



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:53 AM UTC

PDB ID : 1V26 / pdb_00001v26
Title : Crystal structure of tt0168 from *Thermus thermophilus* HB8
Authors : Hisanaga, Y.; Ago, H.; Nakatsu, T.; Hamada, K.; Ida, K.; Kanda, H.; Yamamoto, M.; Hori, T.; Arii, Y.; Sugahara, M.; Kuramitsu, S.; Yokoyama, S.; Miyano, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2003-10-07
Resolution : 2.50 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

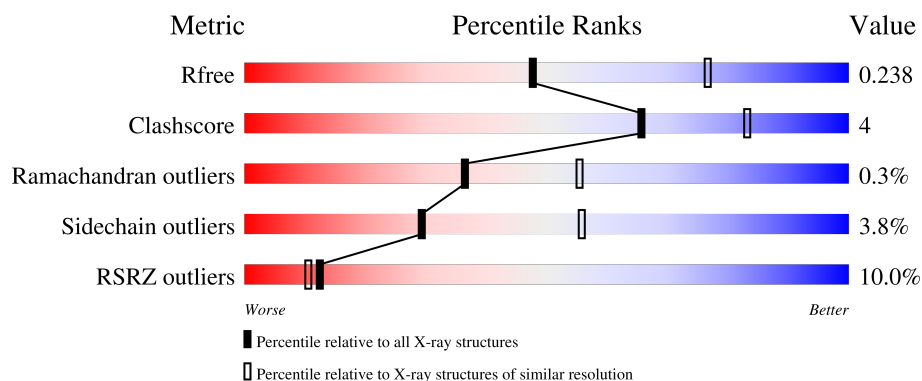
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	541	8% 79% 11% 10%
1	B	541	11% 84% 10% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8316 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.

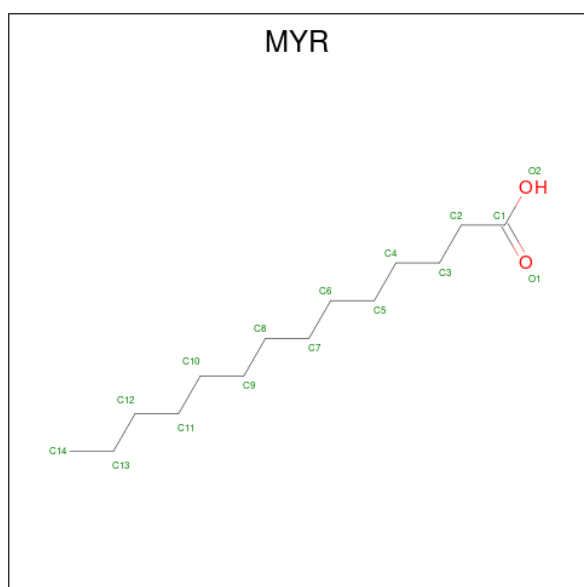
- Molecule 1 is a protein called long-chain-fatty-acid-CoA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3802	2436	661	695	10			
1	B	510	Total	C	N	O	S	0	0	0
			3964	2536	688	730	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

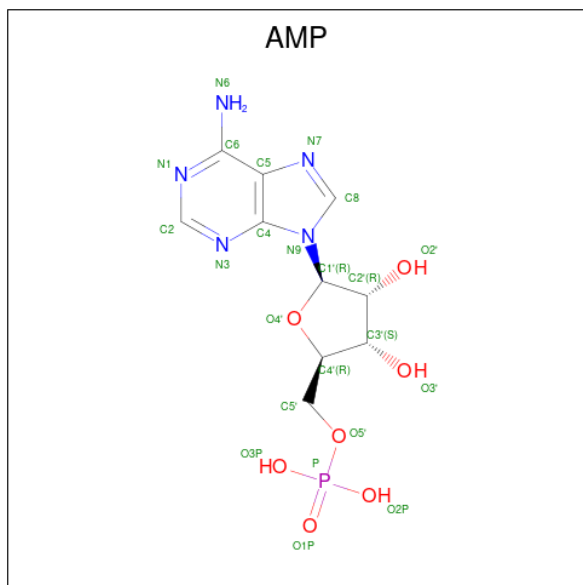
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	14	1		
3	B	1	Total	C	O	0	0
			15	14	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

