



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:24 PM BST

PDB ID : 5GMD  
Title : Crystal structure of Sulfolobus solfataricus diphosphomevalonate decarboxylase in complex with ATP-gamma-S  
Authors : Unno, H.; Hemmi, H.; Hattori, A.  
Deposited on : 2016-07-13  
Resolution : 1.50 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

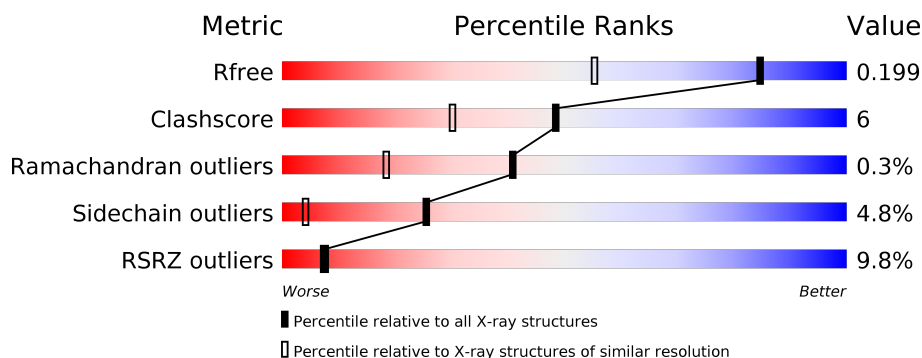
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	325	<div> <div>10%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

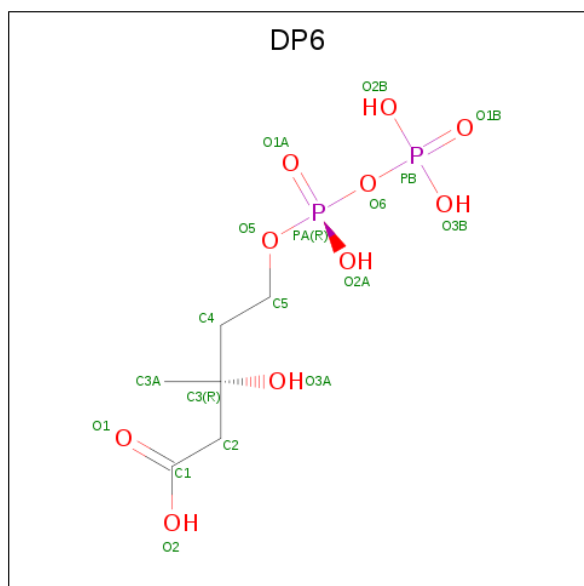
There are 6 unique types of molecules in this entry. The entry contains 2939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

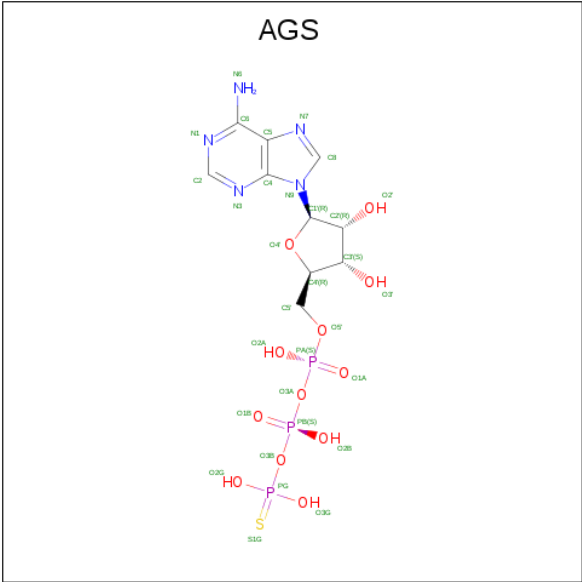
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	2	0
			2614	1665	443	493	13			

- Molecule 2 is (3R)-3-HYDROXY-5-[[[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY]-3-METHYLPENTANOIC ACID (three-letter code: DP6) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>10</sub>P<sub>2</sub>).



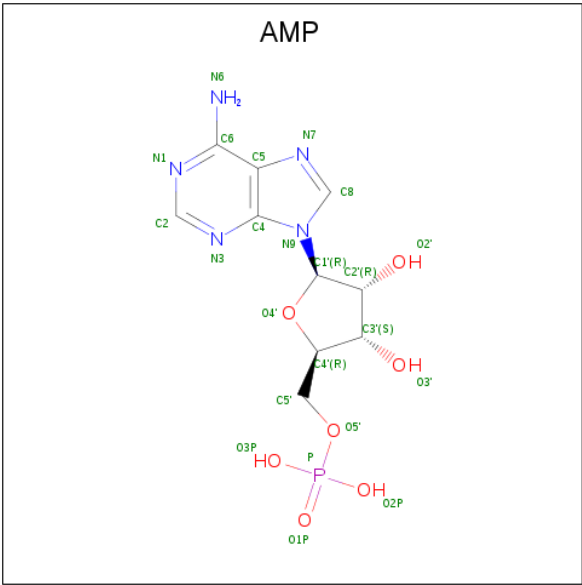
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	6	10	2		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	5	12	3	0	0

