



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:45 PM GMT

PDB ID : 1V25  
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 : 2.30 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

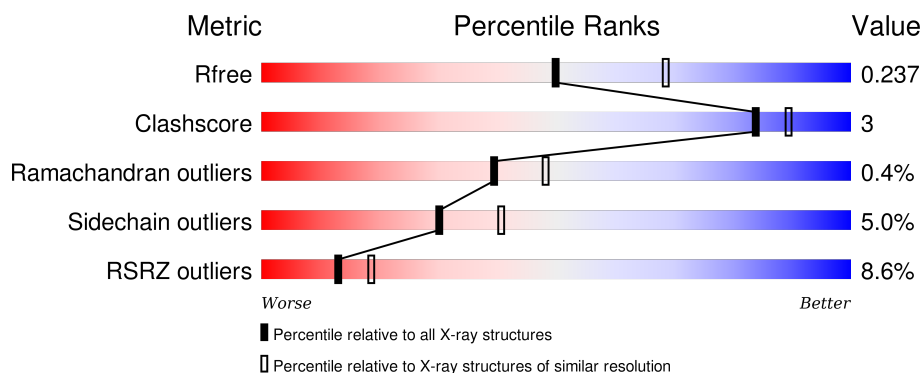
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	541	<div> <div>7%</div> <div>79% 11% • 9%</div> </div>
1	B	541	<div> <div>9%</div> <div>83% 9% • 6%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8236 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.

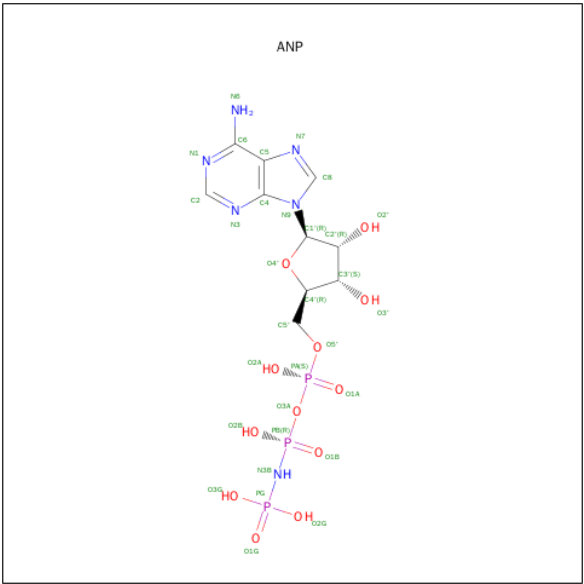
- Molecule 1 is a protein called long-chain-fatty-acid-CoA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3812	2441	663	698	10			
1	B	507	Total	C	N	O	S	0	0	0
			3939	2525	686	717	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

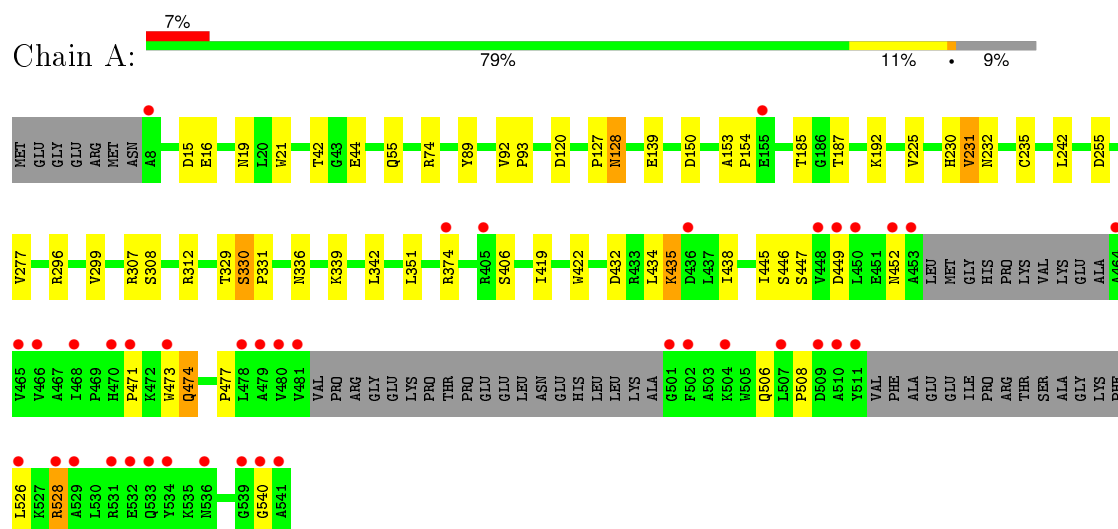
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	196	Total	O	0	0
			196	196		