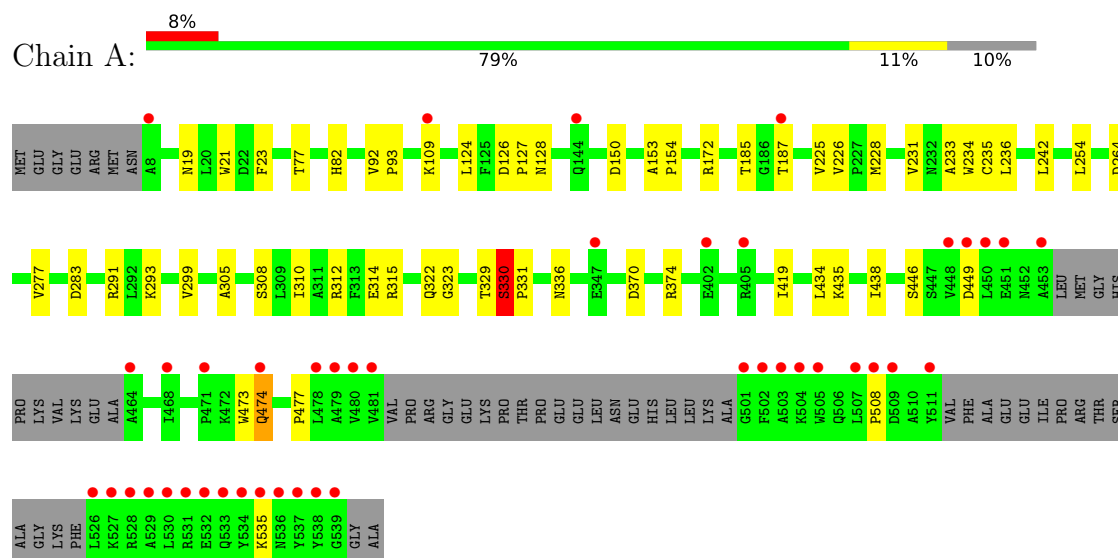
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	251	Total	O	0	0
			251	251		
5	B	221	Total	O	0	0
			221	221		

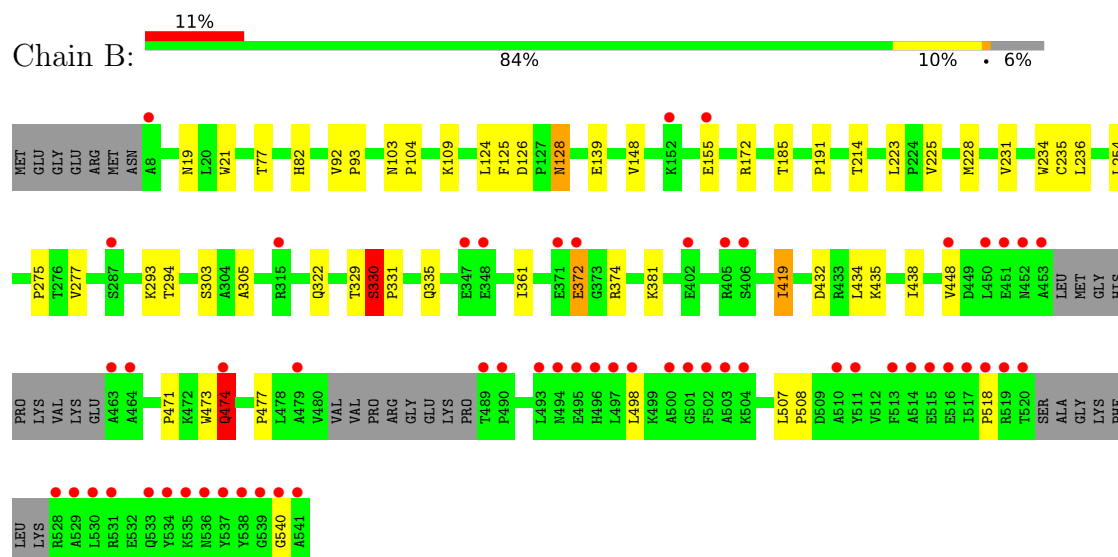
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: long-chain-fatty-acid-CoA synthetase