- 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
			Total	C	N	O	P		
4	A	1	23	10	5	7	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

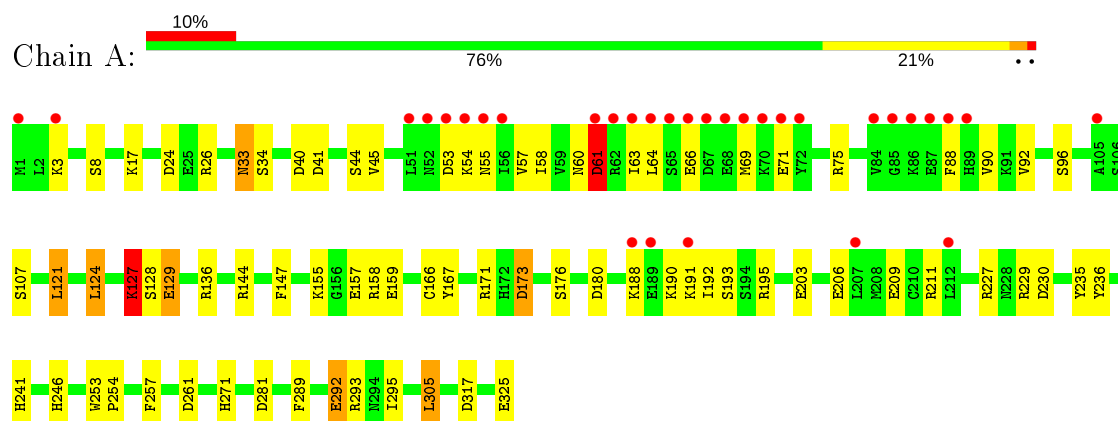
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	243	Total	O		
			243	243	0	0

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

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: Diphosphomevalonate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.24Å 151.24Å 104.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 1.50 48.50 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.50-1.50) 99.1 (48.50-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.93 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.165 , 0.192 0.175 , 0.199	Depositor DCC
$R_{free}$ test set	3638 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.333 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: DP6, AGS, SO4, 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	1.49	16/2668 (0.6%)	1.63	47/3588 (1.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	SER	CB-OG	-10.10	1.29	1.42
1	A	129[A]	GLU	CD-OE1	-7.98	1.16	1.25
1	A	129[B]	GLU	CD-OE1	-7.98	1.16	1.25
1	A	128	SER	CB-OG	6.75	1.51	1.42
1	A	317	ASP	CB-CG	-6.70	1.37	1.51
1	A	144	ARG	CZ-NH1	6.56	1.41	1.33
1	A	173	ASP	CB-CG	6.46	1.65	1.51
1	A	176	SER	CB-OG	-6.29	1.34	1.42
1	A	167	TYR	CE1-CZ	-6.18	1.30	1.38
1	A	33	ASN	CG-ND2	-6.00	1.17	1.32
1	A	325	GLU	N-CA	5.91	1.58	1.46
1	A	227	ARG	CZ-NH1	5.73	1.40	1.33
1	A	157	GLU	CB-CG	5.58	1.62	1.52
1	A	305	LEU	N-CA	-5.53	1.35	1.46
1	A	236	TYR	CE2-CZ	-5.51	1.31	1.38
1	A	167	TYR	CG-CD2	-5.14	1.32	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASP	CB-CG-OD1	12.81	129.82	118.30
1	A	261	ASP	CB-CG-OD2	-12.78	106.80	118.30
1	A	173	ASP	CB-CG-OD2	12.38	129.44	118.30
1	A	158	ARG	NE-CZ-NH2	-10.61	114.99	120.30
1	A	26	ARG	NE-CZ-NH2	10.55	125.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ASP	CB-CG-OD1	9.90	127.21	118.30
1	A	206	GLU	OE1-CD-OE2	-9.29	112.15	123.30
1	A	305	LEU	CB-CG-CD1	8.96	126.23	111.00
1	A	211	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	127	LYS	CD-CE-NZ	8.27	130.72	111.70
1	A	292	GLU	OE1-CD-OE2	-8.25	113.41	123.30
1	A	40	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	211	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	A	41	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	159	GLU	OE1-CD-OE2	-7.54	114.25	123.30
1	A	147	PHE	CB-CG-CD2	-7.17	115.78	120.80
1	A	144	ARG	CD-NE-CZ	7.04	133.46	123.60
1	A	229	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	257	PHE	CB-CG-CD2	6.95	125.66	120.80
1	A	136	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	281	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	171	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	261	ASP	OD1-CG-OD2	6.64	135.92	123.30
1	A	121	LEU	CB-CG-CD1	6.48	122.02	111.00
1	A	24	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	235	TYR	CD1-CE1-CZ	-6.37	114.07	119.80
1	A	144	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	227	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	229	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	26	ARG	CB-CG-CD	5.92	126.98	111.60
1	A	129[A]	GLU	CB-CA-C	5.85	122.10	110.40
1	A	129[B]	GLU	CB-CA-C	5.85	122.10	110.40
1	A	293	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	173	ASP	OD1-CG-OD2	-5.72	112.44	123.30
1	A	144	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	209	GLU	O-C-N	-5.60	113.74	122.70
1	A	180	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	173	ASP	N-CA-CB	-5.40	100.89	110.60
1	A	292	GLU	CG-CD-OE2	5.34	128.99	118.30
1	A	167	TYR	CB-CG-CD2	5.33	124.20	121.00
1	A	41	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	121	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	289	PHE	CB-CG-CD1	5.14	124.40	120.80
1	A	124	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	40	ASP	OD1-CG-OD2	-5.11	113.60	123.30
1	A	195	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	88	PHE	N-CA-C	-5.00	97.49	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	2614	0	2646	28	0
2	A	18	0	10	1	0
3	A	31	0	12	6	0
4	A	23	0	12	0	0
5	A	10	0	0	0	0
6	A	243	0	0	9	2
All	All	2939	0	2680	32	2