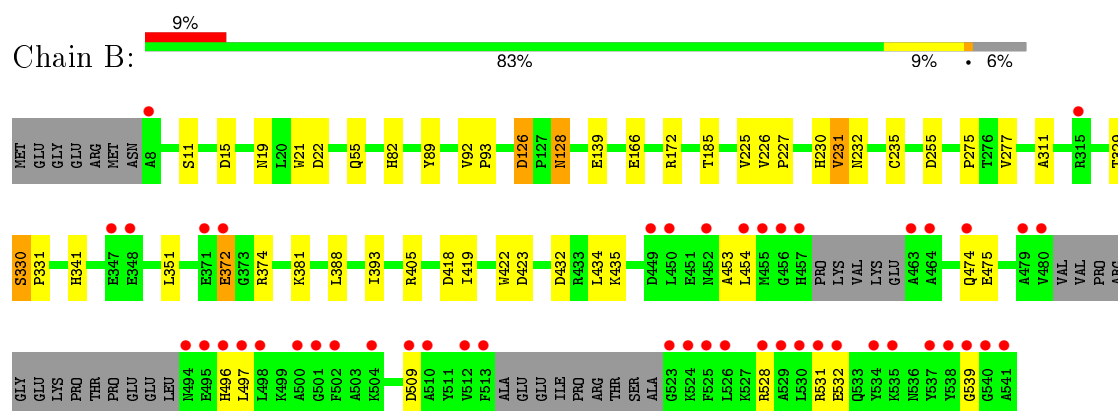
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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, $\alpha$ , $\beta$ , $\gamma$	64.52Å 101.15Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.30 48.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.60-2.30) 99.2 (48.62-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.204 , 0.240 0.204 , 0.237	Depositor DCC
$R_{free}$ test set	5205 reflections (11.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51622 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/3900	0.63	4/5297 (0.1%)
1	B	0.33	0/4031	0.62	7/5471 (0.1%)
All	All	0.33	0/7931	0.62	11/10768 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	432	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	255	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	126	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	120	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	255	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	15	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	15	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	22	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	418	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	423	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3812	0	3822	26	0
1	B	3939	0	3950	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	2	0
3	B	31	0	13	2	0
4	A	225	0	0	3	0
4	B	196	0	0	0	0
All	All	8236	0	7798	47	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 3.

All (47) 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:230:HIS:HA	3:B:1666:ANP:O1G	1.86	0.76
1:A:231:VAL:HG22	3:A:666:ANP:O2G	1.86	0.73
1:A:330:SER:N	1:A:331:PRO:HA	2.08	0.69
1:B:330:SER:N	1:B:331:PRO:HA	2.08	0.69
1:B:231:VAL:HG23	3:B:1666:ANP:HNB1	1.64	0.63
1:A:42:THR:OG1	1:A:44:GLU:HG2	2.00	0.61
1:A:308:SER:O	1:A:312:ARG:HG3	2.00	0.61
1:A:296:ARG:HG2	4:A:1133:HOH:O	2.00	0.60
1:B:225:VAL:HG11	1:B:277:VAL:HG11	1.83	0.60
1:B:275:PRO:HB2	1:B:474:GLN:OE1	2.02	0.59
1:B:19:ASN:HD22	1:B:21:TRP:H	1.50	0.58
1:B:92:VAL:HB	1:B:93:PRO:HD3	1.86	0.57
1:A:474:GLN:NE2	4:A:1154:HOH:O	2.36	0.57
1:A:128:ASN:HD22	1:A:128:ASN:H	1.53	0.57
1:A:307:ARG:NH1	1:A:351:LEU:HD23	2.20	0.56
1:A:89:TYR:OH	1:A:232:ASN:HA	2.07	0.55
1:A:230:HIS:HA	3:A:666:ANP:O1G	2.07	0.55
1:A:438:ILE:HD13	1:A:477:PRO:HG3	1.87	0.54
1:A:445:ILE:HG12	1:A:506:GLN:HG2	1.90	0.53
1:A:471:PRO:HG3	1:A:540:GLY:HA2	1.91	0.53
1:B:329:THR:C	1:B:331:PRO:HA	2.30	0.51
1:A:92:VAL:HB	1:A:93:PRO:HD3	1.92	0.51
1:A:225:VAL:HG11	1:A:277:VAL:HG11	1.93	0.50
1:A:19:ASN:HD22	1:A:21:TRP:H	1.59	0.50
1:B:454:LEU:HG	1:B:497:LEU:HD21	1.93	0.49
1:A:477:PRO:HB2	1:A:508:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASN:HD22	1:B:128:ASN:H	1.60	0.49
1:A:127:PRO:HG3	1:A:150:ASP:HB2	1.95	0.49
1:A:329:THR:C	1:A:331:PRO:HA	2.33	0.49
1:B:419:ILE:HD11	1:B:434:LEU:HG	1.95	0.47
4:A:1222:HOH:O	1:B:341:HIS:HD2	1.97	0.47
1:B:311:ALA:HB2	1:B:351:LEU:HD21	1.97	0.46
1:B:388:LEU:HB3	1:B:393:ILE:HD13	1.97	0.45
1:A:128:ASN:H	1:A:128:ASN:ND2	2.14	0.45
1:B:474:GLN:O	1:B:475:GLU:HG3	2.18	0.43
1:B:82:HIS:HE1	1:B:126:ASP:OD1	2.01	0.43
1:B:372:GLU:HG3	1:B:374:ARG:NH1	2.34	0.43
1:B:128:ASN:ND2	1:B:128:ASN:H	2.17	0.43
1:A:528:ARG:H	1:A:528:ARG:HG2	1.65	0.43
1:B:453:ALA:O	1:B:496:HIS:HE1	2.02	0.43
1:A:419:ILE:HD11	1:A:434:LEU:HG	2.00	0.42
1:A:435:LYS:H	1:A:435:LYS:HG3	1.57	0.41
1:B:89:TYR:OH	1:B:232:ASN:HA	2.21	0.41
1:A:153:ALA:HA	1:A:154:PRO:HD3	1.94	0.41
1:B:226:VAL:HA	1:B:227:PRO:HD3	1.89	0.41
1:A:187:THR:HG21	1:A:192:LYS:HD2	2.03	0.41
1:A:339:LYS:HB2	1:A:342:LEU:HD12	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	483/541 (89%)	465 (96%)	16 (3%)	2 (0%)	39	48
1	B	499/541 (92%)	488 (98%)	9 (2%)	2 (0%)	39	48
All	All	982/1082 (91%)	953 (97%)	25 (2%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	SER
1	B	330	SER
1	B	539	GLY
1	A	473	TRP