- Molecule 1: long-chain-fatty-acid-CoA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.51Å 101.38Å 176.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 2.50 46.10 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.10-2.50) 99.9 (46.10-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.204 , 0.240 (Not available) , 0.238	Depositor DCC
R_{free} test set	4116 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.4	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	0.92	EDS
Total number of atoms	8316	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: MYR, AMP, MG

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	0.37	0/3890	0.82	4/5285 (0.1%)
1	B	0.38	0/4056	0.82	4/5511 (0.1%)
All	All	0.38	0/7946	0.82	8/10796 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	TRP	CA-C-N	-10.78	105.31	122.24
1	A	473	TRP	C-N-CA	-10.78	105.31	122.24
1	B	473	TRP	CA-C-N	-9.48	104.45	121.81
1	B	473	TRP	C-N-CA	-9.48	104.45	121.81
1	A	330	SER	N-CA-C	6.21	123.53	109.81
1	B	330	SER	N-CA-C	5.88	122.81	109.81
1	B	474	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	474	GLN	OE1-CD-NE2	-5.20	117.40	122.60

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	3802	0	3814	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3964	0	3963	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	27	3	0
3	B	15	0	27	2	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
5	A	251	0	0	1	0
5	B	221	0	0	0	0
All	All	8316	0	7855	60	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 4.