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 6.

All (32) 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:1133:HOH:O	0.81	0.98
1:A:127:LYS:HE3	1:A:129[B]:GLU:H	1.32	0.93
1:A:127:LYS:HE3	1:A:129[A]:GLU:H	1.34	0.92
3:A:1002:AGS:S1G	6:A:1141:HOH:O	2.34	0.85
3:A:1002:AGS:O2G	6:A:1102:HOH:O	2.03	0.77
1:A:292:GLU:OE1	1:A:295:ILE:CD1	2.37	0.73
1:A:17:LYS:HG2	6:A:1123:HOH:O	1.89	0.72
1:A:190:LYS:NZ	3:A:1002:AGS:O3G	2.17	0.71
1:A:57:VAL:HG22	1:A:64:LEU:HD22	1.72	0.71
1:A:246:HIS:HD2	6:A:1208:HOH:O	1.74	0.69
1:A:203:GLU:OE1	6:A:1103:HOH:O	2.11	0.68
1:A:190:LYS:HD3	1:A:192:ILE:O	1.95	0.67
1:A:60:ASN:HD21	1:A:96:SER:H	1.41	0.67
1:A:292:GLU:OE1	1:A:295:ILE:HD11	1.97	0.64
1:A:33:ASN:HD22	1:A:155:LYS:H	1.49	0.60
1:A:292:GLU:OE1	1:A:295:ILE:HD12	2.01	0.59
2:A:1001:DP6:O1A	3:A:1002:AGS:S1G	2.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASN:ND2	1:A:155:LYS:H	2.01	0.58
1:A:241:HIS:HB3	6:A:1123:HOH:O	2.04	0.56
1:A:107:SER:N	3:A:1002:AGS:O2B	2.29	0.54
1:A:57:VAL:HB	1:A:92:VAL:HB	1.90	0.53
1:A:129[A]:GLU:HG2	1:A:166:CYS:O	2.10	0.52
1:A:71:GLU:OE1	1:A:75:ARG:NH2	2.45	0.50
3:A:1002:AGS:PG	6:A:1102:HOH:O	2.67	0.50
1:A:58:ILE:HG22	1:A:61:ASP:HA	1.97	0.46
1:A:55:ASN:HD22	1:A:90:VAL:H	1.64	0.44
1:A:8:SER:HA	1:A:45:VAL:O	2.18	0.44
1:A:271:HIS:HE1	6:A:1324:HOH:O	2.02	0.43
1:A:253:TRP:HA	1:A:254:PRO:C	2.38	0.43
1:A:190:LYS:HD2	1:A:193:SER:HA	2.00	0.42
1:A:190:LYS:CD	1:A:193:SER:HA	2.50	0.42
1:A:127:LYS:CE	1:A:129[B]:GLU:H	2.17	0.41

All (2) 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:1210:HOH:O	6:A:1210:HOH:O[4_555]	1.87	0.33
6:A:1298:HOH:O	6:A:1324:HOH:O[4_555]	2.06	0.14

## 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	325/325 (100%)	319 (98%)	5 (2%)	1 (0%)	41 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP

