	0.98
1:B:291:GLN:O	1:B:295:MET:HG2	1.72	0.90
1:A:334:ARG:HG2	1:A:334:ARG:NH1	1.76	0.86
1:A:183:ARG:HG2	1:A:183:ARG:NH1	1.89	0.82
1:B:215:THR:HG21	1:B:338:VAL:O	1.80	0.81
1:C:334:ARG:HH11	1:C:334:ARG:CG	1.93	0.81
1:A:323:ASP:O	1:A:326:ILE:HG22	1.80	0.80
1:B:334:ARG:NH1	1:B:334:ARG:HG2	1.86	0.80
1:B:363:VAL:HA	1:B:401:MET:HG2	1.65	0.79
1:C:334:ARG:HG2	1:C:334:ARG:HH11	1.46	0.78
1:C:404:PHE:O	1:C:408:VAL:HG23	1.83	0.78
2:C:439:ADP:H5'1	2:C:439:ADP:C8	2.18	0.78
1:A:183:ARG:HH11	1:A:183:ARG:CG	1.92	0.78
1:B:327:LEU:HA	1:B:332:PHE:O	1.86	0.76
1:C:353:HIS:HE1	2:C:439:ADP:N3	1.83	0.75
1:B:194:GLU:H	1:B:194:GLU:CD	1.90	0.74
1:B:239:GLU:HA	1:B:242:LYS:HE3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:ARG:HH22	1:B:320:ASP:HB2	1.57	0.70
1:B:184:GLU:HA	1:B:188:LEU:HD22	1.73	0.70
1:A:383:ILE:HG12	1:A:411:ILE:HD12	1.73	0.70
1:A:318:ARG:HH12	1:A:320:ASP:H	1.40	0.69
2:C:439:ADP:H5'	2:C:439:ADP:H8	1.58	0.68
1:B:193:PRO:HD2	1:B:194:GLU:OE2	1.94	0.67
1:A:383:ILE:CG1	1:A:411:ILE:HD12	2.25	0.67
1:C:216:GLY:HA2	2:C:439:ADP:O1A	1.97	0.64
1:B:412:MET:HE2	1:B:412:MET:HA	1.80	0.64
1:A:414:LYS:O	1:A:417:VAL:HG23	1.99	0.63
1:A:409:GLU:HG3	1:A:410:LYS:N	2.14	0.62
1:A:241:VAL:HG12	1:A:241:VAL:O	1.98	0.62
1:B:243:LYS:HB2	1:B:289:GLU:HG2	1.81	0.61
1:B:249:ALA:O	1:B:296:GLN:HG2	2.00	0.61
1:A:269:ILE:CG2	1:A:272:ILE:HG22	2.31	0.61
1:C:244:PHE:HB3	1:C:247:GLU:HB3	1.81	0.61
1:C:163:GLU:O	1:C:164:ARG:C	2.40	0.60
1:A:183:ARG:O	1:A:187:GLU:HB3	2.01	0.60
1:A:231:THR:HB	1:A:265:SER:HB3	1.84	0.59
1:B:413:GLU:HA	1:B:413:GLU:OE1	2.01	0.59
1:A:183:ARG:NH1	1:A:183:ARG:CG	2.56	0.59
1:C:334:ARG:HG2	1:C:334:ARG:NH1	2.10	0.58
1:B:346:ARG:HG2	1:B:380:LEU:HD11	1.86	0.58
1:B:318:ARG:HH12	1:B:320:ASP:H	1.51	0.58
1:A:186:VAL:C	1:A:189:PRO:HD2	2.24	0.57
1:C:270:ASP:O	1:C:271:GLU:HG2	2.03	0.57
1:B:172:ILE:HG12	1:B:219:LEU:HD13	1.86	0.57
1:B:406:LYS:O	1:B:409:GLU:HB3	2.04	0.57
1:B:182:ILE:HD11	1:B:209:LEU:HD11	1.87	0.56
1:B:243:LYS:CB	1:B:289:GLU:HG2	2.36	0.56
2:C:439:ADP:H8	2:C:439:ADP:C5'	2.19	0.55
1:A:269:ILE:HG21	1:A:272:ILE:HG22	1.87	0.55
1:B:215:THR:CG2	1:B:338:VAL:HG12	2.37	0.55
1:B:287:ASP:OD1	1:B:287:ASP:N	2.39	0.55
1:A:172:ILE:HG12	1:A:219:LEU:HD13	1.89	0.55
