



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1G51  
Title : ASPARTYL TRNA SYNTHETASE FROM THERMUS THERMOPHILUS  
AT 2.4 Å RESOLUTION  
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Deposited on : 2000-10-30  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

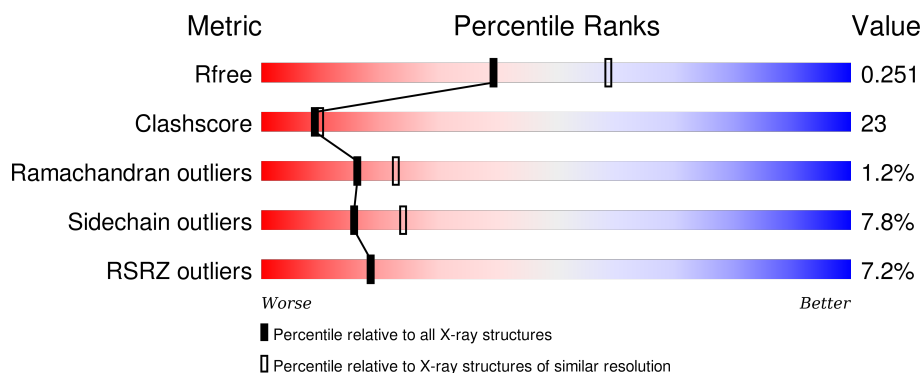
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	580	<div> <div>11%</div> <div>59%</div> <div>36%</div> <div>.</div> </div>
1	B	580	<div> <div>3%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10100 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 ASPARTYL-TRNA SYNTHETASE.

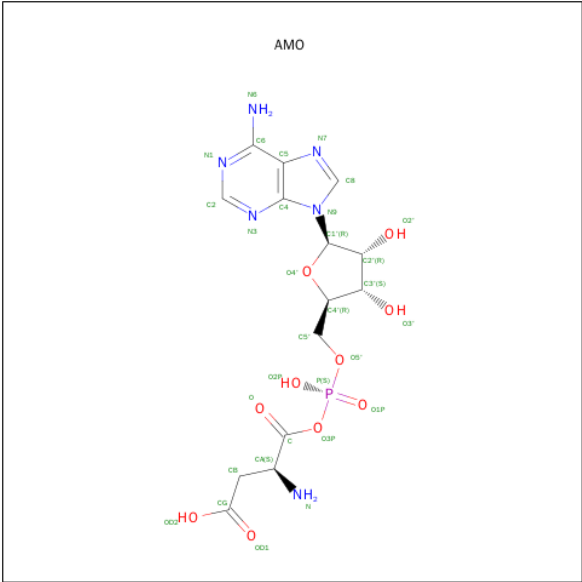
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			
1	B	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



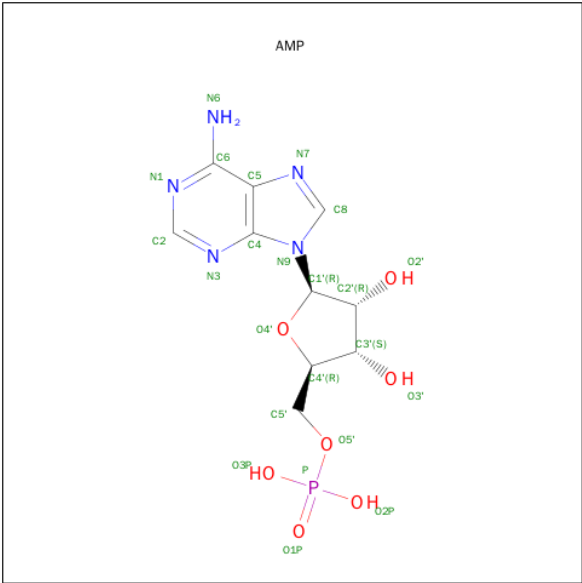
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ASPARTYL-ADENOSINE-5'-MONOPHOSPHATE (three-letter code: AMO) (formula: C<sub>14</sub>H<sub>19</sub>N<sub>6</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	14	6	10	1		
3	B	1	Total	C	N	O	P	0	0
			31	14	6	10	1		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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