All (60) 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:471:PRO:HD3	1:B:540:GLY:HA2	1.24	1.14
1:B:438:ILE:HG21	1:B:477:PRO:HD3	1.48	0.96
1:B:330:SER:N	1:B:331:PRO:HA	2.01	0.76
1:B:225:VAL:HG11	1:B:277:VAL:HG11	1.67	0.75
1:B:471:PRO:HD3	1:B:540:GLY:CA	2.12	0.74
1:A:330:SER:N	1:A:331:PRO:HA	2.04	0.72
1:A:310:ILE:O	1:A:314:GLU:HG2	1.92	0.70
1:B:372:GLU:HB2	1:B:374:ARG:HD3	1.79	0.63
1:A:308:SER:O	1:A:312:ARG:HB2	2.00	0.61
1:B:329:THR:C	1:B:331:PRO:HA	2.26	0.61
1:B:19:ASN:HD22	1:B:21:TRP:H	1.47	0.61
1:B:275:PRO:HB2	1:B:474:GLN:NE2	2.16	0.61
1:A:474:GLN:HG3	5:A:3091:HOH:O	2.01	0.59
1:A:446:SER:HB3	1:A:449:ASP:HB2	1.85	0.58
1:B:305:ALA:H	1:B:322:GLN:NE2	2.01	0.58
1:B:92:VAL:HB	1:B:93:PRO:HD3	1.85	0.57
1:B:335:GLN:HE21	1:B:361:ILE:HG21	1.70	0.56
1:B:82:HIS:HE1	1:B:126:ASP:OD1	1.89	0.56
1:A:329:THR:C	1:A:331:PRO:HA	2.32	0.55
1:B:471:PRO:CD	1:B:540:GLY:HA2	2.17	0.54
1:A:19:ASN:HD22	1:A:21:TRP:H	1.56	0.54
1:B:128:ASN:H	1:B:128:ASN:HD22	1.55	0.52
1:A:264:ASP:HB3	1:A:293:LYS:HE3	1.91	0.52
1:B:293:LYS:HG3	1:B:294:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:HB	1:A:93:PRO:HD3	1.91	0.51
1:B:438:ILE:HD13	1:B:477:PRO:HG3	1.91	0.51
1:A:419:ILE:HD11	1:A:434:LEU:HG	1.94	0.49
1:A:438:ILE:HD13	1:A:477:PRO:HB3	1.94	0.49
1:B:305:ALA:H	1:B:322:GLN:HE22	1.61	0.48
1:B:275:PRO:HB2	1:B:474:GLN:HE22	1.79	0.48
1:B:125:PHE:CZ	1:B:148:VAL:HG22	2.48	0.47
1:B:214:THR:HG21	3:B:2001:MYR:H111	1.96	0.47
1:A:228:MET:HA	1:A:233:ALA:HB2	1.97	0.46
1:A:82:HIS:HE1	1:A:126:ASP:OD1	1.98	0.46
1:A:128:ASN:HD22	1:A:128:ASN:H	1.63	0.46
1:B:477:PRO:HB2	1:B:508:PRO:HA	1.98	0.46
1:A:23:PHE:CE1	1:A:242:LEU:HD13	2.52	0.45
1:A:477:PRO:HG2	1:A:508:PRO:HA	1.99	0.45
1:B:234:TRP:CD2	3:B:2001:MYR:H62	2.51	0.45
1:A:305:ALA:H	1:A:322:GLN:NE2	2.14	0.45
1:A:127:PRO:HG3	1:A:150:ASP:HB2	1.99	0.45
1:A:323:GLY:HA3	3:A:1001:MYR:H72	1.99	0.44
1:B:419:ILE:HB	1:B:432:ASP:HB3	1.99	0.44
1:B:372:GLU:HG3	1:B:374:ARG:NH1	2.33	0.44
1:A:234:TRP:CE2	3:A:1001:MYR:H51	2.53	0.43
1:B:128:ASN:H	1:B:128:ASN:ND2	2.16	0.43
1:A:225:VAL:HG11	1:A:277:VAL:HG11	1.99	0.43
1:B:498:LEU:HD21	1:B:507:LEU:HD11	2.00	0.43
1:A:77:THR:HA	1:A:124:LEU:O	2.18	0.43
1:A:370:ASP:OD2	1:A:374:ARG:HB2	2.19	0.42
1:B:77:THR:HA	1:B:124:LEU:O	2.20	0.42
1:A:128:ASN:H	1:A:128:ASN:ND2	2.18	0.41
1:A:153:ALA:HA	1:A:154:PRO:HD3	1.91	0.41
1:A:305:ALA:H	1:A:322:GLN:HE22	1.69	0.41
1:A:299:VAL:HG11	3:A:1001:MYR:H101	2.03	0.40
1:B:185:THR:HG22	1:B:191:PRO:HG3	2.03	0.40
1:B:225:VAL:HG13	1:B:254:LEU:HD22	2.03	0.40
1:B:419:ILE:HD11	1:B:434:LEU:HG	2.04	0.40
1:B:103:ASN:HA	1:B:104:PRO:HD3	1.89	0.40
1:A:225:VAL:HG13	1:A:254:LEU:HD22	2.03	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	477/541 (88%)	465 (98%)	11 (2%)	1 (0%)	43	63
1	B	502/541 (93%)	489 (97%)	11 (2%)	2 (0%)	30	49
All	All	979/1082 (90%)	954 (97%)	22 (2%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	SER
1	B	330	SER
1	B	518	PRO

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	395/437 (90%)	381 (96%)	14 (4%)	32	58
1	B	411/437 (94%)	394 (96%)	17 (4%)	27	53
All	All	806/874 (92%)	775 (96%)	31 (4%)	29	56

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	172	ARG
1	A	185	THR

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Mol	Chain	Res	Type
1	A	187	THR
1	A	226	VAL
1	A	231	VAL
1	A	235	CYS
1	A	236	LEU
1	A	283	ASP
1	A	291	ARG
1	A	315	ARG
1	A	336	ASN
1	A	435	LYS
1	A	535	LYS
1	B	109	LYS
1	B	128	ASN
1	B	139	GLU
1	B	155	GLU
1	B	172	ARG
1	B	223	LEU
1	B	228	MET
1	B	231	VAL
1	B	235	CYS
1	B	236	LEU
1	B	303	SER
1	B	372	GLU
1	B	381	LYS
1	B	419	ILE
1	B	435	LYS
1	B	448	VAL
1	B	474	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	82	HIS
1	A	128	ASN
1	A	247	GLN
1	A	322	GLN
1	A	335	GLN
1	A	336	ASN
1	A	474	GLN
1	A	536	ASN
1	B	19	ASN