### 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	291/289 (101%)	277 (95%)	14 (5%)	25 4

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	53	ASP
1	A	54	LYS
1	A	61	ASP
1	A	63	ILE
1	A	66	GLU
1	A	69	MET
1	A	121	LEU
1	A	124	LEU
1	A	127	LYS
1	A	173	ASP
1	A	188	LYS
1	A	191	LYS
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 ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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$
5	SO4	A	1005	-	4,4,4	2.21	1 (25%)	6,6,6	1.72	2 (33%)
2	DP6	A	1001	-	11,17,17	1.29	2 (18%)	14,26,26	0.85	0
4	AMP	A	1003	-	22,25,25	1.81	6 (27%)	25,38,38	1.91	9 (36%)
3	AGS	A	1002	-	26,33,33	1.39	4 (15%)	26,52,52	1.35	3 (11%)
5	SO4	A	1004	-	4,4,4	1.65	2 (50%)	6,6,6	1.47	1 (16%)

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	-	-	3/17/19/19	-
4	AMP	A	1003	-	-	0/6/26/26	0/3/3/3
3	AGS	A	1002	-	-	3/17/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	AMP	C8-N7	4.02	1.41	1.34
5	A	1005	SO4	O2-S	-3.68	1.26	1.46
4	A	1003	AMP	P-O1P	3.42	1.61	1.50
3	A	1002	AGS	PG-S1G	3.30	1.97	1.90
4	A	1003	AMP	C4-N3	2.77	1.39	1.35
4	A	1003	AMP	C5-C4	2.75	1.48	1.40
3	A	1002	AGS	C2-N3	2.70	1.36	1.32
4	A	1003	AMP	P-O5'	2.67	1.68	1.60
3	A	1002	AGS	C5-C4	2.66	1.48	1.40
2	A	1001	DP6	C4-C5	-2.46	1.38	1.50
5	A	1004	SO4	O2-S	2.40	1.59	1.46
4	A	1003	AMP	C2-N3	2.37	1.35	1.32
3	A	1002	AGS	C4-N3	-2.32	1.32	1.35
5	A	1004	SO4	O3-S	2.07	1.64	1.47
2	A	1001	DP6	C2-C3	-2.03	1.51	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	AMP	N3-C2-N1	-4.48	121.67	128.68
4	A	1003	AMP	O5'-P-O1P	-3.43	96.85	106.47
3	A	1002	AGS	PA-O3A-PB	-3.26	121.64	132.83
4	A	1003	AMP	C1'-N9-C4	-2.87	121.60	126.64
3	A	1002	AGS	C1'-N9-C4	-2.83	121.66	126.64
3	A	1002	AGS	C3'-C2'-C1'	2.82	105.23	100.98
4	A	1003	AMP	O2P-P-O5'	2.74	114.03	106.73
5	A	1005	SO4	O4-S-O3	-2.62	97.87	109.06
4	A	1003	AMP	C4-C5-N7	2.41	111.91	109.40
5	A	1004	SO4	O4-S-O2	2.39	121.78	109.31
5	A	1005	SO4	O4-S-O2	2.30	121.30	109.31
4	A	1003	AMP	C2-N1-C6	2.19	122.50	118.75
4	A	1003	AMP	C5-C6-N6	-2.19	117.02	120.35
4	A	1003	AMP	O3P-P-O2P	2.18	115.96	107.64
4	A	1003	AMP	N6-C6-N1	2.01	122.74	118.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DP6	C5-O5-PA-O1A
2	A	1001	DP6	C2-C3-C4-C5

