



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:37 PM EST

PDB ID : 5GME
Title : Crystal structure of Sulfolobus solfataricus Diphosphomevalonate decarboxylase in complex with ADP
Authors : Unno, H.; Hemmi, H.; Hattori, A.
Deposited on : 2016-07-13
Resolution : 1.70 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

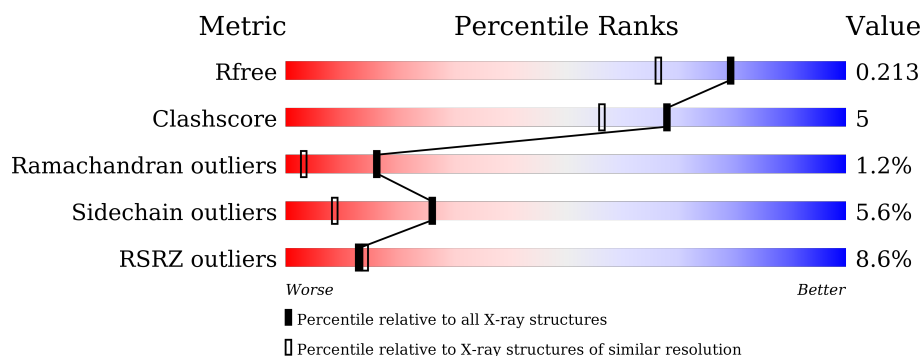
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	325	<div> <div>9%</div> <div>81%</div> <div>14%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1005	-	-	-	X

2 Entry composition [i](#)

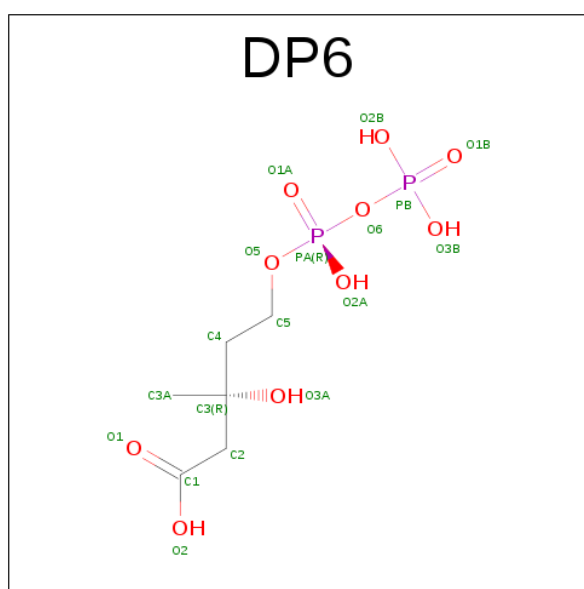
There are 6 unique types of molecules in this entry. The entry contains 2932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Diphosphomevalonate decarboxylase.

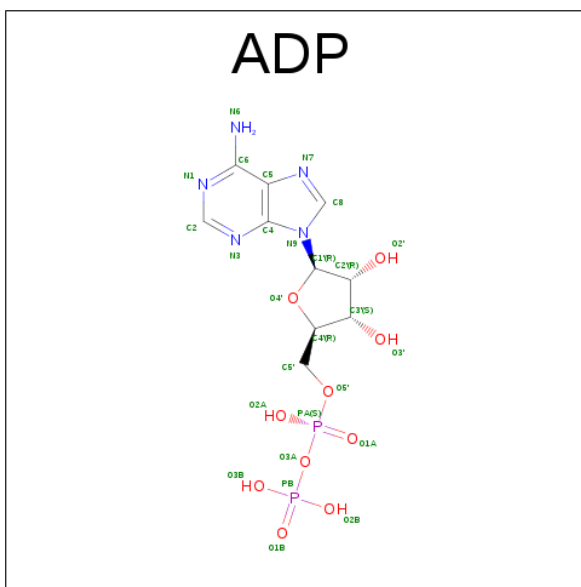
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2597	1654	442	490	11			

- Molecule 2 is (3R)-3-HYDROXY-5-[[[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY]-3-METHYLPENTANOIC ACID (three-letter code: DP6) (formula: C₆H₁₄O₁₀P₂).



