



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:42 am GMT

PDB ID : 4A59
Title : Crystal structure of Toxoplasma gondii nucleoside triphosphate diphosphohydrolase 3 (NTPDase3) in complex with AMP
Authors : Krug, U.; Zebisch, M.; Straeter, N.
Deposited on : 2011-10-24
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

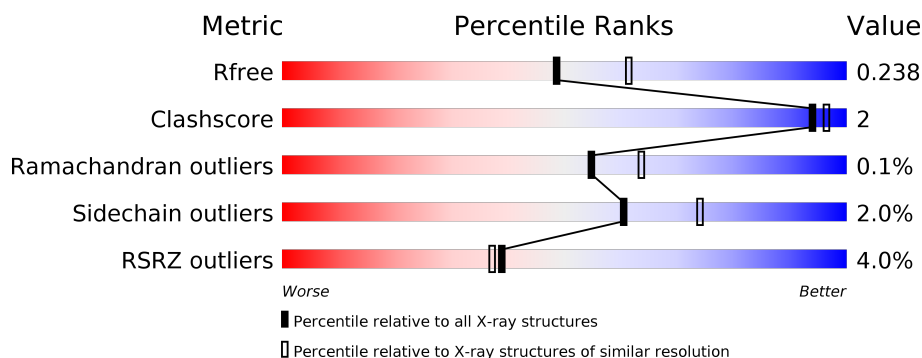
1 Overall quality at a glance

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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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 ≥ 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	611	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	B	611	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>
1	C	611	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>
1	D	611	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19482 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 NUCLEOSIDE-TRIPHOSPHATASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	7	0
			4650	2923	825	875	27			
1	B	593	Total	C	N	O	S	0	2	0
			4612	2899	818	868	27			
1	C	590	Total	C	N	O	S	0	1	0
			4584	2883	812	862	27			
1	D	595	Total	C	N	O	S	0	3	0
			4629	2910	820	872	27			

There are 32 discrepancies between the modelled and reference sequences:

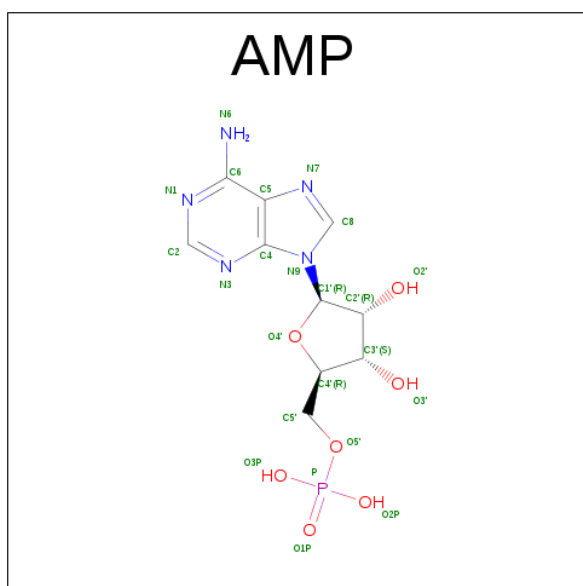
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	EXPRESSION TAG	UNP Q27893
A	629	GLU	-	EXPRESSION TAG	UNP Q27893
A	630	HIS	-	EXPRESSION TAG	UNP Q27893
A	631	HIS	-	EXPRESSION TAG	UNP Q27893
A	632	HIS	-	EXPRESSION TAG	UNP Q27893
A	633	HIS	-	EXPRESSION TAG	UNP Q27893
A	634	HIS	-	EXPRESSION TAG	UNP Q27893
A	635	HIS	-	EXPRESSION TAG	UNP Q27893
B	25	MET	-	EXPRESSION TAG	UNP Q27893
B	629	GLU	-	EXPRESSION TAG	UNP Q27893
B	630	HIS	-	EXPRESSION TAG	UNP Q27893
B	631	HIS	-	EXPRESSION TAG	UNP Q27893
B	632	HIS	-	EXPRESSION TAG	UNP Q27893
B	633	HIS	-	EXPRESSION TAG	UNP Q27893
B	634	HIS	-	EXPRESSION TAG	UNP Q27893
B	635	HIS	-	EXPRESSION TAG	UNP Q27893
C	25	MET	-	EXPRESSION TAG	UNP Q27893
C	629	GLU	-	EXPRESSION TAG	UNP Q27893
C	630	HIS	-	EXPRESSION TAG	UNP Q27893
C	631	HIS	-	EXPRESSION TAG	UNP Q27893
C	632	HIS	-	EXPRESSION TAG	UNP Q27893