### 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%)	373 (94%)	22 (6%)	26	35
1	B	407/437 (93%)	389 (96%)	18 (4%)	35	46
All	All	802/874 (92%)	762 (95%)	40 (5%)	30	41

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	55	GLN
1	A	74	ARG
1	A	128	ASN
1	A	139	GLU
1	A	185	THR
1	A	231	VAL
1	A	235	CYS
1	A	242	LEU
1	A	299	VAL
1	A	336	ASN
1	A	374	ARG
1	A	406	SER
1	A	422	TRP
1	A	435	LYS
1	A	446	SER
1	A	447	SER
1	A	449	ASP
1	A	452	ASN

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Mol	Chain	Res	Type
1	A	474	GLN
1	A	526	LEU
1	A	528	ARG
1	B	11	SER
1	B	55	GLN
1	B	128	ASN
1	B	139	GLU
1	B	166	GLU
1	B	172	ARG
1	B	185	THR
1	B	231	VAL
1	B	235	CYS
1	B	372	GLU
1	B	381	LYS
1	B	405	ARG
1	B	422	TRP
1	B	435	LYS
1	B	509	ASP
1	B	528	ARG
1	B	531	ARG
1	B	532	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	41	HIS
1	A	55	GLN
1	A	82	HIS
1	A	128	ASN
1	A	145	HIS
1	A	232	ASN
1	A	290	HIS
1	A	335	GLN
1	A	336	ASN
1	B	19	ASN
1	B	41	HIS
1	B	82	HIS
1	B	128	ASN
1	B	232	ASN
1	B	290	HIS
1	B	322	GLN

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Mol	Chain	Res	Type
1	B	335	GLN
1	B	336	ASN
1	B	341	HIS
1	B	496	HIS