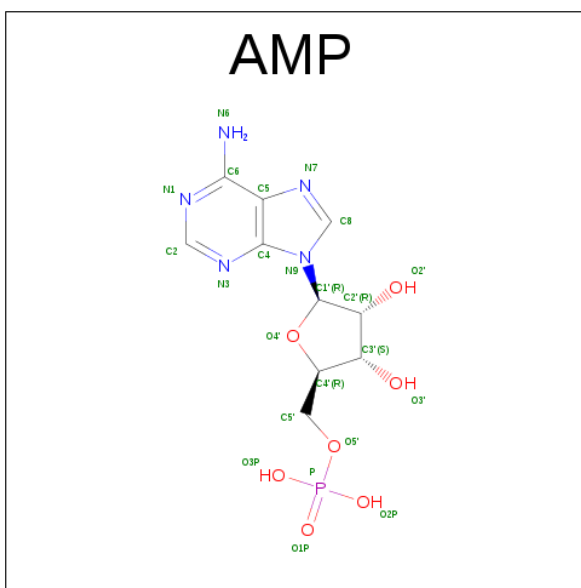
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	6	10	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: 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		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

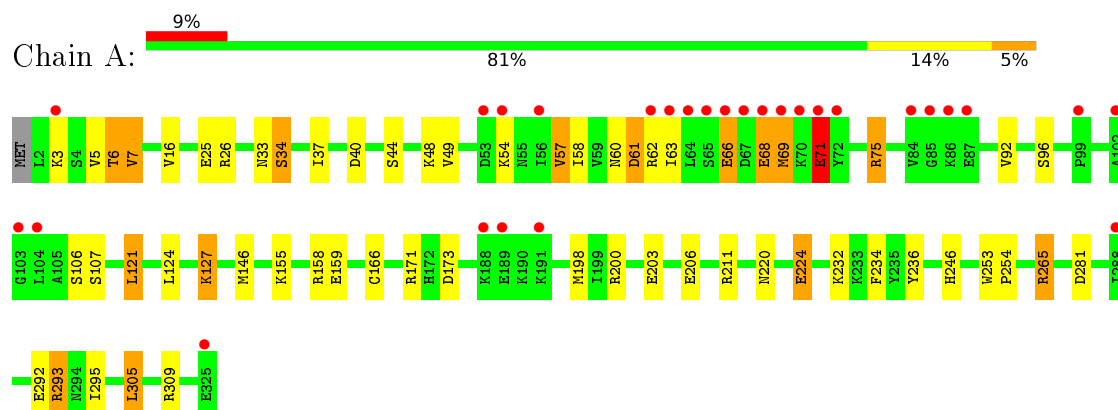
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	257	Total	O	0	0
			257	257		

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: Diphosphomevalonate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	151.29 Å 151.29 Å 104.42 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.75 – 1.70 27.75 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.75-1.70) 99.8 (27.75-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.169 , 0.202 0.180 , 0.213	Depositor DCC
R_{free} test set	2551 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2932	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DP6, SO4, ADP, 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	1.30	4/2645 (0.2%)	1.37	27/3558 (0.8%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	SER	CB-OG	-10.80	1.28	1.42
1	A	198	MET	CB-CG	-6.25	1.31	1.51
1	A	211	ARG	CZ-NH2	-5.80	1.25	1.33
1	A	71	GLU	N-CA	5.78	1.57	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	A	198	MET	CG-SD-CE	-11.75	81.40	100.20
1	A	309	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	305	LEU	CB-CG-CD1	8.98	126.26	111.00
1	A	265	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	159	GLU	OE1-CD-OE2	-7.66	114.10	123.30
1	A	309	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	198	MET	CB-CA-C	-7.01	96.38	110.40
1	A	7	VAL	CG1-CB-CG2	6.99	122.09	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	211	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	206	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	293	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	158	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	236	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	A	265	ARG	CD-NE-CZ	5.81	131.73	123.60
1	A	281	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	200	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	146	MET	CG-SD-CE	5.66	109.26	100.20
1	A	40	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	309	ARG	CG-CD-NE	-5.42	100.41	111.80
1	A	75	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	171	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	127	LYS	CD-CE-NZ	5.28	123.85	111.70
1	A	166	CYS	CA-CB-SG	-5.23	104.58	114.00
1	A	121	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	7	VAL	N-CA-CB	-5.14	100.19	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	GLU	Peptide