1:B:185:VAL:HG12	1:B:186:VAL:HG12	1.89	0.55
1:B:334:ARG:HH11	1:B:334:ARG:HG3	1.64	0.54
1:C:391:ALA:HA	1:C:396:ARG:NH2	2.22	0.54
1:C:204:PRO:HG3	1:C:334:ARG:NH1	2.22	0.54
1:B:180:GLN:NE2	1:B:184:GLU:OE1	2.40	0.54
1:A:376:VAL:HG22	1:A:379:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:THR:HB	2:C:439:ADP:O2A	2.08	0.54
1:A:163:GLU:O	1:A:164:ARG:HG2	2.08	0.54
1:B:353:HIS:CD2	1:B:381:LYS:HG2	2.43	0.53
1:A:334:ARG:NH1	1:A:334:ARG:CG	2.46	0.53
1:A:396:ARG:NH2	1:A:403:ASP:OD2	2.41	0.53
1:A:303:GLY:O	1:A:305:ASP:N	2.41	0.53
1:A:318:ARG:NH1	1:A:320:ASP:H	2.05	0.53
1:A:220:LEU:O	1:A:224:VAL:HG23	2.09	0.53
1:B:334:ARG:NH1	1:B:334:ARG:CG	2.39	0.53
1:B:175:LEU:HB3	1:B:178:GLN:HG2	1.91	0.53
1:A:279:ARG:HH11	1:A:284:THR:HA	1.73	0.52
1:B:210:TYR:CZ	1:B:337:GLU:HB2	2.45	0.52
1:B:307:ARG:O	1:B:309:ASP:HB2	2.08	0.52
1:C:160:GLU:HB2	1:C:234:ARG:HB3	1.92	0.51
1:B:328:ARG:O	1:B:328:ARG:HD3	2.10	0.51
1:C:161:VAL:HG22	1:C:233:ILE:HG12	1.93	0.51
1:C:260:LYS:NZ	1:C:304:PHE:HB3	2.26	0.51
1:B:307:ARG:HG2	1:B:309:ASP:HB2	1.91	0.51
2:C:439:ADP:C8	2:C:439:ADP:C5'	2.91	0.51
1:B:353:HIS:CD2	1:B:381:LYS:HE3	2.46	0.51
1:A:353:HIS:CD2	1:A:381:LYS:HG3	2.46	0.50
1:A:280:THR:O	1:A:281:ASP:HB3	2.11	0.50
1:B:186:VAL:HG22	1:B:224:VAL:HG11	1.94	0.50
1:B:159:MET:HG2	1:B:255:ILE:HG12	1.94	0.50
1:C:325:ALA:O	1:C:328:ARG:HB3	2.12	0.50
1:C:208:LEU:HD23	1:C:335:ILE:HG12	1.93	0.50
1:C:308:GLY:O	1:C:309:ASP:HB2	2.13	0.49
1:A:377:GLY:HA3	2:A:439:ADP:N7	2.28	0.49
1:C:178:GLN:NE2	1:C:178:GLN:H	2.11	0.49
1:B:374:GLY:O	1:B:415:LYS:NZ	2.35	0.49
1:C:327:LEU:HD22	1:C:335:ILE:HD11	1.95	0.49
1:A:215:THR:HG21	1:A:338:VAL:O	2.12	0.49
1:C:194:GLU:H	1:C:194:GLU:CD	2.15	0.48
1:C:308:GLY:HA2	1:C:311:LYS:HE2	1.94	0.48
1:C:216:GLY:CA	2:C:439:ADP:O1A	2.62	0.48
1:C:247:GLU:HA	1:C:250:SER:HB2	1.96	0.48
1:B:215:THR:HG22	1:B:338:VAL:HG12	1.96	0.47
1:B:164:ARG:HH22	1:C:193:PRO:HD2	1.79	0.47
1:A:297:LEU:HG	1:A:301:MET:CE	2.44	0.47
1:A:354:THR:HA	1:A:357:MET:HG2	1.97	0.47
1:C:354:THR:HA	1:C:357:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:CG	1:C:334:ARG:NH1	2.62	0.47
1:A:189:PRO:HG3	1:A:196:PHE:CZ	2.50	0.47
1:A:353:HIS:NE2	1:A:381:LYS:HG3	2.30	0.47
