



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2024 – 11:42 pm BST

PDB ID : 4CVN
Title : Structure of the Fap7-Rps14 complex
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Deposited on : 2014-03-28
Resolution : 2.12 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

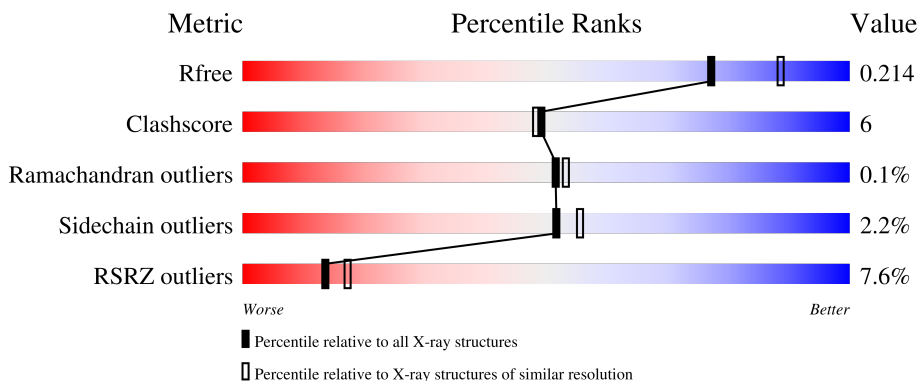
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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.



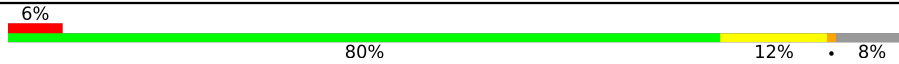

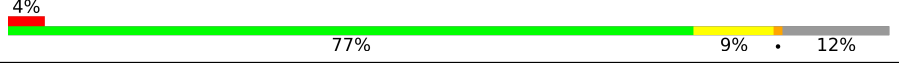

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	191	 4% 81% 13% • 6%
1	B	191	 3% 76% 14% • 9%
1	C	191	 14% 79% 14% • 6%
1	D	191	 16% 70% 14% • 14%

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Mol	Chain	Length	Quality of chain
2	E	137	
2	F	137	
2	G	137	
2	H	137	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9759 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 PUTATIVE ADENYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1412	897	237	275	3	0	0	0
1	B	174	1384	882	231	268	3	0	2	0
1	C	179	1412	897	237	275	3	0	0	0
1	D	165	1304	833	218	251	2	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q9UZK4
A	-9	LYS	-	expression tag	UNP Q9UZK4
A	-8	HIS	-	expression tag	UNP Q9UZK4
A	-7	HIS	-	expression tag	UNP Q9UZK4
A	-6	HIS	-	expression tag	UNP Q9UZK4
A	-5	HIS	-	expression tag	UNP Q9UZK4
A	-4	HIS	-	expression tag	UNP Q9UZK4
A	-3	HIS	-	expression tag	UNP Q9UZK4
A	-2	ALA	-	expression tag	UNP Q9UZK4
A	-1	MET	-	expression tag	UNP Q9UZK4
A	0	GLY	-	expression tag	UNP Q9UZK4
B	-10	MET	-	expression tag	UNP Q9UZK4
B	-9	LYS	-	expression tag	UNP Q9UZK4
B	-8	HIS	-	expression tag	UNP Q9UZK4
B	-7	HIS	-	expression tag	UNP Q9UZK4
B	-6	HIS	-	expression tag	UNP Q9UZK4
B	-5	HIS	-	expression tag	UNP Q9UZK4
B	-4	HIS	-	expression tag	UNP Q9UZK4
B	-3	HIS	-	expression tag	UNP Q9UZK4
B	-2	ALA	-	expression tag	UNP Q9UZK4
B	-1	MET	-	expression tag	UNP Q9UZK4