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Mol	Chain	Res	Type
1	B	55	GLN
1	B	82	HIS
1	B	128	ASN
1	B	145	HIS
1	B	322	GLN
1	B	335	GLN
1	B	336	ASN
1	B	474	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	MYR	B	2001	4	13,14,15	0.24	0	12,13,15	0.67	0
4	AMP	B	2002	2,3	25,25,25	1.08	2 (8%)	37,38,38	2.03	8 (21%)
3	MYR	A	1001	4	13,14,15	0.26	0	12,13,15	0.67	0
4	AMP	A	1002	2,3	25,25,25	1.07	2 (8%)	37,38,38	1.98	8 (21%)

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
3	MYR	B	2001	4	-	7/12/12/13	-
4	AMP	B	2002	2,3	-	0/10/26/26	0/3/3/3
3	MYR	A	1001	4	-	7/12/12/13	-
4	AMP	A	1002	2,3	-	0/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	AMP	P-O1P	2.84	1.59	1.50
4	A	1002	AMP	P-O1P	2.79	1.59	1.50
4	A	1002	AMP	C8-N7	2.30	1.36	1.31
4	B	2002	AMP	C8-N7	2.17	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	AMP	C5-C4-N3	-5.01	119.82	126.72
4	B	2002	AMP	C5-C4-N3	-4.87	120.02	126.72
4	B	2002	AMP	N3-C2-N1	-4.85	121.23	128.58
4	B	2002	AMP	C4-N9-C8	4.70	110.68	105.74
4	A	1002	AMP	N3-C2-N1	-4.57	121.66	128.58
4	A	1002	AMP	C4-N9-C8	4.50	110.46	105.74
4	B	2002	AMP	N9-C8-N7	-4.31	107.83	113.94
4	A	1002	AMP	N9-C8-N7	-4.19	107.99	113.94
4	A	1002	AMP	N3-C4-N9	3.79	133.62	127.17
4	B	2002	AMP	N3-C4-N9	3.75	133.55	127.17
4	B	2002	AMP	C2-N3-C4	3.41	120.16	111.83
4	A	1002	AMP	C2-N3-C4	3.36	120.03	111.83
4	B	2002	AMP	C4-C5-N7	-2.89	107.28	110.58
4	A	1002	AMP	C4-C5-N7	-2.87	107.30	110.58
4	B	2002	AMP	C5-N7-C8	2.76	107.79	103.45
4	A	1002	AMP	C5-N7-C8	2.70	107.69	103.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