1:C:273:ASP:N	1:C:273:ASP:OD1	2.48	0.47
1:A:160:GLU:OE1	1:A:234:ARG:NH1	2.47	0.46
1:B:408:VAL:O	1:B:409:GLU:C	2.54	0.46
1:B:230:ALA:HB1	1:B:265:SER:HA	1.98	0.46
1:A:273:ASP:OD1	1:A:273:ASP:N	2.48	0.46
1:B:281:ASP:N	1:B:281:ASP:OD1	2.49	0.46
1:C:353:HIS:CE1	2:C:439:ADP:N3	2.74	0.46
1:A:230:ALA:HB1	1:A:265:SER:HA	1.96	0.46
1:C:185:VAL:HG13	1:C:204:PRO:HG2	1.97	0.46
1:C:207:ILE:HG12	1:C:313:ILE:HG12	1.96	0.46
1:C:272:ILE:C	1:C:274:ALA:H	2.19	0.46
1:A:186:VAL:HG22	1:A:224:VAL:HG11	1.96	0.46
1:C:175:LEU:HD22	1:C:178:GLN:HG3	1.96	0.46
1:B:244:PHE:HD1	1:B:245:ILE:H	1.63	0.46
1:B:355:ARG:HG2	1:B:355:ARG:O	2.14	0.46
1:B:318:ARG:HD2	1:B:318:ARG:HA	1.70	0.46
1:A:214:GLY:O	1:A:376:VAL:HB	2.16	0.46
1:B:194:GLU:CD	1:B:194:GLU:N	2.66	0.45
1:C:202:GLU:HG2	1:C:307:ARG:HG2	1.99	0.45
1:A:405:ARG:O	1:A:409:GLU:HB3	2.16	0.45
1:B:354:THR:O	1:B:357:MET:HG2	2.17	0.45
1:C:249:ALA:HB2	1:C:293:THR:HA	1.97	0.45
1:C:365:LEU:HD23	1:C:368:ILE:HD12	1.98	0.45
1:B:360:ALA:HB3	1:B:363:VAL:HG23	1.97	0.45
1:A:364:ASN:OD1	1:A:366:GLU:HB2	2.16	0.45
1:C:163:GLU:HG2	1:C:163:GLU:H	1.61	0.45
1:C:243:LYS:HD3	1:C:243:LYS:H	1.80	0.45
1:C:208:LEU:CD1	1:C:272:ILE:HD11	2.47	0.45
1:C:367:GLU:O	1:C:371:MET:HB2	2.17	0.45
1:A:269:ILE:CG2	1:A:272:ILE:CG2	2.96	0.44
1:B:231:THR:HB	1:B:265:SER:HB3	1.99	0.44
1:A:272:ILE:HG21	1:A:272:ILE:HD13	1.73	0.44
1:C:175:LEU:O	1:C:176:GLU:C	2.55	0.44
1:A:362:ASP:O	1:A:401:MET:HG2	2.16	0.44
1:B:236:VAL:HG23	1:B:239:GLU:HB2	2.00	0.44
1:A:318:ARG:HA	1:A:318:ARG:HD2	1.76	0.44
1:A:194:GLU:O	1:A:198:LYS:HD3	2.18	0.44
1:A:304:PHE:C	1:A:304:PHE:CD1	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:GLU:CA	1:B:413:GLU:OE1	2.65	0.43
1:A:279:ARG:HB3	1:A:280:THR:H	1.59	0.43
1:A:169:TYR:C	1:A:171:ASP:H	2.21	0.43
1:B:207:ILE:HD12	1:B:336:ILE:HD12	2.00	0.43
1:B:206:GLY:O	1:B:332:PHE:HA	2.18	0.43
1:B:318:ARG:NH2	1:B:320:ASP:HB2	2.30	0.43
1:C:230:ALA:HB1	1:C:265:SER:HA	2.00	0.43
1:B:180:GLN:O	1:B:184:GLU:HG2	2.18	0.43
1:C:188:LEU:HB3	1:C:189:PRO:HD3	1.99	0.43
1:C:363:VAL:HA	1:C:401:MET:HG2	2.00	0.43
1:A:245:ILE:HG13	1:A:245:ILE:H	1.38	0.43
1:A:301:MET:C	1:A:303:GLY:N	2.71	0.43
1:C:390:ASN:ND2	1:C:403:ASP:O	2.52	0.43
1:B:182:ILE:O	1:B:186:VAL:HG13	2.19	0.43