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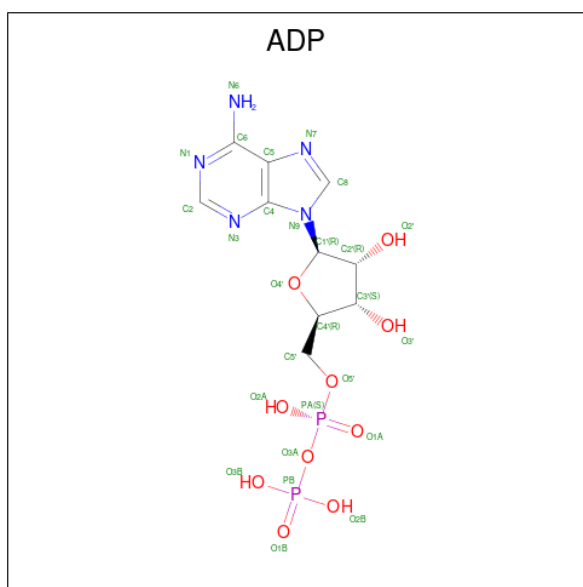
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q9UZK4
C	-10	MET	-	expression tag	UNP Q9UZK4
C	-9	LYS	-	expression tag	UNP Q9UZK4
C	-8	HIS	-	expression tag	UNP Q9UZK4
C	-7	HIS	-	expression tag	UNP Q9UZK4
C	-6	HIS	-	expression tag	UNP Q9UZK4
C	-5	HIS	-	expression tag	UNP Q9UZK4
C	-4	HIS	-	expression tag	UNP Q9UZK4
C	-3	HIS	-	expression tag	UNP Q9UZK4
C	-2	ALA	-	expression tag	UNP Q9UZK4
C	-1	MET	-	expression tag	UNP Q9UZK4
C	0	GLY	-	expression tag	UNP Q9UZK4
D	-10	MET	-	expression tag	UNP Q9UZK4
D	-9	LYS	-	expression tag	UNP Q9UZK4
D	-8	HIS	-	expression tag	UNP Q9UZK4
D	-7	HIS	-	expression tag	UNP Q9UZK4
D	-6	HIS	-	expression tag	UNP Q9UZK4
D	-5	HIS	-	expression tag	UNP Q9UZK4
D	-4	HIS	-	expression tag	UNP Q9UZK4
D	-3	HIS	-	expression tag	UNP Q9UZK4
D	-2	ALA	-	expression tag	UNP Q9UZK4
D	-1	MET	-	expression tag	UNP Q9UZK4
D	0	GLY	-	expression tag	UNP Q9UZK4

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	126	Total	C	N	O	S	0	0	0
			947	586	189	170	2			
2	F	118	Total	C	N	O	S	0	0	0
			882	550	168	162	2			
2	G	120	Total	C	N	O	S	0	0	0
			895	558	171	164	2			
2	H	119	Total	C	N	O	S	0	0	0
			903	559	180	162	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	93	Total	O	0	0
			93	93		

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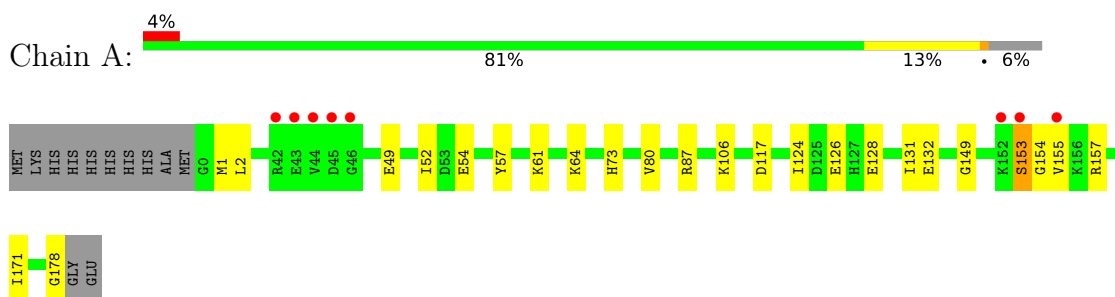
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	99	Total O 99 99	0	0
5	C	41	Total O 41 41	0	0
5	D	62	Total O 62 62	0	0
5	E	55	Total O 55 55	0	0
5	F	45	Total O 45 45	0	0
5	G	46	Total O 46 46	0	0
5	H	67	Total O 67 67	0	0

