WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 06:49 PM 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)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.263
Clashscore		16
Ramachandran outliers		2.3%
Sidechain outliers		14.8%
RSRZ outliers		0.6%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
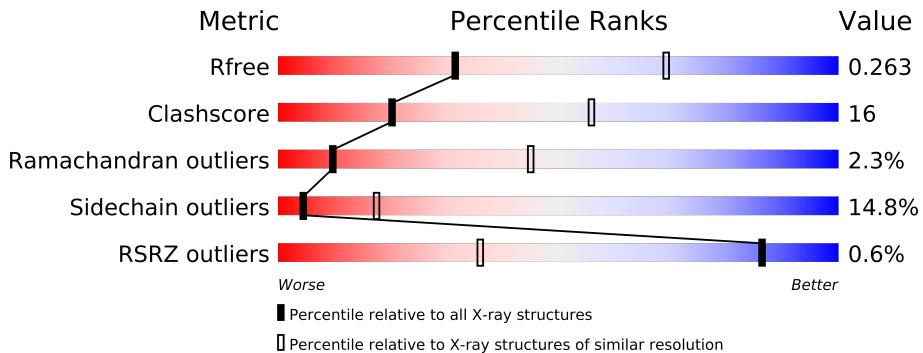
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	
1	C	285	
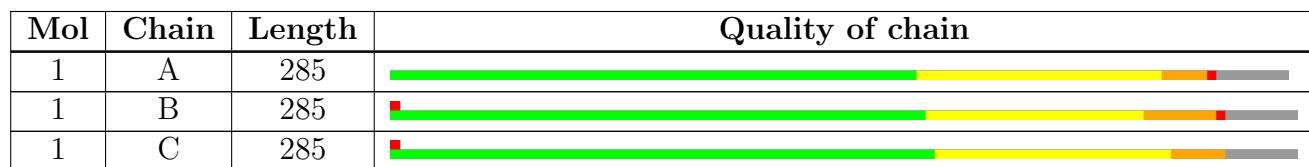
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6162 atoms, of which 0 are hydrogen and 0 are deuterium.

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-activatingnucleotidase.

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: $C_{10}H_{15}N_5O_{10}P_2$).
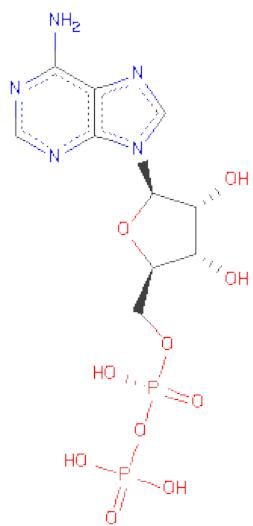

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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-activatingnucleotidase

Chain A:
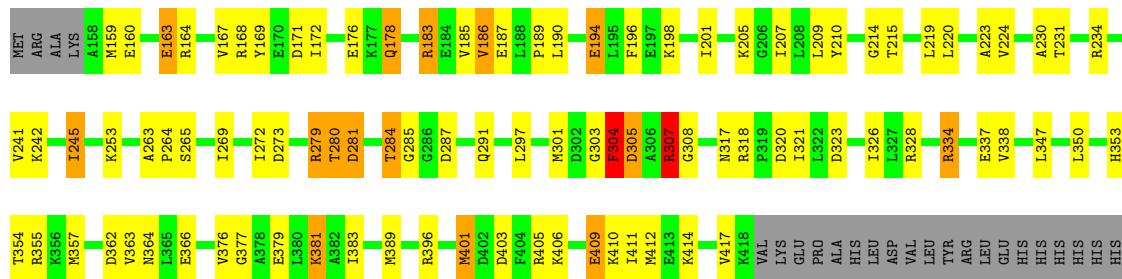
- Molecule 1: Proteasome-activatingnucleotidase

Chain B:
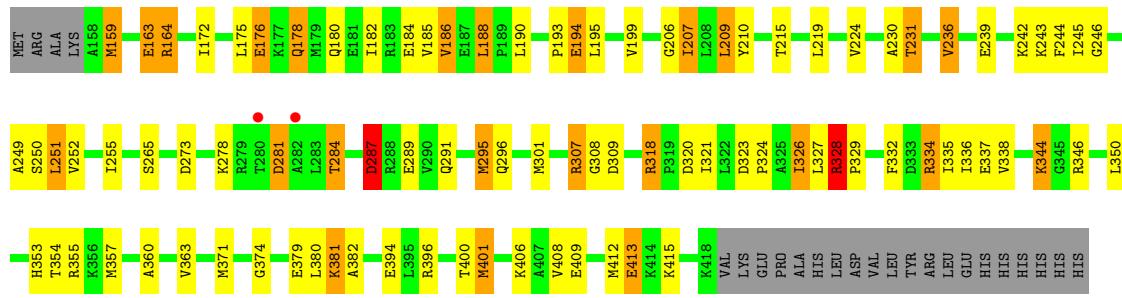
- Molecule 1: Proteasome-activatingnucleotidase

Chain C:
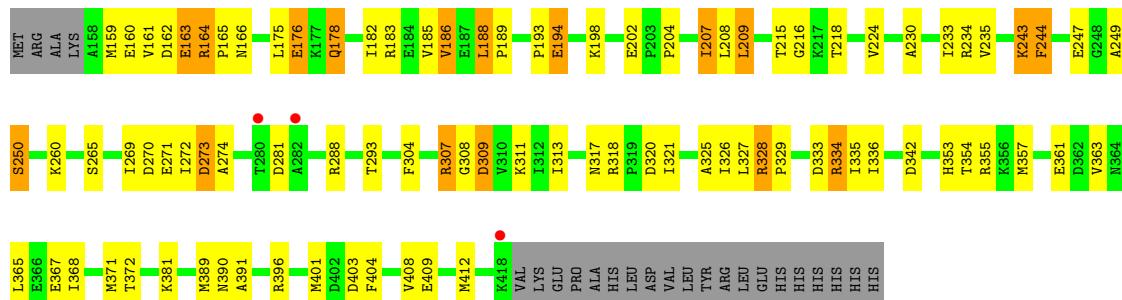
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.82 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.221 , 0.277 0.216 , 0.263	Depositor DCC
R_{free} test set	1092 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	86.7	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 96.7	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 22731 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.