### 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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ANP	A	666	2	27,33,33	1.64	3 (11%)	30,52,52	2.23	6 (20%)
3	ANP	B	1666	2	27,33,33	1.72	3 (11%)	30,52,52	2.12	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	666	2	-	0/12/38/38	0/3/3/3
3	ANP	B	1666	2	-	0/12/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	666	ANP	O4'-C1'	3.74	1.45	1.41
3	B	1666	ANP	O4'-C1'	3.88	1.46	1.41
3	A	666	ANP	PB-O1B	4.20	1.50	1.46
3	B	1666	ANP	PB-O1B	4.87	1.51	1.46
3	A	666	ANP	PG-O1G	4.90	1.51	1.46
3	B	1666	ANP	PG-O1G	5.16	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	666	ANP	N3-C2-N1	-9.88	121.33	128.89
3	B	1666	ANP	N3-C2-N1	-9.62	121.53	128.89
3	A	666	ANP	C2'-C1'-N9	-3.54	108.89	114.29
3	A	666	ANP	PA-O3A-PB	-2.66	123.75	132.67
3	B	1666	ANP	O2G-PG-O1G	-2.53	106.76	113.49
3	B	1666	ANP	PA-O3A-PB	-2.41	124.58	132.67
3	B	1666	ANP	C4-C5-N7	-2.29	107.37	109.48
3	A	666	ANP	O3G-PG-O1G	-2.07	108.00	113.49
3	A	666	ANP	C4-C5-N7	-2.06	107.58	109.48
3	B	1666	ANP	C2'-C1'-N9	-2.06	111.15	114.29
3	B	1666	ANP	O3A-PA-O5'	2.50	109.57	102.94
3	A	666	ANP	O3A-PA-O5'	2.62	109.89	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	666	ANP	2	0
3	B	1666	ANP	2	0

## 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, 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	491/541 (90%)	0.34	39 (7%)	15 22	7, 16, 58, 98	0
1	B	507/541 (93%)	0.26	47 (9%)	11 16	7, 16, 72, 96	0
All	All	998/1082 (92%)	0.30	86 (8%)	13 18	7, 16, 65, 98	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ALA	9.0
1	A	540	GLY	9.0
1	B	523	GLY	8.8
1	A	529	ALA	7.7
1	B	526	LEU	7.6
1	A	481	VAL	7.0
1	B	539	GLY	6.7
1	A	526	LEU	6.6
1	B	525	PHE	6.1
1	B	454	LEU	6.0
1	B	512	VAL	5.7
1	B	464	ALA	5.4
1	A	528	ARG	5.4
1	B	529	ALA	5.4
1	B	497	LEU	5.3
1	A	531	ARG	5.2
1	A	502	PHE	5.2
1	B	456	GLY	5.2
1	A	534	TYR	5.1
1	B	513	PHE	5.1
1	A	532	GLU	4.9
1	B	528	ARG	4.8
1	B	463	ALA	4.7
1	A	473	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	450	LEU	4.6
1	B	500	ALA	4.6
1	A	539	GLY	4.5
1	A	480	VAL	4.3
1	B	501	GLY	4.1
1	A	501	GLY	4.0
1	B	8	ALA	4.0
1	B	480	VAL	3.8
1	B	371	GLU	3.7
1	A	504	LYS	3.6
1	B	455	MET	3.6
1	A	478	LEU	3.6
1	A	510	ALA	3.5
1	A	468	ILE	3.5
1	B	524	LYS	3.4
1	B	495	GLU	3.2
1	B	531	ARG	3.2
1	B	498	LEU	3.2
1	A	448	VAL	3.2
1	B	532	GLU	3.2
1	B	494	ASN	3.1
1	A	533	GLN	3.1
1	B	530	LEU	3.0
1	A	453	ALA	3.0
1	B	540	GLY	3.0
1	A	436	ASP	3.0
1	B	534	TYR	2.9
1	A	511	TYR	2.9
1	A	452	ASN	2.9
1	A	507	LEU	2.8
1	A	449	ASP	2.7
1	B	348	GLU	2.7
1	B	504	LYS	2.7
1	B	474	GLN	2.7
1	A	374	ARG	2.6
1	B	538	TYR	2.6
1	B	347	GLU	2.5
1	B	537	TYR	2.5
1	A	509	ASP	2.5
1	B	496	HIS	2.4
1	A	464	ALA	2.4
1	A	479	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	449	ASP	2.4
1	B	510	ALA	2.3
1	B	450	LEU	2.3
1	B	457	HIS	2.3
1	A	8	ALA	2.3
1	A	155	GLU	2.3
1	A	465	VAL	2.2
1	B	372	GLU	2.2
1	B	535	LYS	2.2
1	B	315	ARG	2.2
1	B	452	ASN	2.2
1	A	471	PRO	2.1
1	B	479	ALA	2.1
1	A	536	ASN	2.1
1	A	470	HIS	2.1
1	B	502	PHE	2.1
1	A	405	ARG	2.0
1	A	466	VAL	2.0
1	B	509	ASP	2.0
1	B	541	ALA	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
3	ANP	B	1666	31/31	0.88	0.18	1.77	15,16,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ANP	A	666	31/31	0.89	0.18	1.17	10,11,40,42	0
2	MG	A	1001	1/1	0.97	0.16	0.16	23,23,23,23	0
2	MG	B	1002	1/1	0.95	0.07	-	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.