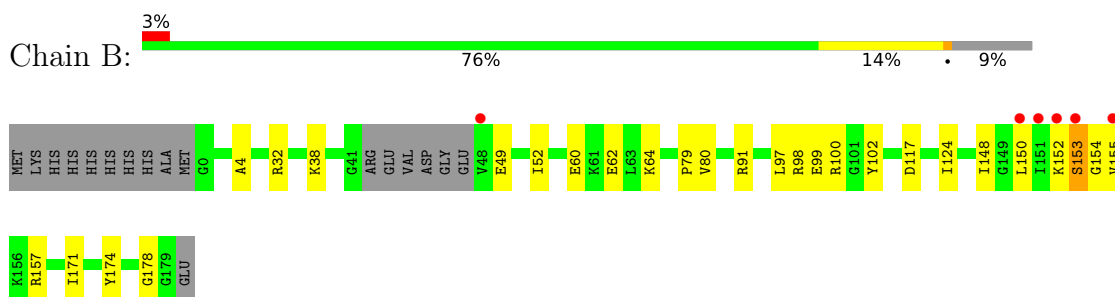
3 Residue-property plots [i](#)

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.

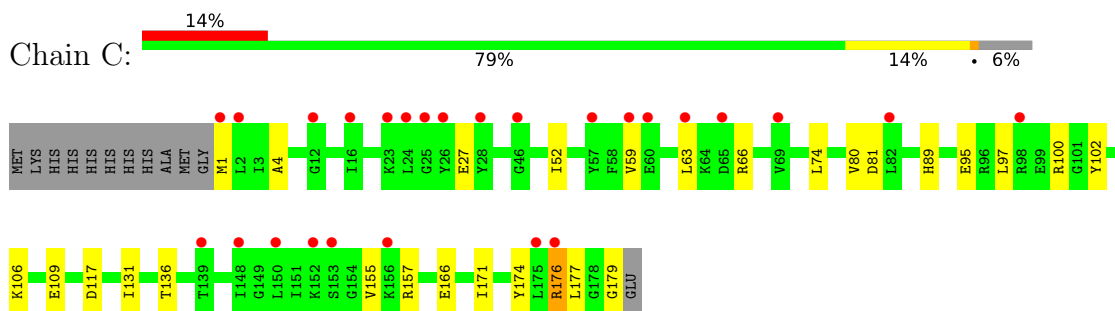
- Molecule 1: PUTATIVE ADENYLATE KINASE



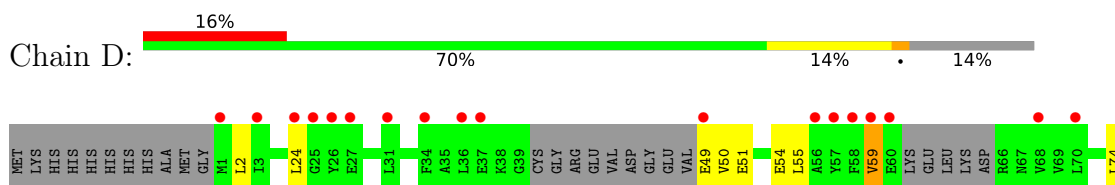
- Molecule 1: PUTATIVE ADENYLATE KINASE



- Molecule 1: PUTATIVE ADENYLATE KINASE

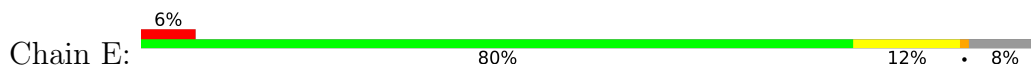


- Molecule 1: PUTATIVE ADENYLATE KINASE

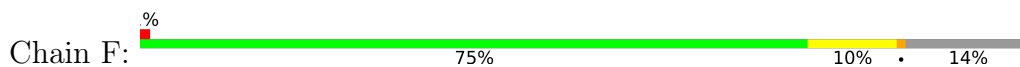




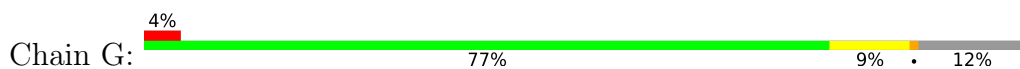
- Molecule 2: 30S RIBOSOMAL PROTEIN S11



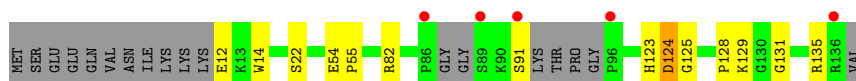
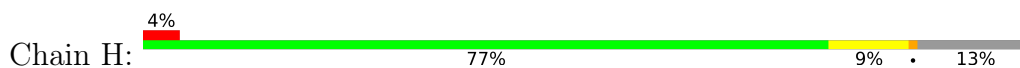
- Molecule 2: 30S RIBOSOMAL PROTEIN S11