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Chain	Residue	Modelled	Actual	Comment	Reference
C	633	HIS	-	EXPRESSION TAG	UNP Q27893
C	634	HIS	-	EXPRESSION TAG	UNP Q27893
C	635	HIS	-	EXPRESSION TAG	UNP Q27893
D	25	MET	-	EXPRESSION TAG	UNP Q27893
D	629	GLU	-	EXPRESSION TAG	UNP Q27893
D	630	HIS	-	EXPRESSION TAG	UNP Q27893
D	631	HIS	-	EXPRESSION TAG	UNP Q27893
D	632	HIS	-	EXPRESSION TAG	UNP Q27893
D	633	HIS	-	EXPRESSION TAG	UNP Q27893
D	634	HIS	-	EXPRESSION TAG	UNP Q27893
D	635	HIS	-	EXPRESSION TAG	UNP Q27893

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

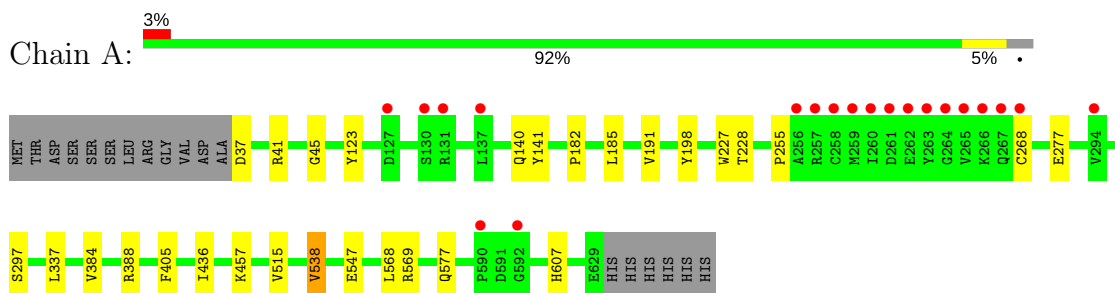
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	307	Total 310	O 310	0	3
3	B	166	Total 169	O 169	0	3
3	C	225	Total 226	O 226	0	1
3	D	186	Total 187	O 187	0	1

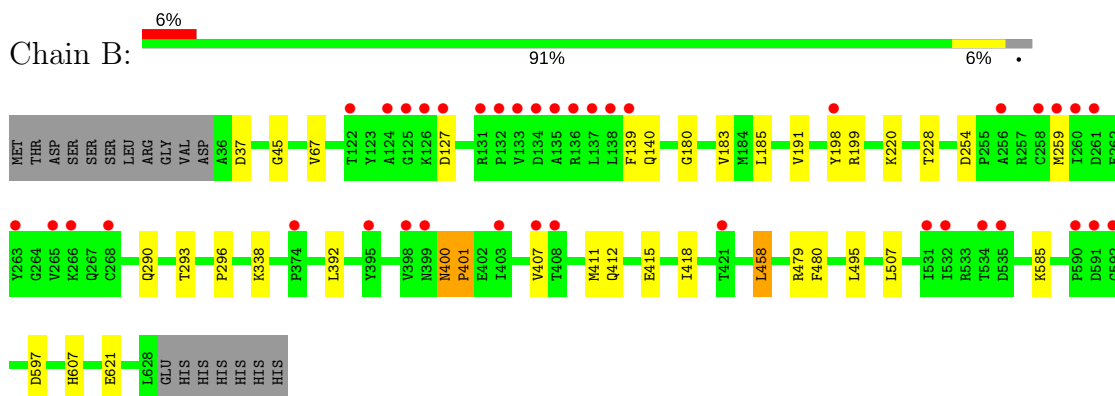
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