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	0.55	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(^{o})	Ideal(^{o})
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 Close contacts (i)

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (198) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:H5'1	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
1:C:218:THR:HB	2:C:439:ADP:O2A	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	259/285 (91%)	220 (85%)	34 (13%)	5 (2%)	12	51
1	B	259/285 (91%)	222 (86%)	31 (12%)	6 (2%)	10	45
1	C	259/285 (91%)	226 (87%)	26 (10%)	7 (3%)	8	39
All	All	777/855 (91%)	668 (86%)	91 (12%)	18 (2%)	10	45

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
1	C	309	ASP
1	C	355	ARG
1	A	281	ASP
1	A	304	PHE
1	B	329	PRO
1	C	273	ASP

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Mol	Chain	Res	Type
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%)	4	15
1	B	216/239 (90%)	180 (83%)	36 (17%)	3	11
1	C	216/239 (90%)	189 (88%)	27 (12%)	7	25
All	All	648/717 (90%)	552 (85%)	96 (15%)	4	17

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	-	29,29,29	1.11	2 (6%)	45,45,45	1.93	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ADP	B	439	-	29,29,29	1.17	2 (6%)	45,45,45	1.93	8 (17%)
2	ADP	C	439	-	29,29,29	1.02	2 (6%)	45,45,45	1.85	9 (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	A	439	-	-	0/16/32/32	0/1/3/3
2	ADP	B	439	-	-	0/16/32/32	0/1/3/3
2	ADP	C	439	-	-	0/16/32/32	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	439	ADP	C4-N9	-3.86	1.32	1.37
2	A	439	ADP	C5-C4	3.03	1.47	1.40
2	C	439	ADP	C5-C4	2.94	1.47	1.40
2	A	439	ADP	C4-N9	-2.71	1.33	1.37
2	C	439	ADP	C4-N9	-2.48	1.34	1.37
2	B	439	ADP	C5-C4	2.28	1.45	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	ADP	N3-C2-N1	-7.34	122.57	128.71
2	A	439	ADP	N3-C2-N1	-6.78	123.04	128.71
2	C	439	ADP	N3-C2-N1	-5.78	123.88	128.71
2	C	439	ADP	N3-C4-N9	5.53	135.41	125.43
2	B	439	ADP	N3-C4-N9	5.33	135.06	125.43
2	A	439	ADP	N3-C4-N9	5.20	134.82	125.43
2	C	439	ADP	PA-O3A-PB	-4.04	119.84	131.68
2	A	439	ADP	C4-C5-N7	-3.66	106.39	109.52
2	A	439	ADP	PA-O3A-PB	-3.62	121.08	131.68
2	B	439	ADP	PA-O3A-PB	-3.51	121.39	131.68
2	B	439	ADP	C5-C4-N3	-3.47	118.14	125.70
2	C	439	ADP	C4'-O4'-C1'	3.24	113.27	109.75
2	C	439	ADP	C5-C4-N3	-3.23	118.67	125.70
2	A	439	ADP	C5-C4-N3	-3.20	118.72	125.70
2	A	439	ADP	O4'-C1'-N9	3.16	111.38	108.44
2	B	439	ADP	C2-N3-C4	2.91	122.29	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	439	ADP	C4-C5-N7	-2.86	107.08	109.52
2	C	439	ADP	C4-C5-N7	-2.80	107.13	109.52
2	A	439	ADP	C2-N3-C4	2.73	121.78	114.01
2	B	439	ADP	C3'-C2'-C1'	2.52	104.86	100.91
2	A	439	ADP	O3B-PB-O1B	2.44	118.43	110.44
2	C	439	ADP	C2-N3-C4	2.36	120.73	114.01
2	C	439	ADP	C3'-C2'-C1'	2.28	104.48	100.91
2	A	439	ADP	C8-N9-C4	2.19	108.57	106.90
2	C	439	ADP	C8-N9-C4	2.12	108.52	106.90
2	B	439	ADP	C2'-C1'-N9	-2.08	107.93	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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^2)	Q<0.9
1	A	261/285 (91%)	-0.32	0	100	100	88, 100, 113, 124	0
1	B	261/285 (91%)	-0.27	2 (0%)	83	28	86, 100, 113, 120	0
1	C	261/285 (91%)	-0.14	3 (1%)	77	22	87, 100, 113, 123	0
All	All	783/855 (91%)	-0.24	5 (0%)	86	36	86, 100, 113, 124	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	THR	4.1
1	C	418	LYS	4.0
1	C	282	ALA	2.4
1	B	280	THR	2.3
1	B	282	ALA	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 ⓘ

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. 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, 95th 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	ADP	B	439	27/27	0.17	-0.02	60,65,70,71	0
2	ADP	A	439	27/27	0.17	-0.20	72,81,84,84	0
2	ADP	C	439	27/27	0.15	-0.24	89,91,95,97	0

6.5 Other polymers ⓘ

There are no such residues in this entry.