- Molecule 2: 30S RIBOSOMAL PROTEIN S11



- Molecule 2: 30S RIBOSOMAL PROTEIN S11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.05Å 139.55Å 83.08Å 90.00° 105.51° 90.00°	Depositor
Resolution (Å)	44.77 – 2.12 44.83 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.77-2.12) 99.5 (44.83-2.12)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.12Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.172 , 0.212 0.173 , 0.214	Depositor DCC
R_{free} test set	4133 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtrriage
Anisotropy	0.313	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9759	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: ADP, 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	0.39	0/1430	0.59	0/1933
1	B	0.40	0/1400	0.61	0/1890
1	C	0.34	0/1430	0.60	0/1933
1	D	0.36	0/1320	0.58	0/1784
2	E	0.38	0/965	0.65	1/1301 (0.1%)
2	F	0.39	0/900	0.62	0/1219
2	G	0.39	0/913	0.62	0/1235
2	H	0.43	0/918	0.65	0/1235
All	All	0.39	0/9276	0.61	1/12530 (0.0%)

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
1	B	0	1
1	D	0	1
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	125	GLY	N-CA-C	-5.56	99.21	113.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	SER	Peptide
1	B	153	SER	Peptide
1	D	153	SER	Peptide
2	E	123	HIS	Peptide
2	F	123	HIS	Peptide
2	G	123	HIS	Peptide
2	H	123	HIS	Peptide

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	1412	0	1443	22	0
1	B	1384	0	1416	18	0
1	C	1412	0	1443	20	0
1	D	1304	0	1336	21	0
2	E	947	0	972	13	0
2	F	882	0	898	24	0
2	G	895	0	914	12	0
2	H	903	0	922	10	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	93	0	0	1	0
5	B	99	0	0	1	0
5	C	41	0	0	2	0
5	D	62	0	0	1	0
5	E	55	0	0	4	0
5	F	45	0	0	2	0
5	G	46	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	67	0	0	0	0
All	All	9759	0	9392	109	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 6.