1:B:350:LEU:O	1:B:354:THR:HG23	2.19	0.43
1:A:307:ARG:HB2	1:A:308:GLY:H	1.46	0.42
1:B:164:ARG:NH2	1:C:194:GLU:OE2	2.52	0.42
1:B:207:ILE:CD1	1:B:336:ILE:HD12	2.49	0.42
1:C:328:ARG:HA	1:C:329:PRO:HD2	1.70	0.42
1:A:406:LYS:HA	1:A:409:GLU:HG2	2.00	0.42
1:A:164:ARG:O	1:A:164:ARG:CG	2.67	0.42
1:C:260:LYS:HZ1	1:C:304:PHE:HB3	1.84	0.42
1:A:167:VAL:O	1:A:223:ALA:HA	2.19	0.42
1:B:239:GLU:O	1:B:242:LYS:HD2	2.19	0.42
1:C:318:ARG:HH12	1:C:320:ASP:H	1.68	0.42
1:C:164:ARG:HA	1:C:165:PRO:HD2	1.91	0.42
1:C:235:VAL:HB	1:C:269:ILE:HG23	2.01	0.42
1:B:379:GLU:O	1:B:382:ALA:HB3	2.19	0.42
1:B:163:GLU:O	1:B:164:ARG:HG2	2.20	0.42
1:C:186:VAL:HG22	1:C:224:VAL:HG11	2.01	0.42
1:C:209:LEU:HD12	1:C:336:ILE:HB	2.01	0.42
1:B:400:THR:HG22	1:B:401:MET:N	2.35	0.41
1:B:252:VAL:HA	1:B:255:ILE:HD12	2.02	0.41
1:A:263:ALA:HA	1:A:264:PRO:C	2.40	0.41
1:C:162:ASP:OD2	1:C:165:PRO:HB3	2.20	0.41
1:A:210:TYR:CZ	1:A:337:GLU:HB2	2.54	0.41
1:A:363:VAL:HA	1:A:401:MET:HG2	2.01	0.41
1:A:178:GLN:H	1:A:178:GLN:HE21	1.68	0.41
1:A:178:GLN:NE2	1:A:178:GLN:H	2.18	0.41
1:B:195:LEU:O	1:B:199:VAL:HG23	2.19	0.41
1:B:188:LEU:HA	1:B:188:LEU:HD12	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLY:O	1:A:304:PHE:C	2.59	0.41
1:B:344:LYS:H	1:B:344:LYS:HG2	1.49	0.41
1:A:205:LYS:HD3	1:A:305:ASP:HB2	2.03	0.41
1:A:383:ILE:HG13	1:A:411:ILE:HD12	2.00	0.41
1:B:324:PRO:C	1:B:326:ILE:H	2.22	0.41
1:B:295:MET:HA	1:B:295:MET:CE	2.51	0.41
1:B:251:LEU:O	1:B:255:ILE:HG13	2.21	0.40
1:C:182:ILE:O	1:C:186:VAL:HG13	2.21	0.40
1:A:347:LEU:HA	1:A:350:LEU:HD12	2.02	0.40
1:C:216:GLY:N	2:C:439:ADP:O1A	2.55	0.40
1:A:163:GLU:H	1:A:163:GLU:HG2	1.60	0.40
1:C:272:ILE:C	1:C:274:ALA:N	2.75	0.40
1:C:317:ASN:HD22	1:C:317:ASN:N	2.18	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	259/285 (91%)	220 (85%)	34 (13%)	5 (2%)	10	40
1	B	259/285 (91%)	222 (86%)	31 (12%)	6 (2%)	8	35
1	C	259/285 (91%)	226 (87%)	26 (10%)	7 (3%)	6	31
All	All	777/855 (91%)	668 (86%)	91 (12%)	18 (2%)	8	35

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ARG
1	A	285	GLY
1	B	176	GLU
1	C	307	ARG

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Mol	Chain	Res	Type
1	C	309	ASP
1	C	355	ARG
1	A	281	ASP
1	A	304	PHE
1	B	329	PRO
1	C	273	ASP