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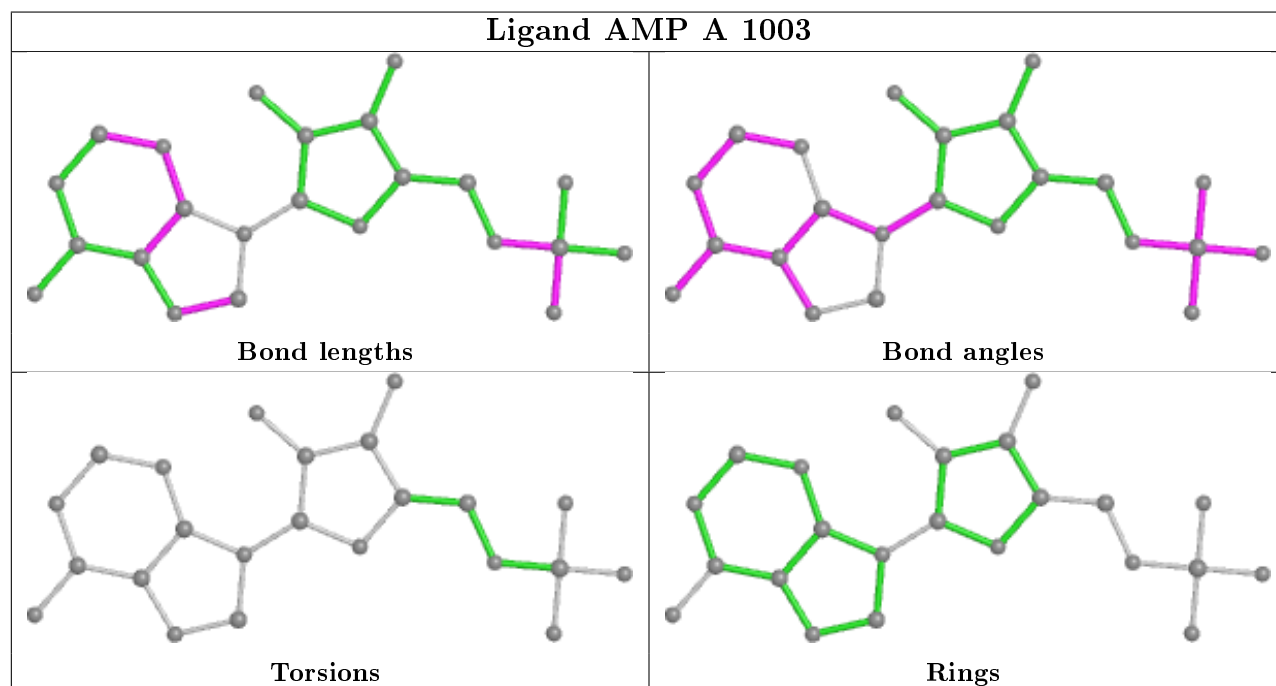
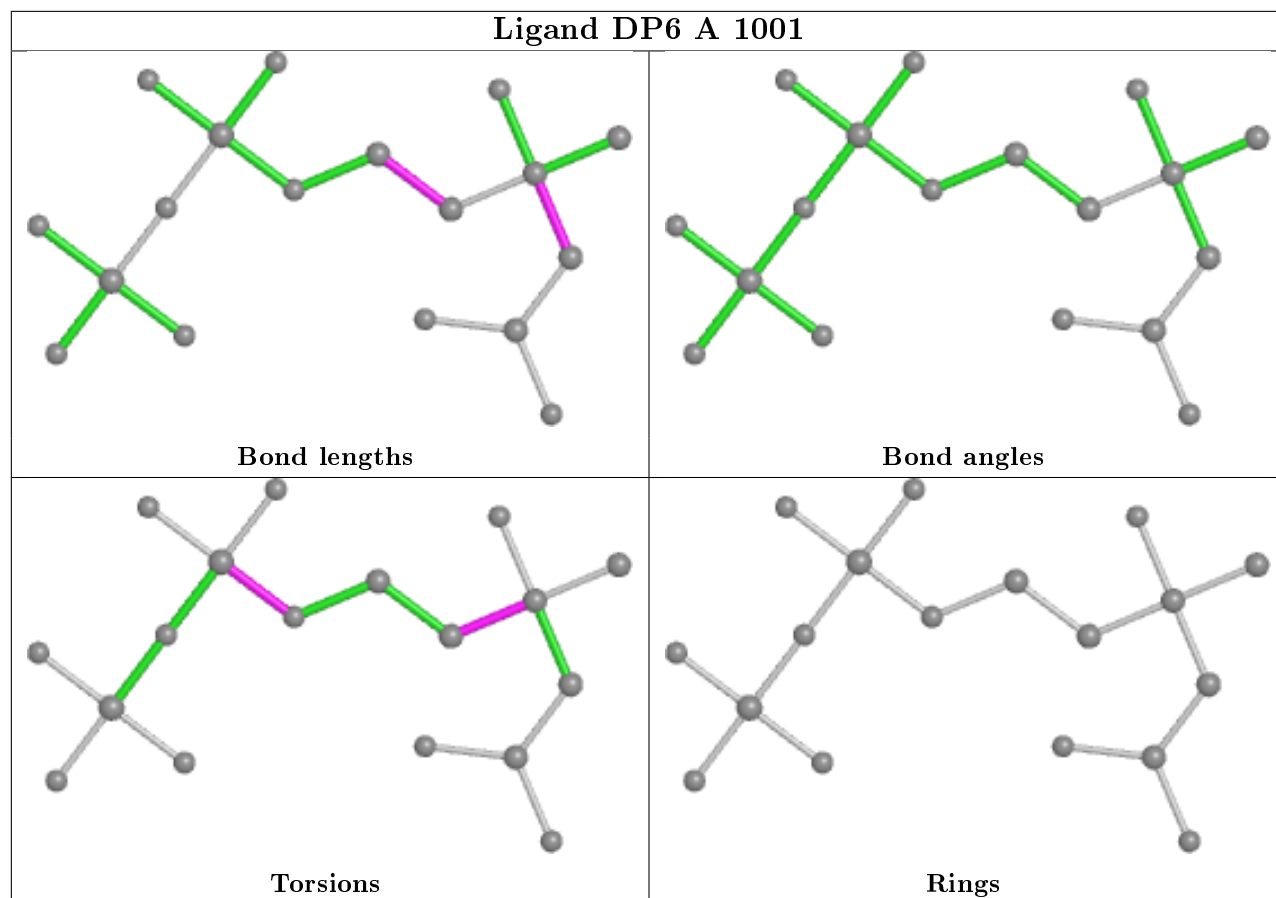
Mol	Chain	Res	Type	Atoms
3	A	1002	AGS	PB-O3B-PG-O2G
2	A	1001	DP6	C3A-C3-C4-C5
3	A	1002	AGS	C5'-O5'-PA-O1A
3	A	1002	AGS	C5'-O5'-PA-O3A