All (109) 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:54:GLU:OE2	2:F:93:THR:HG23	1.78	0.83
1:C:157:ARG:NH1	5:C:2022:HOH:O	2.03	0.82
2:G:92:LYS:NZ	5:G:2038:HOH:O	2.12	0.81
1:D:166:GLU:OE2	5:D:2047:HOH:O	1.99	0.81
1:C:95:GLU:OE2	1:C:174:TYR:OH	1.99	0.79
1:B:98:ARG:NH2	1:B:174:TYR:OH	2.16	0.79
1:B:38:LYS:NZ	1:B:62:GLU:OE1	2.16	0.78
1:A:157:ARG:NH2	5:A:2061:HOH:O	2.15	0.77
1:B:100:ARG:NH2	3:B:1001:ADP:O3B	2.13	0.74
2:E:53:ASP:OD1	5:E:2029:HOH:O	2.06	0.73
1:A:57:TYR:OH	2:F:117:ASP:OD2	2.04	0.72
1:D:90:PRO:HB2	1:D:171:ILE:HG21	1.73	0.71
2:E:90:LYS:NZ	5:E:2027:HOH:O	2.07	0.70
1:C:166:GLU:OE2	5:C:2032:HOH:O	2.08	0.70
1:B:124:ILE:HG23	1:B:157:ARG:HH22	1.59	0.68
1:D:161:ILE:HD12	1:D:162:VAL:HG13	1.76	0.67
2:E:69:GLU:OE2	5:E:2032:HOH:O	2.14	0.66
1:C:27:GLU:OE1	1:C:66:ARG:NH2	2.22	0.65
2:G:127:ARG:HD2	2:G:128:PRO:HD2	1.80	0.63
1:D:2:LEU:N	1:D:81:ASP:OD2	2.31	0.63
1:C:179:GLY:HA2	2:G:82:ARG:HH22	1.65	0.62
1:A:149:GLY:O	1:A:153:SER:OG	2.18	0.61
1:D:100:ARG:NH2	3:D:1001:ADP:O1B	2.24	0.60
1:A:61:LYS:NZ	2:F:117:ASP:OD2	2.34	0.59
1:D:128:GLU:N	1:D:128:GLU:OE1	2.31	0.58
1:B:153:SER:OG	1:B:155:VAL:HG23	2.04	0.58
1:D:74:LEU:HD11	2:F:128:PRO:HG3	1.86	0.57
2:F:103:ARG:CZ	2:F:107:ARG:HH11	2.17	0.57
1:D:153:SER:N	1:D:154:GLY:HA2	2.21	0.56
1:D:55:LEU:O	1:D:59:VAL:HG12	2.05	0.56
1:A:131:ILE:HD11	1:A:155:VAL:O	2.05	0.56
1:B:32:ARG:HA	2:E:126:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:SER:N	1:B:154:GLY:HA2	2.22	0.55
1:B:49[A]:GLU:HA	2:E:127:ARG:O	2.07	0.55
1:C:59:VAL:HG13	1:C:63:LEU:HD12	1.89	0.53
1:B:97:LEU:HD22	1:B:102:TYR:CE2	2.44	0.53
1:D:179:GLY:HA2	2:F:82:ARG:NH2	2.24	0.53
1:A:153:SER:N	1:A:154:GLY:HA2	2.23	0.53
1:A:57:TYR:OH	1:A:61:LYS:NZ	2.43	0.52
1:C:179:GLY:HA2	2:G:82:ARG:NH2	2.25	0.51
1:C:109:GLU:HA	1:C:176:ARG:NH2	2.25	0.51
1:B:91:ARG:NH2	5:B:2046:HOH:O	2.28	0.51
1:C:100:ARG:NH2	3:C:1001:ADP:O1B	2.32	0.50
1:B:178:GLY:C	2:E:82:ARG:HH12	2.15	0.49
2:F:103:ARG:NE	2:F:107:ARG:HH11	2.09	0.49
1:A:178:GLY:C	2:H:82:ARG:HH22	2.15	0.49
1:C:117:ASP:OD2	2:G:22:SER:HB2	2.12	0.49
1:D:76:HIS:NE2	1:D:122:GLU:OE1	2.36	0.49
1:B:148:ILE:O	1:B:152:LYS:HG2	2.12	0.49
1:A:54:GLU:OE2	2:F:93:THR:CG2	2.58	0.48
1:D:179:GLY:HA2	2:F:82:ARG:HH22	1.78	0.48
1:A:2:LEU:HG	1:A:80:VAL:HG12	1.94	0.48
1:A:126:GLU:OE2	2:F:103:ARG:NH1	2.39	0.48
1:C:4:ALA:HB2	1:C:80:VAL:HG11	1.96	0.48
2:E:65:ARG:O	2:E:69:GLU:HG3	2.14	0.47
2:F:103:ARG:NE	2:F:107:ARG:NH1	2.62	0.47
1:D:51:GLU:HG3	1:D:54:GLU:H	1.79	0.47
1:C:52:ILE:HD11	2:G:128:PRO:HB3	1.96	0.47
1:D:178:GLY:O	2:F:82:ARG:NH2	2.36	0.47
1:A:52:ILE:CD1	2:H:135:ARG:HA	2.45	0.47
1:C:177:LEU:HA	2:G:18:HIS:CE1	2.50	0.46
1:D:24:LEU:HD21	1:D:148:ILE:HG12	1.97	0.46