1	B	284	THR
1	B	328	ARG
1	C	164	ARG
1	C	342	ASP
1	A	280	THR
1	C	281	ASP
1	B	287	ASP
1	B	246	GLY

### 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	216/239 (90%)	183 (85%)	33 (15%)	3	14
1	B	216/239 (90%)	180 (83%)	36 (17%)	3	11
1	C	216/239 (90%)	189 (88%)	27 (12%)	6	22
All	All	648/717 (90%)	552 (85%)	96 (15%)	4	16

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	MET
1	A	163	GLU
1	A	168	ARG
1	A	176	GLU
1	A	178	GLN
1	A	183	ARG
1	A	185	VAL
1	A	186	VAL

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Mol	Chain	Res	Type
1	A	190	LEU
1	A	194	GLU
1	A	201	ILE
1	A	207	ILE
1	A	209	LEU
1	A	242	LYS
1	A	245	ILE
1	A	253	LYS
1	A	279	ARG
1	A	284	THR
1	A	287	ASP
1	A	291	GLN
1	A	304	PHE
1	A	305	ASP
1	A	307	ARG
1	A	317	ASN
1	A	321	ILE
1	A	328	ARG
1	A	334	ARG
1	A	355	ARG
1	A	381	LYS
1	A	389	MET
1	A	401	MET
1	A	409	GLU
1	A	412	MET
1	B	159	MET
1	B	163	GLU
1	B	164	ARG
1	B	176	GLU
1	B	178	GLN
1	B	186	VAL
1	B	188	LEU
1	B	190	LEU
1	B	194	GLU
1	B	207	ILE
1	B	209	LEU
1	B	231	THR
1	B	236	VAL
1	B	250	SER
1	B	251	LEU
1	B	273	ASP
1	B	278	LYS

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Mol	Chain	Res	Type
1	B	281	ASP
1	B	284	THR
1	B	287	ASP
1	B	295	MET
1	B	301	MET
1	B	307	ARG
1	B	318	ARG
1	B	321	ILE
1	B	323	ASP
1	B	326	ILE
1	B	328	ARG
1	B	334	ARG
1	B	335	ILE
1	B	344	LYS
1	B	371	MET
1	B	381	LYS
1	B	394	GLU
1	B	401	MET
1	B	413	GLU
1	C	159	MET
1	C	163	GLU
1	C	166	ASN
1	C	176	GLU
1	C	178	GLN
1	C	183	ARG
1	C	186	VAL
1	C	188	LEU
1	C	194	GLU
1	C	198	LYS
1	C	207	ILE
1	C	209	LEU
1	C	215	THR
1	C	243	LYS
1	C	244	PHE
1	C	250	SER
1	C	321	ILE
1	C	326	ILE
1	C	328	ARG
1	C	333	ASP
1	C	334	ARG
1	C	361	GLU
1	C	372	THR

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Mol	Chain	Res	Type
1	C	381	LYS
1	C	389	MET
1	C	409	GLU
1	C	412	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	192	HIS
1	A	353	HIS
1	A	358	ASN
1	B	178	GLN
1	B	229	ASN
1	B	291	GLN
1	B	353	HIS
1	C	166	ASN
1	C	178	GLN
1	C	291	GLN
1	C	317	ASN
1	C	353	HIS

### 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 ⓘ

3 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	A	439	-	22,29,29	1.04	1 (4%)	27,45,45	2.12	5 (18%)
2	ADP	B	439	-	22,29,29	0.95	1 (4%)	27,45,45	2.18	4 (14%)