There are no ring outliers.

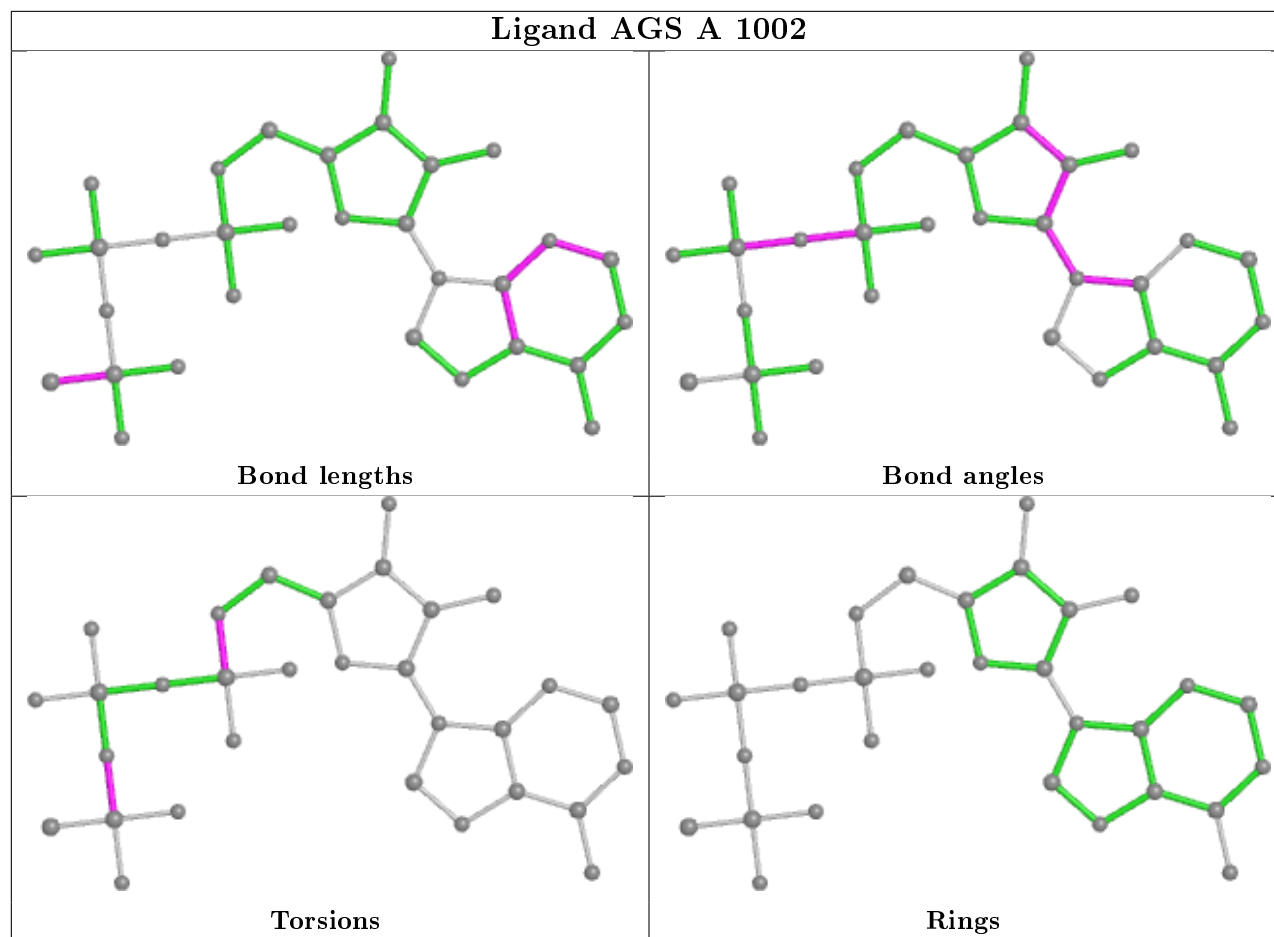
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DP6	1	0
3	A	1002	AGS	6	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, 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	325/325 (100%)	0.71	32 (9%) 7 7	8, 15, 43, 72	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ASP	6.0
1	A	85	GLY	5.5
1	A	56	ILE	5.0
1	A	54	LYS	4.9
1	A	67	ASP	4.6
1	A	1	MET	4.6
1	A	87	GLU	4.3
1	A	51	LEU	4.2
1	A	66	GLU	4.1
1	A	72	TYR	3.9
1	A	188	LYS	3.8
1	A	68	GLU	3.7
1	A	191	LYS	3.6
1	A	63	ILE	3.5
1	A	64	LEU	3.4
1	A	86	LYS	3.3
1	A	189	GLU	3.2
1	A	62	ARG	3.1
1	A	70	LYS	2.9
1	A	88	PHE	2.9
1	A	52	ASN	2.9
1	A	55	ASN	2.7
1	A	61	ASP	2.6
1	A	84	VAL	2.5
1	A	3	LYS	2.5
1	A	65	SER	2.5
1	A	89	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	MET	2.3
1	A	212	LEU	2.2
1	A	105	ALA	2.2
1	A	207	LEU	2.2
1	A	71	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