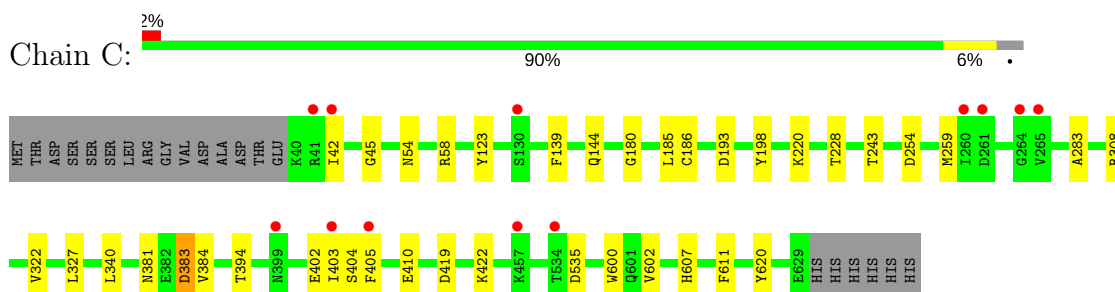
• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1

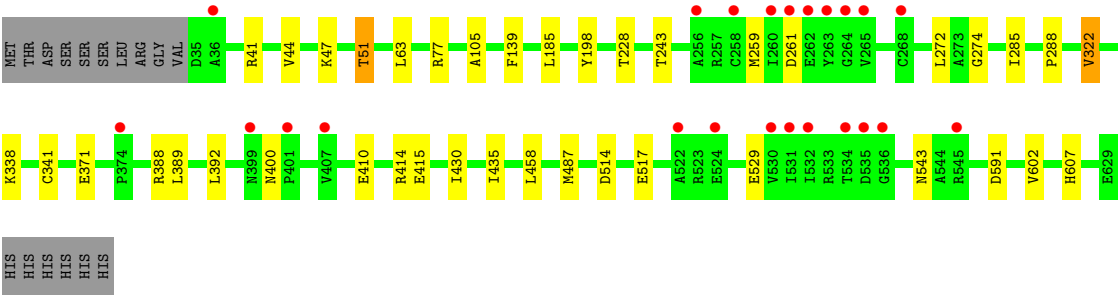


• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.17Å 166.03Å 97.94Å 90.00° 97.15° 90.00°	Depositor
Resolution (Å)	42.30 – 2.20 42.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.30-2.20) 99.7 (42.30-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.180 , 0.228 0.189 , 0.238	Depositor DCC
R_{free} test set	1399 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19482	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	0/4760	0.68	0/6439
1	B	0.48	0/4707	0.69	0/6369
1	C	0.50	0/4676	0.69	0/6327
1	D	0.49	0/4727	0.68	0/6397
All	All	0.50	0/18870	0.68	0/25532

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 [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 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	4650	0	4644	15	0
1	B	4612	0	4597	18	0
1	C	4584	0	4568	16	0
1	D	4629	0	4612	17	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	46	0	24	0	0
3	A	310	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	169	0	0	0	0
3	C	226	0	0	0	0
3	D	187	0	0	2	0
All	All	19482	0	18481	58	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 2.