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	2597	0	2623	24	0
2	A	18	0	10	1	0
3	A	27	0	12	2	0
4	A	23	0	12	0	0
5	A	10	0	0	0	0
6	A	257	0	0	9	4
All	All	2932	0	2657	25	4

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 5.

All (25) 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:44:SER:HB2	6:A:1112:HOH:O	0.99	1.15
2:A:1001:DP6:O1A	6:A:1101:HOH:O	1.90	0.89
1:A:224:GLU:OE1	6:A:1102:HOH:O	2.02	0.76
1:A:246:HIS:HD2	6:A:1239:HOH:O	1.80	0.63
1:A:107:SER:N	3:A:1002:ADP:O3B	2.33	0.61
1:A:6:THR:HG22	1:A:48:LYS:HG3	1.83	0.60
1:A:33:ASN:ND2	1:A:155:LYS:H	2.00	0.60
1:A:49:VAL:HG12	1:A:92:VAL:HG22	1.84	0.59
1:A:293:ARG:NH2	6:A:1106:HOH:O	2.38	0.57
1:A:33:ASN:HD22	1:A:155:LYS:H	1.53	0.55
1:A:25:GLU:OE1	1:A:26:ARG:HD3	2.08	0.54
1:A:58:ILE:HG22	1:A:61:ASP:HA	1.89	0.53
1:A:44:SER:CB	6:A:1112:HOH:O	1.86	0.51
1:A:57:VAL:HG13	1:A:69:MET:HG3	1.93	0.49
1:A:71:GLU:OE1	1:A:75:ARG:NH1	2.46	0.49
1:A:60:ASN:HD21	1:A:96:SER:H	1.62	0.46
1:A:220:ASN:OD1	6:A:1103:HOH:O	2.20	0.45
1:A:203:GLU:HG3	6:A:1297:HOH:O	2.16	0.45
1:A:232:LYS:HG2	6:A:1263:HOH:O	2.17	0.44
1:A:253:TRP:HA	1:A:254:PRO:C	2.39	0.42
1:A:37:ILE:HD11	1:A:234:PHE:HZ	1.84	0.42
1:A:292:GLU:OE1	1:A:295:ILE:CD1	2.68	0.42
1:A:106:SER:HA	3:A:1002:ADP:O3B	2.21	0.41
1:A:16:VAL:O	1:A:34:SER:HB2	2.21	0.41
1:A:57:VAL:HG13	1:A:69:MET:CG	2.50	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1295:HOH:O	6:A:1314:HOH:O[4_555]	1.58	0.62
6:A:1235:HOH:O	6:A:1301:HOH:O[4_555]	1.83	0.37
6:A:1248:HOH:O	6:A:1248:HOH:O[4_555]	1.93	0.27
6:A:1164:HOH:O	6:A:1279:HOH:O[3_555]	2.03	0.17

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	322/325 (99%)	311 (97%)	7 (2%)	4 (1%)	16 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	66	GLU
1	A	71	GLU
1	A	69	MET

5.3.2 Protein sidechains [i](#)

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	288/289 (100%)	272 (94%)	16 (6%)	26 9

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	VAL
1	A	6	THR
1	A	7	VAL
1	A	54	LYS
1	A	57	VAL
1	A	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	63	ILE
1	A	66	GLU
1	A	68	GLU
1	A	121	LEU
1	A	124	LEU
1	A	127	LYS
1	A	224	GLU
1	A	265	ARG
1	A	305	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	33	ASN
1	A	55	ASN
1	A	60	ASN
1	A	154	ASN
1	A	246	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](#)