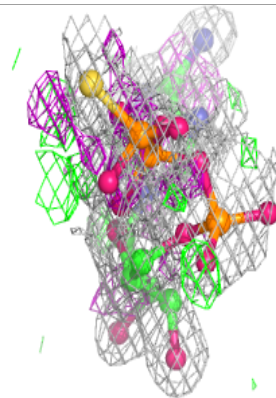
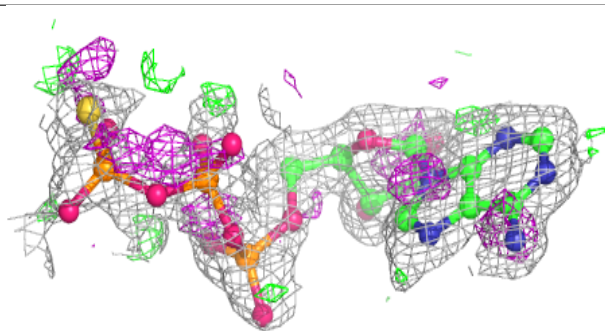
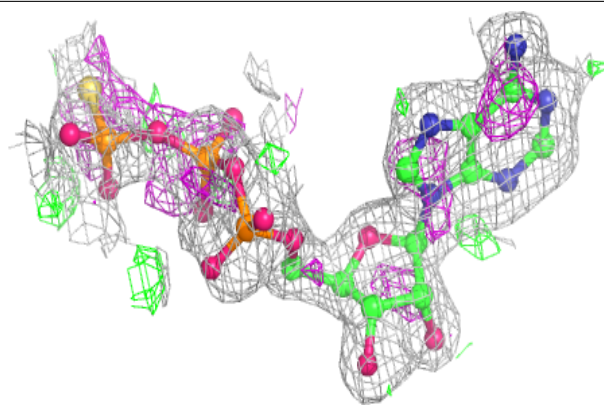
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	1004	5/5	0.79	0.21	32,34,49,56	0
3	AGS	A	1002	31/31	0.87	0.27	24,35,94,108	0
5	SO4	A	1005	5/5	0.91	0.21	15,29,34,36	0
4	AMP	A	1003	23/23	0.92	0.17	18,32,54,68	0
2	DP6	A	1001	18/18	0.98	0.08	11,12,16,18	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.