All (58) 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:277[B]:GLU:OE1	3:A:2106[B]:HOH:O	1.54	1.23
1:B:191:VAL:HG12	1:B:199:ARG:HG3	1.71	0.71
1:B:185:LEU:HB3	1:B:228:THR:HG23	1.82	0.61
1:B:180:GLY:HA2	1:B:220:LYS:HB2	1.84	0.59
1:A:185:LEU:HB3	1:A:228:THR:HG23	1.85	0.59
1:C:185:LEU:HB3	1:C:228:THR:HG23	1.85	0.58
1:A:337:LEU:HD22	1:A:436:ILE:HD13	1.86	0.58
1:D:274:GLY:HA3	1:D:487:MET:HE1	1.84	0.58
1:D:410:GLU:HG2	1:D:414:ARG:HE	1.69	0.57
1:D:392:LEU:HG	3:D:2138:HOH:O	2.04	0.56
1:A:515:VAL:HG11	1:A:569:ARG:HG3	1.87	0.56
1:B:400:ASN:HB3	1:B:401:PRO:HD3	1.88	0.56
1:A:45:GLY:HA3	1:D:139:PHE:O	2.06	0.55
1:C:381:ASN:OD1	1:C:383:ASP:HB2	2.07	0.55
1:C:402:GLU:HA	1:C:405:PHE:CE2	2.42	0.55
1:A:457:LYS:O	1:B:407:VAL:HG21	2.06	0.54
1:A:191:VAL:HG23	3:A:2030:HOH:O	2.08	0.54
1:D:47:LYS:O	1:D:51:THR:HG23	2.08	0.53
1:B:45:GLY:HA3	1:C:139:PHE:O	2.08	0.52
1:C:123:TYR:OH	1:C:144:GLN:HG2	2.09	0.52
1:B:338:LYS:HE2	1:B:418:ILE:HG13	1.92	0.51
1:D:415:GLU:HG3	1:D:458:LEU:HD12	1.93	0.49
1:A:515:VAL:HG22	1:A:568:LEU:HB3	1.96	0.48
1:D:77:ARG:HE	1:D:105:ALA:HB1	1.79	0.48
1:A:405:PHE:CE1	1:B:296:PRO:HG2	2.50	0.47
1:C:419:ASP:HB3	1:C:422:LYS:HD2	1.96	0.46
1:A:123:TYR:HB3	1:A:141:TYR:CD2	2.51	0.46
1:D:322[A]:VAL:HG23	3:D:2117:HOH:O	2.16	0.46
1:B:479:ARG:HD2	1:B:480:PHE:CE1	2.51	0.46
1:A:255:PRO:HB3	1:A:268:CYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:THR:HG23	1:C:602:VAL:HB	1.98	0.46
1:C:193:ASP:HB2	1:C:394:THR:HG21	1.98	0.45
1:C:186:CYS:HB2	1:C:600:TRP:CH2	2.51	0.45
1:B:495:LEU:HD22	1:B:585:LYS:HB3	1.98	0.45
1:D:272:LEU:HB2	1:D:288:PRO:HG3	2.00	0.44
1:D:41:ARG:HA	1:D:44:VAL:HG22	1.99	0.44
1:D:514:ASP:OD2	1:D:517:GLU:HB2	2.18	0.44
1:B:412:GLN:HG3	1:B:458:LEU:HD23	2.00	0.43
1:B:67:VAL:HB	1:B:183:VAL:HG22	2.01	0.43
1:C:54:ASN:HB3	1:C:58:ARG:HE	1.83	0.43
1:A:538:VAL:HG13	1:A:547:GLU:HB2	2.01	0.43
1:D:341:CYS:HB2	1:D:430:ILE:HG21	2.01	0.43
1:D:285:ILE:HB	1:D:322[B]:VAL:HG22	2.02	0.42
1:B:290:GLN:O	1:B:293:THR:HB	2.20	0.41
1:A:182:PRO:HB3	1:A:227:TRP:CZ3	2.55	0.41
1:B:621:GLU:HG2	1:C:620:TYR:HB2	2.01	0.41
1:B:507:LEU:HD23	1:B:507:LEU:HA	1.95	0.41
1:D:243:THR:HG23	1:D:602:VAL:HB	2.02	0.41
1:D:338:LYS:HD3	1:D:389:LEU:HD11	2.02	0.41
1:D:185:LEU:HB3	1:D:228:THR:HG23	2.02	0.41
1:B:411:MET:O	1:B:415:GLU:HG2	2.21	0.41
1:B:139:PHE:O	1:C:45:GLY:HA3	2.20	0.41
1:A:37:ASP:HB2	1:A:41:ARG:HH12	1.85	0.41
1:C:308:ARG:HD2	1:C:611:PHE:CE2	2.56	0.40
1:A:140:GLN:HB2	1:D:41:ARG:HB3	2.04	0.40
1:C:283:ALA:HB3	1:C:327:LEU:HB2	2.03	0.40
1:C:180:GLY:HA2	1:C:220:LYS:HB2	2.04	0.40
1:B:140:GLN:HG3	1:C:42:ILE:HG22	2.03	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	598/611 (98%)	585 (98%)	12 (2%)	1 (0%)	51	58
1	B	593/611 (97%)	583 (98%)	8 (1%)	2 (0%)	44	49
1	C	589/611 (96%)	584 (99%)	5 (1%)	0	100	100
1	D	596/611 (98%)	584 (98%)	12 (2%)	0	100	100
All	All	2376/2444 (97%)	2336 (98%)	37 (2%)	3 (0%)	55	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	PRO
1	B	400	ASN
1	A	297	SER