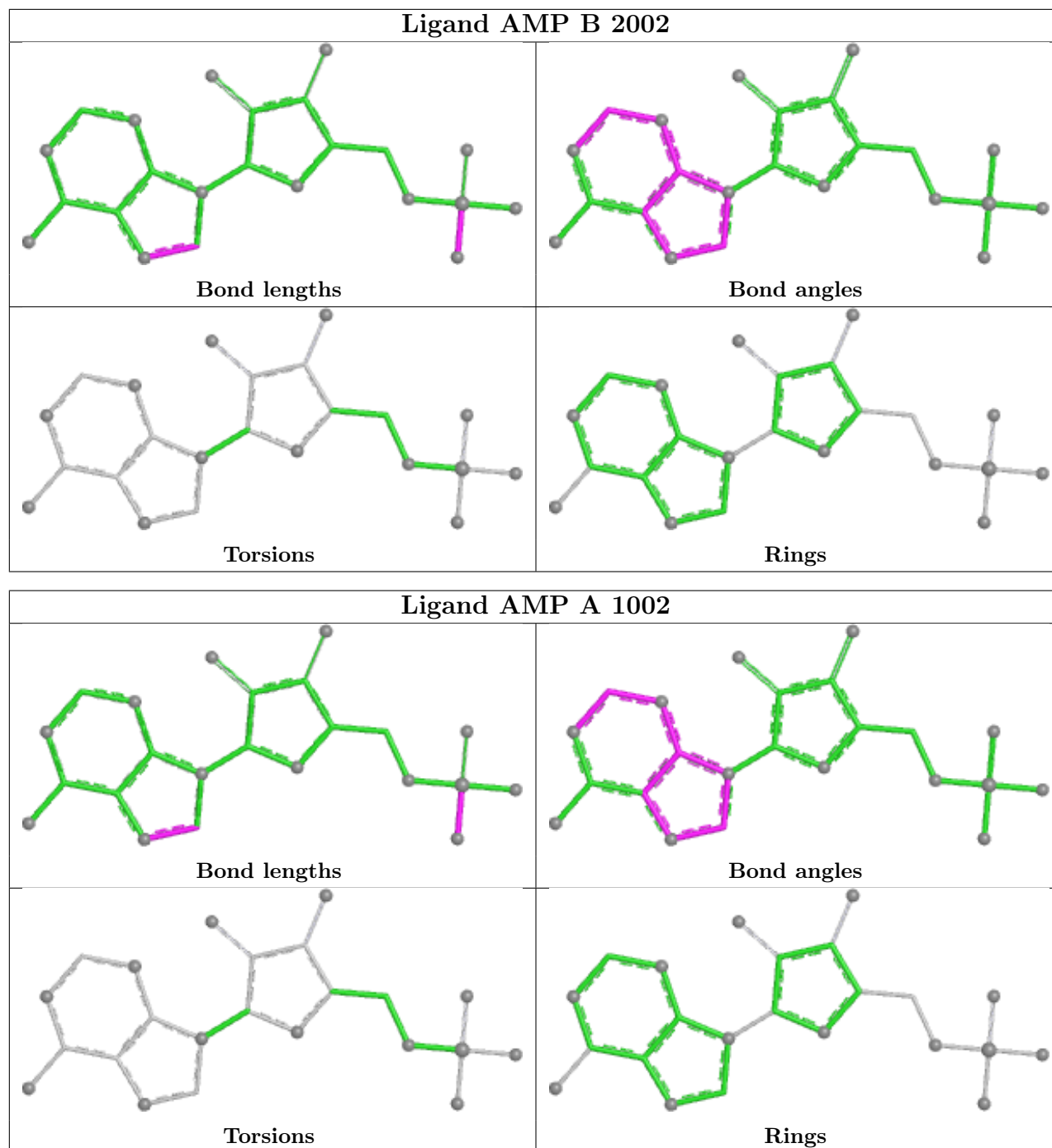
Mol	Chain	Res	Type	Atoms
3	B	2001	MYR	C5-C6-C7-C8
3	B	2001	MYR	C7-C8-C9-C10
3	A	1001	MYR	C6-C7-C8-C9
3	B	2001	MYR	C6-C7-C8-C9
3	A	1001	MYR	C9-C10-C11-C12
3	B	2001	MYR	C4-C5-C6-C7
3	A	1001	MYR	C5-C6-C7-C8
3	B	2001	MYR	C3-C4-C5-C6
3	A	1001	MYR	C2-C3-C4-C5
3	A	1001	MYR	C10-C11-C12-C13
3	B	2001	MYR	C11-C12-C13-C14
3	A	1001	MYR	C11-C12-C13-C14
3	A	1001	MYR	C1-C2-C3-C4
3	B	2001	MYR	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	MYR	2	0
3	A	1001	MYR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [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, 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	489/541 (90%)	0.35	43 (8%)	15 14	10, 21, 70, 100	0
1	B	510/541 (94%)	0.35	57 (11%)	10 8	11, 21, 71, 102	0
All	All	999/1082 (92%)	0.35	100 (10%)	12 10	10, 21, 70, 102	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	LEU	7.9
1	B	520	THR	5.9
1	B	541	ALA	5.8
1	A	501	GLY	5.7
1	A	539	GLY	5.4
1	B	463	ALA	5.1
1	A	464	ALA	4.8
1	B	528	ARG	4.6
1	B	493	LEU	4.5
1	A	481	VAL	4.4
1	B	517	ILE	4.3
1	A	530	LEU	4.2
1	B	8	ALA	4.1
1	B	500	ALA	4.0
1	B	498	LEU	3.9
1	A	480	VAL	3.9
1	A	8	ALA	3.9
1	A	507	LEU	3.9
1	B	489	THR	3.8
1	A	528	ARG	3.8
1	B	518	PRO	3.7
1	A	453	ALA	3.6
1	B	497	LEU	3.6
1	A	511	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	453	ALA	3.4
1	A	534	TYR	3.4
1	B	474	GLN	3.3
1	A	531	ARG	3.3
1	B	510	ALA	3.3
1	B	448	VAL	3.3
1	B	531	ARG	3.2
1	A	505	TRP	3.2
1	A	504	LYS	3.2
1	B	513	PHE	3.1
1	A	402	GLU	3.1
1	B	516	GLU	3.1
1	B	503	ALA	3.1
1	A	502	PHE	3.1
1	A	449	ASP	3.1
1	A	537	TYR	3.1
1	B	514	ALA	3.0
1	B	502	PHE	3.0
1	B	501	GLY	3.0
1	B	452	ASN	3.0
1	A	527	LYS	3.0
1	A	508	PRO	2.9
1	B	490	PRO	2.9
1	B	287	SER	2.9
1	A	529	ALA	2.8
1	A	451	GLU	2.8
1	A	478	LEU	2.8
1	A	503	ALA	2.7
1	B	494	ASN	2.7
1	B	530	LEU	2.7
1	A	533	GLN	2.7
1	B	533	GLN	2.7
1	A	187	THR	2.7
1	B	371	GLU	2.7
1	A	535	LYS	2.6
1	A	448	VAL	2.6
1	B	155	GLU	2.6
1	A	538	TYR	2.6
1	B	534	TYR	2.6
1	B	450	LEU	2.6
1	B	464	ALA	2.6
1	B	515	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	539	GLY	2.5
1	B	540	GLY	2.4
1	B	511	TYR	2.4
1	B	315	ARG	2.4
1	B	348	GLU	2.4
1	A	450	LEU	2.4
1	B	536	ASN	2.4
1	A	479	ALA	2.4
1	A	532	GLU	2.4
1	A	468	ILE	2.3
1	B	519	ARG	2.3
1	B	496	HIS	2.3
1	B	479	ALA	2.3
1	B	372	GLU	2.3
1	B	406	SER	2.3
1	B	402	GLU	2.3
1	B	537	TYR	2.3
1	A	474	GLN	2.2
1	A	509	ASP	2.2
1	B	347	GLU	2.2
1	B	538	TYR	2.2
1	B	535	LYS	2.2
1	A	347	GLU	2.2
1	B	495	GLU	2.2
1	A	471	PRO	2.2
1	A	536	ASN	2.1
1	A	405	ARG	2.1
1	A	109	LYS	2.1
1	B	451	GLU	2.1
1	B	152	LYS	2.1
1	A	144	GLN	2.1
1	B	405	ARG	2.1
1	B	504	LYS	2.1
1	B	529	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