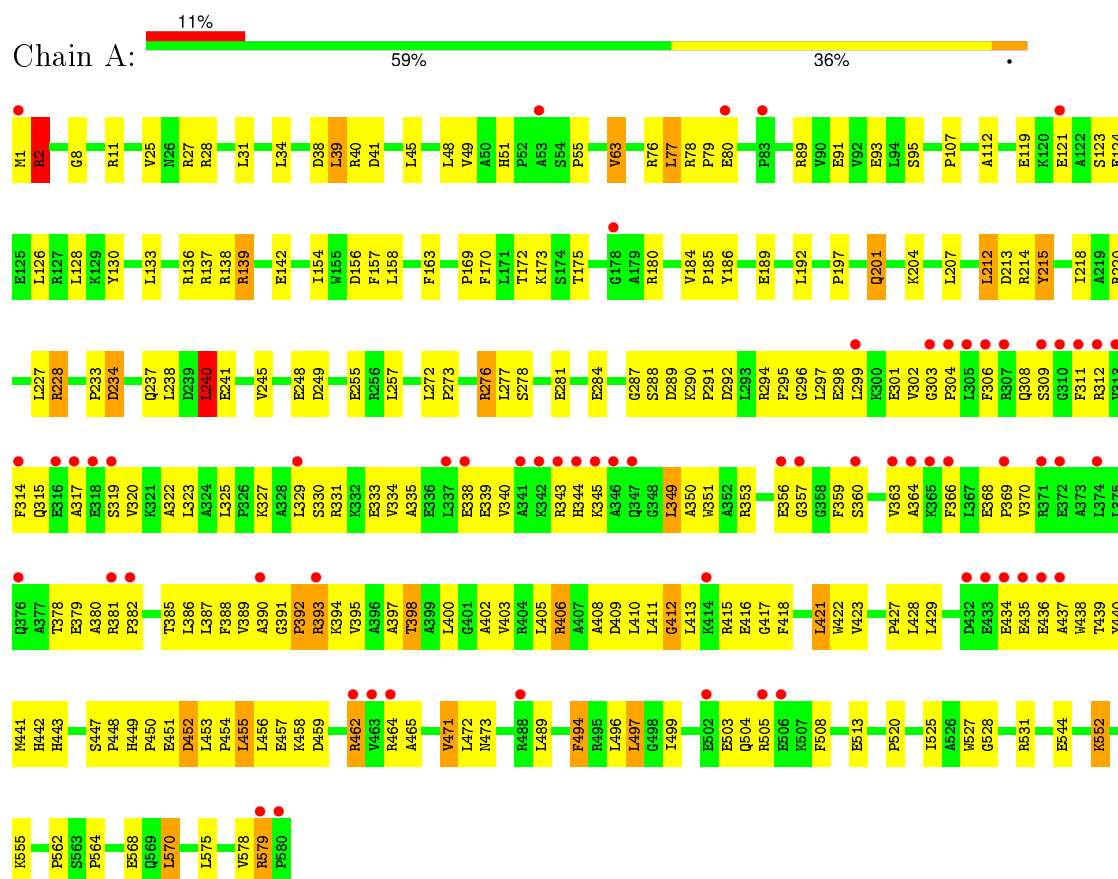
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	288	Total 288	O 288	0	0
5	B	381	Total 381	O 381	0	0

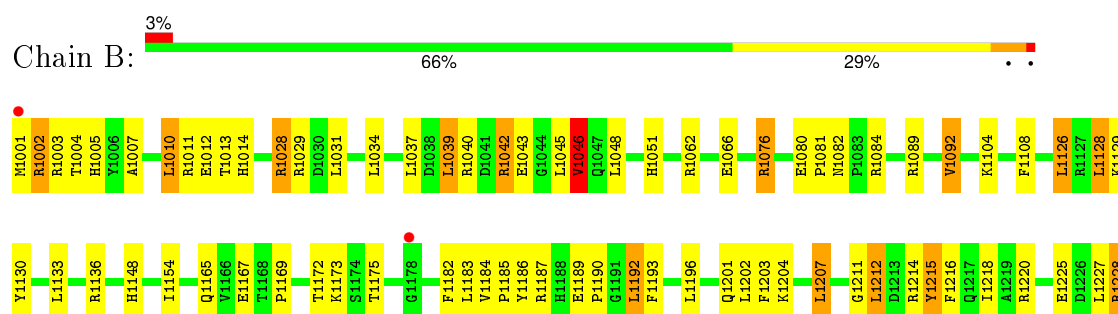
### 3 Residue-property plots

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

#### • Molecule 1: ASPARTYL-TRNA SYNTHETASE



#### • Molecule 1: ASPARTYL-TRNA SYNTHETASE



A1229	R1343	L1437	R1531
P1233	H1344	W1438	L1532
D1234	K1345	T1439	L1533
Q1237	A1346	M1441	F1548
L1238	G1348	H1442	D1566
D1239	L1349	H1443	P1567
L1240	A1350	F1444	L1558
E1241	W1351	F1445	G1560
V1245	E1356	S1447	A1561
D1249	E1368	P1448	P1562
L1253	P1369	H1449	S1563
L1257	E1372	E1451	P1564
R1263	A1373	L1453	E1568
E1269	L1374	P1454	L1573
L1277	L1375	L1455	G1574
K1290	Q1376	L1456	L1575
P1291	Q1376	E1457	M1576
L1297	L1386	K1458	P1580
E1298	L1387	D1459	
L1299	F1388	R1462	
V1302	P1392	W1463	
G1303	R1393	R1464	
P1304	K1394	A1465	
L1305	V1395	V1471	
F1306	L1400	L1472	
R1307	V1403	M1473	
Q1308	R1404	R1483	
V1312	L1405	D1486	
V1313	L1410	P1487	
E1316	L1411	R1492	
V1320	G1412	V1493	
L1323	L1413	F1494	
A1324	K1414	L1497	
L1325	R1415	G1500	
F1326	E1416	E1501	
K1327	R1419	E1502	
A1328	F1420	R1505	
L1329	L1421	E1513	
S1330	W1422	E1516	
R1331	V1423	H1522	
L1337	P1427	T1525	
E1338	L1428	A1526	
E1339	W1431	W1527	
	D1432	G1528	
	E1433		
	E1434		
	E1435		
	E1436		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.13Å 155.50Å 171.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.00 – 2.40 14.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.3 (14.00-2.40) 91.4 (14.00-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.194 , 0.251 0.194 , 0.251	Depositor DCC
$R_{free}$ test set	4443 reflections (7.67%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 60454 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: AMP, SO4, AMO