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	512/521 (98%)	505 (99%)	7 (1%)	71	84
1	B	506/521 (97%)	497 (98%)	9 (2%)	64	77
1	C	503/521 (96%)	491 (98%)	12 (2%)	54	67
1	D	508/521 (98%)	493 (97%)	15 (3%)	46	58
All	All	2029/2084 (97%)	1986 (98%)	43 (2%)	60	72

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	TYR
1	A	384	VAL
1	A	388[A]	ARG
1	A	388[B]	ARG
1	A	538	VAL
1	A	577	GLN
1	A	607	HIS
1	B	37	ASP

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Mol	Chain	Res	Type
1	B	127	ASP
1	B	198	TYR
1	B	254	ASP
1	B	259	MET
1	B	392	LEU
1	B	458	LEU
1	B	597	ASP
1	B	607	HIS
1	C	198	TYR
1	C	254	ASP
1	C	259	MET
1	C	322	VAL
1	C	340	LEU
1	C	383	ASP
1	C	384	VAL
1	C	403	ILE
1	C	404	SER
1	C	410	GLU
1	C	535	ASP
1	C	607	HIS
1	D	51	THR
1	D	63	LEU
1	D	198	TYR
1	D	259	MET
1	D	261	ASP
1	D	322[A]	VAL
1	D	322[B]	VAL
1	D	371	GLU
1	D	388	ARG
1	D	400	ASN
1	D	435	ILE
1	D	529	GLU
1	D	543	ASN
1	D	591	ASP
1	D	607	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	ASN
1	B	43	ASN
1	B	400	ASN

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Mol	Chain	Res	Type
1	C	54	ASN
1	D	43	ASN
1	D	400	ASN
1	D	548	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	AMP	A	700	-	22,25,25	1.58	2 (9%)	24,38,38	1.48	4 (16%)
2	AMP	B	700	-	22,25,25	1.62	2 (9%)	24,38,38	1.05	2 (8%)
2	AMP	C	700	-	22,25,25	1.35	3 (13%)	24,38,38	1.38	2 (8%)
2	AMP	D	700	-	22,25,25	1.23	2 (9%)	24,38,38	1.30	2 (8%)
2	AMP	D	701	-	22,25,25	1.47	3 (13%)	24,38,38	1.31	3 (12%)