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	DP6	A	1001	-	11,17,17	1.04	1 (9%)	9,26,26	1.09	0
3	ADP	A	1002	-	24,29,29	1.25	1 (4%)	23,45,45	1.94	5 (21%)
4	AMP	A	1003	-	22,25,25	1.46	5 (22%)	22,38,38	2.81	6 (27%)
5	SO4	A	1004	-	4,4,4	2.09	2 (50%)	6,6,6	1.16	1 (16%)
5	SO4	A	1005	-	4,4,4	1.97	1 (25%)	6,6,6	1.04	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	DP6	A	1001	-	-	0/17/19/19	0/0/0/0
3	ADP	A	1002	-	-	0/12/32/32	0/3/3/3
4	AMP	A	1003	-	-	0/6/26/26	0/3/3/3
5	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1005	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1005	SO4	O1-S	-3.02	1.36	1.47
4	A	1003	AMP	P-O2P	-3.01	1.44	1.54
2	A	1001	DP6	C4-C5	-2.01	1.44	1.51
4	A	1003	AMP	O2'-C2'	2.03	1.47	1.43
4	A	1003	AMP	P-O5'	2.05	1.65	1.59
4	A	1003	AMP	C5-C4	2.49	1.46	1.40
5	A	1004	SO4	O1-S	2.52	1.56	1.47
5	A	1004	SO4	O2-S	3.00	1.57	1.47
4	A	1003	AMP	P-O1P	3.29	1.61	1.50
3	A	1002	ADP	C5-C4	3.79	1.49	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	AMP	N3-C2-N1	-7.57	122.92	128.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	1003	AMP	C1'-N9-C4	-6.90	119.11	126.81
3	A	1002	ADP	N3-C2-N1	-6.86	123.48	128.87
4	A	1003	AMP	O5'-P-O1P	-4.59	95.55	107.08
3	A	1002	ADP	C1'-N9-C4	-2.83	123.65	126.81
5	A	1004	SO4	O4-S-O3	-2.69	98.25	109.09
4	A	1003	AMP	O2P-P-O5'	2.07	112.76	106.72
3	A	1002	ADP	O2B-PB-O1B	2.09	117.45	110.63
3	A	1002	ADP	C2-N1-C6	2.12	122.55	118.77
4	A	1003	AMP	C2-N1-C6	2.86	123.86	118.77
3	A	1002	ADP	O4'-C1'-N9	2.89	113.57	108.11
4	A	1003	AMP	N6-C6-N1	4.26	125.66	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DP6	1	0
3	A	1002	ADP	2	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 ⓘ

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	324/325 (99%)	0.30	28 (8%) 13 14	10, 22, 59, 92	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ASP	6.3
1	A	85	GLY	5.7
1	A	189	GLU	4.3
1	A	67	ASP	4.1
1	A	66	GLU	3.9
1	A	68	GLU	3.4
1	A	86	LYS	3.2
1	A	103	GLY	3.2
1	A	70	LYS	3.1
1	A	87	GLU	3.0
1	A	84	VAL	2.9
1	A	188	LYS	2.9
1	A	3	LYS	2.9
1	A	54	LYS	2.8
1	A	69	MET	2.7
1	A	65	SER	2.6
1	A	325	GLU	2.5
1	A	104	LEU	2.5
1	A	63	ILE	2.5
1	A	71	GLU	2.5
1	A	62	ARG	2.4
1	A	191	LYS	2.3
1	A	72	TYR	2.3
1	A	64	LEU	2.2
1	A	102	ALA	2.2
1	A	288	ILE	2.1
1	A	99	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	56	ILE	2.1

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, 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
5	SO4	A	1005	5/5	0.98	0.20	2.59	24,33,35,38	0
4	AMP	A	1003	23/23	0.94	0.13	1.69	20,36,47,54	0
3	ADP	A	1002	27/27	0.73	0.25	1.45	39,74,100,102	0
2	DP6	A	1001	18/18	0.98	0.06	-1.60	14,19,24,29	0
5	SO4	A	1004	5/5	0.94	0.21	-	23,27,30,32	5

6.5 Other polymers [i](#)

There are no such residues in this entry.