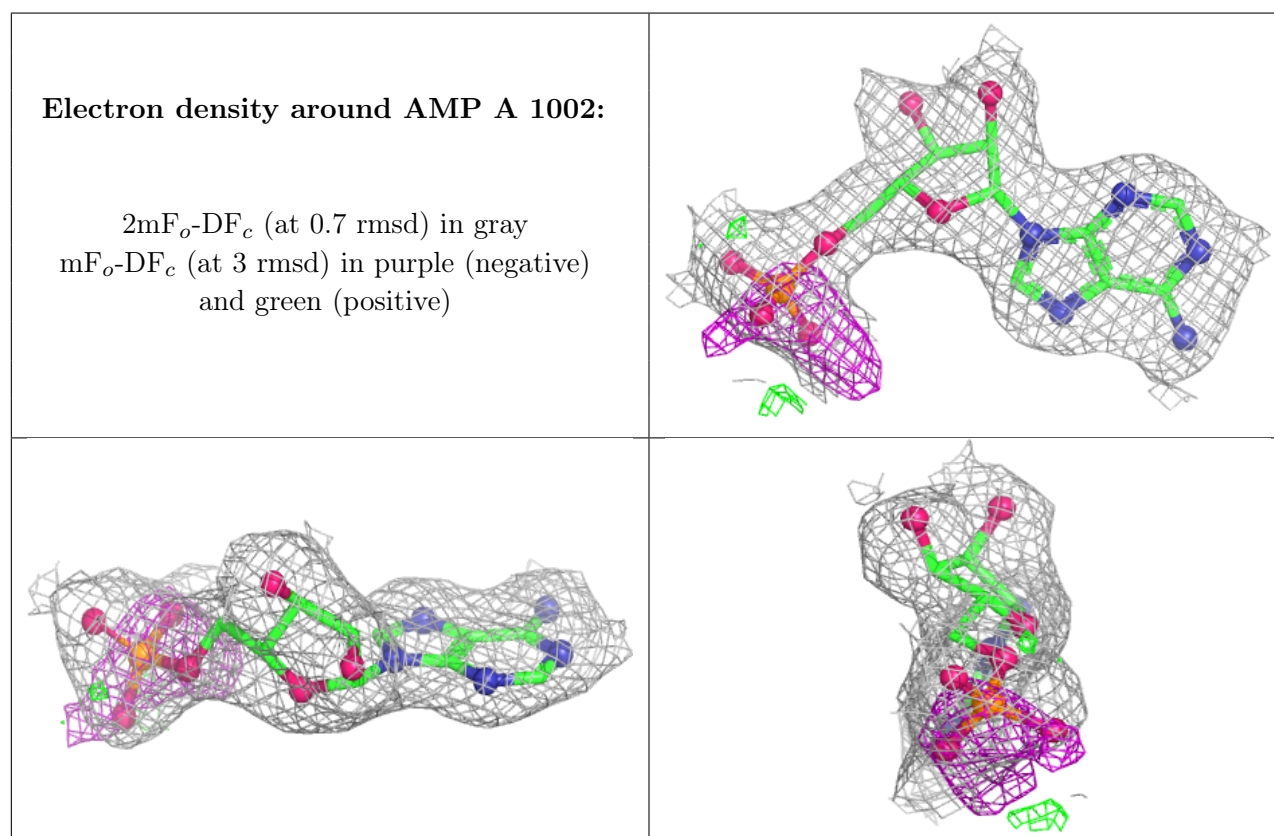
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