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	AMP	A	700	-	-	0/6/26/26	0/3/3/3
2	AMP	B	700	-	-	0/6/26/26	0/3/3/3
2	AMP	C	700	-	-	0/6/26/26	0/3/3/3
2	AMP	D	700	-	-	0/6/26/26	0/3/3/3
2	AMP	D	701	-	-	0/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	AMP	C2-N1	2.34	1.38	1.33
2	C	700	AMP	C2-N1	2.35	1.38	1.33
2	D	701	AMP	C2-N3	2.70	1.36	1.32
2	C	700	AMP	C2-N3	2.84	1.36	1.32
2	D	700	AMP	C2-N3	2.98	1.37	1.32
2	D	700	AMP	O4'-C1'	3.15	1.45	1.41
2	C	700	AMP	O4'-C1'	3.16	1.45	1.41
2	B	700	AMP	C2-N3	4.05	1.38	1.32
2	A	700	AMP	C2-N3	4.22	1.39	1.32
2	D	701	AMP	O4'-C1'	4.69	1.47	1.41
2	A	700	AMP	O4'-C1'	5.20	1.48	1.41
2	B	700	AMP	O4'-C1'	5.44	1.48	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	AMP	N3-C2-N1	-4.20	125.20	128.86
2	C	700	AMP	N3-C2-N1	-3.51	125.80	128.86
2	A	700	AMP	C1'-N9-C4	-3.32	120.89	126.64
2	D	700	AMP	N3-C2-N1	-3.07	126.18	128.86
2	A	700	AMP	O2'-C2'-C1'	-2.73	103.06	111.61
2	D	701	AMP	C4'-O4'-C1'	-2.70	106.89	109.77
2	D	701	AMP	C1'-N9-C4	-2.65	122.06	126.64
2	D	701	AMP	N3-C2-N1	-2.43	126.74	128.86
2	B	700	AMP	N3-C2-N1	-2.41	126.75	128.86
2	C	700	AMP	O5'-P-O1P	-2.06	100.70	106.47
2	B	700	AMP	C4-C5-N7	2.15	111.49	109.41
2	A	700	AMP	C4-C5-N7	2.32	111.66	109.41
2	D	700	AMP	O5'-P-O1P	2.68	113.99	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	593/611 (97%)	-0.15	20 (3%) 46 43	19, 30, 64, 98	0
1	B	593/611 (97%)	0.11	39 (6%) 19 18	23, 42, 80, 141	0
1	C	590/611 (96%)	-0.25	12 (2%) 65 63	21, 36, 64, 108	0
1	D	595/611 (97%)	-0.09	23 (3%) 40 38	19, 40, 76, 106	0
All	All	2371/2444 (97%)	-0.09	94 (3%) 39 37	19, 37, 74, 141	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	8.0
1	B	137	LEU	7.8
1	A	260	ILE	7.6
1	A	259	MET	6.9
1	C	405	PHE	5.8
1	B	260	ILE	5.5
1	D	535	ASP	5.3
1	A	592	GLY	5.1
1	B	256	ALA	5.1
1	D	265	VAL	5.0
1	D	258	CYS	4.9
1	D	534	THR	4.8
1	A	264	GLY	4.7
1	B	265	VAL	4.7
1	D	263	TYR	4.6
1	A	268	CYS	4.5
1	A	267	GLN	4.4
1	D	374	PRO	4.4
1	B	132	PRO	4.4
1	A	294	VAL	4.2
1	C	265	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	258	CYS	4.2
1	A	258	CYS	4.1
1	C	260	ILE	4.1
1	C	42	ILE	4.0
1	B	125	GLY	4.0
1	B	259	MET	4.0
1	B	135	ALA	3.8
1	B	407	VAL	3.8
1	B	591	ASP	3.7
1	A	131	ARG	3.7
1	B	266	LYS	3.6
1	B	408	THR	3.5
1	B	535	ASP	3.4
1	B	133	VAL	3.3
1	C	264	GLY	3.2
1	C	41	ARG	3.2
1	D	532	ILE	3.1
1	A	256	ALA	3.1
1	B	531	ILE	3.1
1	A	127	ASP	3.1
1	B	124	ALA	3.1
1	A	263	TYR	3.1
1	B	398	VAL	3.1
1	B	138	LEU	3.0
1	D	399	ASN	3.0
1	A	130	SER	3.0
1	A	590	PRO	3.0
1	B	399	ASN	2.9
1	B	534	THR	2.9
1	B	268	CYS	2.9
1	B	134	ASP	2.9
1	B	127	ASP	2.9
1	B	421	THR	2.8
1	B	395	TYR	2.8
1	B	592	GLY	2.7
1	A	137	LEU	2.7
1	B	532	ILE	2.7
1	B	403	ILE	2.7
1	D	268	CYS	2.6
1	B	590	PRO	2.6
1	C	130	SER	2.6
1	D	262	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	374	PRO	2.5
1	D	530	VAL	2.5
1	D	36	ALA	2.5
1	A	257	ARG	2.5
1	D	536	GLY	2.5
1	C	261	ASP	2.4
1	D	264	GLY	2.4
1	B	126	LYS	2.4
1	D	260	ILE	2.4
1	A	266	LYS	2.3
1	D	531	ILE	2.3
1	C	457	LYS	2.3
1	B	263	TYR	2.3
1	D	545	ARG	2.3
1	A	261	ASP	2.2
1	D	522	ALA	2.2
1	B	122	THR	2.2
1	B	139	PHE	2.2
1	C	399	ASN	2.2
1	B	261	ASP	2.2
1	D	524	GLU	2.1
1	C	403	ILE	2.1
1	B	198	TYR	2.1
1	C	534	THR	2.1
1	B	131	ARG	2.1
1	A	262	GLU	2.1
1	D	256	ALA	2.1
1	D	401	PRO	2.0
1	D	407	VAL	2.0
1	B	136	ARG	2.0
1	D	261	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	AMP	D	701	23/23	0.89	0.22	0.51	57,75,88,90	0
2	AMP	B	700	23/23	0.95	0.13	-0.40	28,43,57,58	0
2	AMP	C	700	23/23	0.96	0.12	-0.62	29,35,47,48	0
2	AMP	D	700	23/23	0.95	0.12	-0.70	36,45,50,53	0
2	AMP	A	700	23/23	0.98	0.09	-1.45	23,30,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.