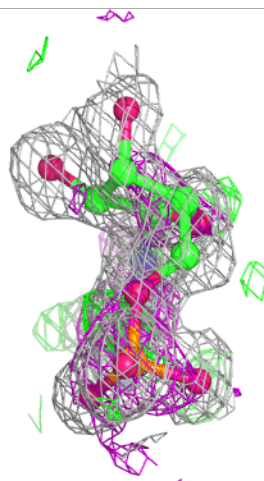
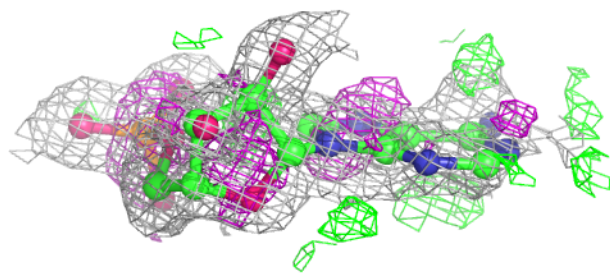
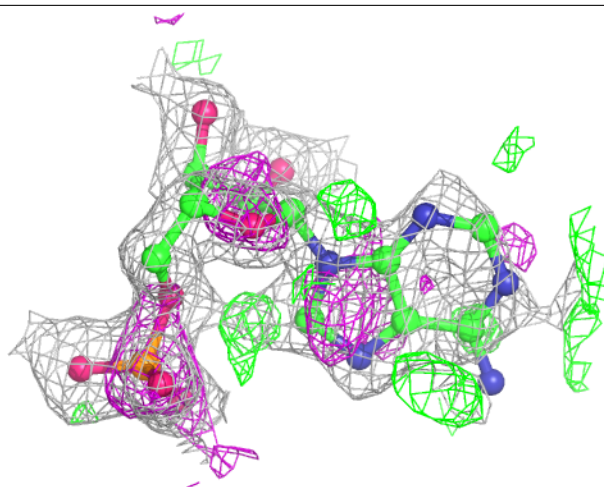
**Electron density around AGS A 1002:**

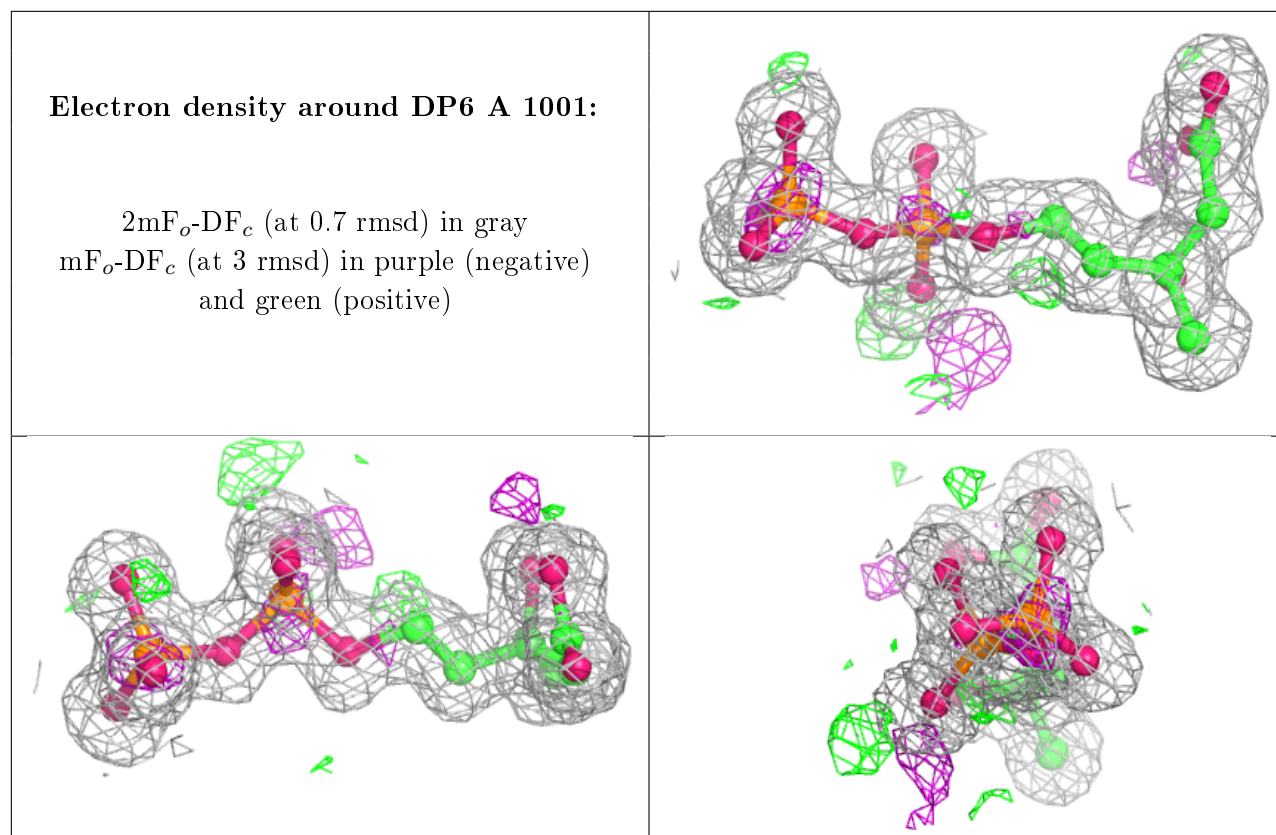
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AMP A 1003:**

$2mF_o-DF_c$  (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.