2	ADP	C	439	-	22,29,29	0.95	1 (4%)	27,45,45	1.91	5 (18%)

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	A	439	-	-	0/12/32/32	0/3/3/3
2	ADP	B	439	-	-	0/12/32/32	0/3/3/3
2	ADP	C	439	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	439	ADP	C5-C4	2.28	1.45	1.40
2	C	439	ADP	C5-C4	2.94	1.47	1.40
2	A	439	ADP	C5-C4	3.03	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	ADP	N3-C2-N1	-8.26	122.57	128.89
2	A	439	ADP	N3-C2-N1	-7.64	123.04	128.89
2	C	439	ADP	N3-C2-N1	-6.55	123.88	128.89
2	B	439	ADP	C2'-C1'-N9	-4.16	107.93	114.29
2	C	439	ADP	PA-O3A-PB	-3.83	119.84	132.67
2	A	439	ADP	PA-O3A-PB	-3.46	121.08	132.67
2	A	439	ADP	C2'-C1'-N9	-3.45	109.02	114.29
2	A	439	ADP	C4-C5-N7	-3.36	106.39	109.48
2	B	439	ADP	PA-O3A-PB	-3.36	121.39	132.67
2	B	439	ADP	C4-C5-N7	-2.61	107.08	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	439	ADP	C4-C5-N7	-2.56	107.13	109.48
2	C	439	ADP	C2'-C1'-N9	-2.20	110.93	114.29
2	A	439	ADP	O3B-PB-O1B	2.44	118.43	110.58
2	C	439	ADP	C4'-O4'-C1'	3.23	113.27	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	439	ADP	1	0
2	C	439	ADP	10	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	261/285 (91%)	-0.20	3 (1%) 82 66	88, 100, 113, 124	0
1	B	261/285 (91%)	-0.14	6 (2%) 64 40	86, 100, 113, 120	0
1	C	261/285 (91%)	0.08	18 (6%) 20 7	87, 100, 113, 123	0
All	All	783/855 (91%)	-0.09	27 (3%) 49 24	86, 100, 113, 124	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	THR	6.3
1	C	280	THR	6.1
1	C	282	ALA	5.5
1	A	283	LEU	4.1
1	B	158	ALA	3.4
1	C	304	PHE	3.3
1	C	307	ARG	3.3
1	A	304	PHE	3.2
1	B	282	ALA	3.2
1	C	418	LYS	3.1
1	C	318	ARG	3.0
1	A	280	THR	2.9
1	C	283	LEU	2.9
1	C	158	ALA	2.9
1	B	246	GLY	2.8
1	C	356	LYS	2.6
1	C	250	SER	2.5
1	C	281	ASP	2.5
1	C	306	ALA	2.5
1	C	343	GLU	2.4
1	C	159	MET	2.3
1	B	159	MET	2.3
1	C	277	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	278	LYS	2.1
1	B	281	ASP	2.1
1	C	245	ILE	2.0
1	C	279	ARG	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(Å <sup>2</sup> )	Q<0.9
2	ADP	C	439	27/27	0.90	0.15	-0.95	89,91,95,97	0
2	ADP	A	439	27/27	0.93	0.16	-1.36	72,81,84,84	0
2	ADP	B	439	27/27	0.95	0.12	-1.79	60,65,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.