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	0.62	0/4780	0.84	7/6467 (0.1%)
1	B	0.65	0/4780	0.91	14/6467 (0.2%)
All	All	0.63	0/9560	0.88	21/12934 (0.2%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	LEU	CA-CB-CG	8.87	135.71	115.30
1	B	1240	LEU	CA-CB-CG	8.74	135.40	115.30
1	A	2	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	1212	LEU	C-N-CA	-6.83	104.62	121.70
1	A	212	LEU	N-CA-C	-6.36	93.82	111.00

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	4668	0	4679	276	0
1	B	4668	0	4676	181	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	17	5	0
3	B	31	0	17	3	0
4	B	23	0	12	0	0
5	A	288	0	0	21	0
5	B	381	0	0	25	0
All	All	10100	0	9401	435	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 23.

The worst 5 of 435 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:1431:TRP:CH2	1:B:1436:GLU:HA	1.92	1.04
1:A:301:GLU:OE2	1:A:319:SER:HB2	1.59	1.00
1:A:214:ARG:HG2	5:B:2657:HOH:O	1.61	1.00
1:A:394:LYS:HE2	1:A:398:THR:HG21	1.42	1.00
1:A:499:ILE:HG13	1:A:503:GLU:HB3	1.48	0.95

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	578/580 (100%)	536 (93%)	33 (6%)	9 (2%)	12	16
1	B	578/580 (100%)	543 (94%)	30 (5%)	5 (1%)	21	30
All	All	1156/1160 (100%)	1079 (93%)	63 (5%)	14 (1%)	16	23

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	392	PRO
1	A	436	GLU
1	A	452	ASP
1	B	1414	LYS

### 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	483/483 (100%)	448 (93%)	35 (7%)	18	28
1	B	483/483 (100%)	443 (92%)	40 (8%)	14	21
All	All	966/966 (100%)	891 (92%)	75 (8%)	16	24

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	LEU
1	B	1092	VAL
1	B	1497	LEU
1	A	579	ARG
1	B	1042	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	HIS
1	B	1344	HIS
1	B	1047	GLN
1	A	442	HIS
1	B	1014	HIS

### 5.3.3 RNA ⓘ

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	SO4	A	1901	-	4,4,4	0.39	0	6,6,6	0.18	0
3	AMO	A	831	-	23,33,33	0.91	1 (4%)	24,49,49	0.73	1 (4%)
3	AMO	B	1831	-	23,33,33	0.87	1 (4%)	24,49,49	0.96	2 (8%)
4	AMP	B	800	-	20,25,25	0.74	0	22,38,38	1.07	2 (9%)
2	SO4	B	901	-	4,4,4	0.35	0	6,6,6	0.15	0

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	SO4	A	1901	-	-	0/0/0/0	0/0/0/0
3	AMO	A	831	-	-	0/15/39/39	0/3/3/3
3	AMO	B	1831	-	-	0/15/39/39	0/3/3/3
4	AMP	B	800	-	-	0/6/26/26	0/3/3/3
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1831	AMO	P-O3P	2.60	1.66	1.60
3	A	831	AMO	P-O3P	3.20	1.67	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	AMP	O3'-C3'-C2'	-2.58	103.45	111.83
3	B	1831	AMO	O3P-P-O1P	-2.19	101.15	108.38
3	A	831	AMO	O2P-P-O3P	2.11	110.69	104.16
4	B	800	AMP	O3P-P-O1P	2.75	119.43	110.58
3	B	1831	AMO	O3P-P-O5'	2.88	110.36	102.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	831	AMO	5	0
3	B	1831	AMO	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	580/580 (100%)	0.13	64 (11%) <b>7</b> <b>7</b>	14, 39, 86, 102	0
1	B	580/580 (100%)	-0.37	20 (3%) 49 49	13, 31, 64, 93	0
All	All	1160/1160 (100%)	-0.12	84 (7%) <b>18</b> <b>18</b>	13, 34, 81, 102	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	PRO	6.2
1	B	1434	GLU	5.5
1	A	434	GLU	5.2
1	A	307	ARG	5.2
1	A	365	LYS	5.1

### 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( $\text{\AA}^2$ )	Q<0.9
4	AMP	B	800	23/23	0.77	0.25	1.65	73,82,96,98	0
2	SO4	B	901	5/5	0.98	0.15	0.32	68,69,70,70	0
3	AMO	B	1831	31/31	0.98	0.10	-0.19	17,26,29,30	0
3	AMO	A	831	31/31	0.97	0.09	-0.68	25,28,30,32	0
2	SO4	A	1901	5/5	0.96	0.10	-	69,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.