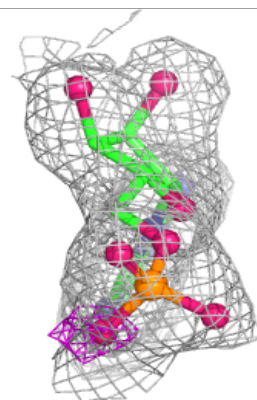
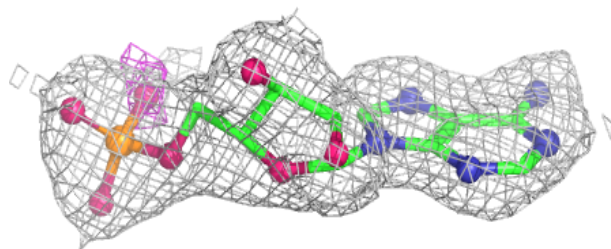
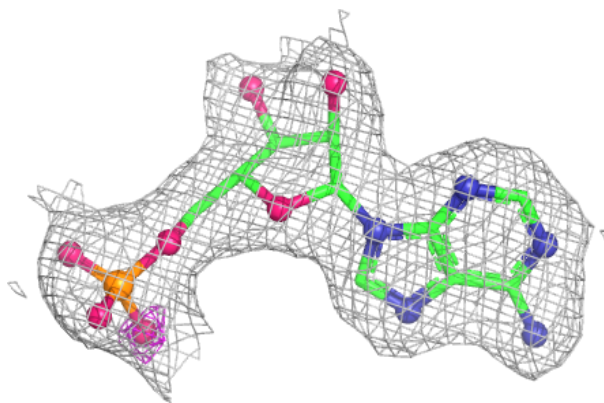
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MYR	A	1001	15/16	0.88	0.13	6,7,9,9	0
3	MYR	B	2001	15/16	0.90	0.12	17,18,20,20	0
4	AMP	A	1002	23/23	0.94	0.08	7,13,13,14	0
4	AMP	B	2002	23/23	0.96	0.07	16,17,19,20	0
2	MG	A	3001	1/1	0.97	0.15	35,35,35,35	0
2	MG	B	3002	1/1	0.98	0.11	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around AMP B 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.