2:F:103:ARG:NH2	2:F:107:ARG:HH11	2.13	0.46
2:F:103:ARG:NH2	2:F:107:ARG:NH1	2.63	0.46
2:G:54:GLU:N	2:G:55:PRO:HD2	2.30	0.46
2:G:65:ARG:O	2:G:69:GLU:HG3	2.16	0.46
2:H:12:GLU:HG3	2:H:14:TRP:HE1	1.81	0.46
1:A:49:GLU:HB3	2:H:129:LYS:HA	1.98	0.45
2:G:103:ARG:O	2:G:107:ARG:HG2	2.17	0.45
2:F:103:ARG:HE	2:F:107:ARG:NH1	2.14	0.45
1:A:52:ILE:HD11	2:H:135:ARG:HA	1.98	0.45
1:A:126:GLU:CD	2:F:103:ARG:HH12	2.19	0.45
2:F:107:ARG:NH2	5:F:2041:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLU:O	1:D:157:ARG:NH1	2.46	0.44
2:E:89:SER:OG	2:E:90:LYS:N	2.50	0.44
1:B:150:LEU:O	1:B:153:SER:OG	2.29	0.44
1:D:128:GLU:OE2	1:D:129:ASN:ND2	2.51	0.44
2:F:52:ARG:HG2	5:F:2020:HOH:O	2.18	0.44
2:F:65:ARG:NH1	2:F:69:GLU:OE1	2.31	0.44
1:A:106:LYS:NZ	2:H:124:ASP:CG	2.71	0.44
1:C:89:HIS:H	1:C:136:THR:CG2	2.31	0.44
1:C:106:LYS:NZ	2:G:124:ASP:CG	2.72	0.43
1:D:106:LYS:NZ	2:F:124:ASP:CG	2.72	0.43
1:D:150:LEU:HD22	1:D:155:VAL:HG21	2.00	0.43
2:F:65:ARG:HH11	2:F:65:ARG:HG3	1.82	0.43
1:D:129:ASN:OD1	1:D:156:LYS:HB3	2.17	0.43
1:C:1:MET:HA	1:C:81:ASP:OD2	2.19	0.43
1:C:131:ILE:HD11	1:C:155:VAL:O	2.18	0.43
1:B:4:ALA:HB2	1:B:80:VAL:HG11	2.00	0.43
2:F:103:ARG:HH21	2:F:107:ARG:NH1	2.17	0.43
1:C:97:LEU:HD22	1:C:102:TYR:CE2	2.54	0.43
1:C:109:GLU:HA	1:C:176:ARG:HH21	1.84	0.42
1:B:117:ASP:OD2	2:E:22:SER:HB2	2.20	0.42
1:A:87:ARG:NH1	1:A:132:GLU:OE2	2.48	0.42
2:E:54:GLU:N	2:E:55:PRO:HD2	2.35	0.41
2:E:69:GLU:HG2	5:E:2036:HOH:O	2.21	0.41
1:A:73:HIS:CD2	2:H:125:GLY:HA3	2.56	0.41
1:D:148:ILE:O	1:D:152:LYS:HB2	2.21	0.41
1:B:60:GLU:HB2	1:B:79:PRO:HG2	2.03	0.41
2:F:57:PRO:O	2:F:61:MET:HG3	2.20	0.41
2:H:128:PRO:HG2	2:H:131:GLY:O	2.21	0.41
1:A:117:ASP:OD2	2:H:22:SER:HB2	2.21	0.41
1:A:124:ILE:HG23	1:A:157:ARG:HH22	1.85	0.41
1:C:74:LEU:HD11	2:G:128:PRO:HD3	2.03	0.41
1:B:52:ILE:HD11	2:E:128:PRO:HB3	2.02	0.41
1:A:61:LYS:CE	2:F:117:ASP:OD2	2.69	0.41
2:E:135:ARG:O	2:E:136:ARG:HB3	2.21	0.40
1:B:148:ILE:HG23	1:B:152:LYS:HE2	2.03	0.40
2:H:54:GLU:N	2:H:55:PRO:HD2	2.36	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	177/191 (93%)	176 (99%)	1 (1%)	0	100	100
1	B	170/191 (89%)	169 (99%)	1 (1%)	0	100	100
1	C	177/191 (93%)	172 (97%)	4 (2%)	1 (1%)	25	20
1	D	159/191 (83%)	158 (99%)	1 (1%)	0	100	100
2	E	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
2	F	116/137 (85%)	115 (99%)	1 (1%)	0	100	100
2	G	118/137 (86%)	117 (99%)	1 (1%)	0	100	100
2	H	113/137 (82%)	112 (99%)	1 (1%)	0	100	100
All	All	1154/1312 (88%)	1142 (99%)	11 (1%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	176	ARG

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	154/164 (94%)	150 (97%)	4 (3%)	46	49
1	B	151/164 (92%)	148 (98%)	3 (2%)	55	59
1	C	154/164 (94%)	153 (99%)	1 (1%)	86	90
1	D	142/164 (87%)	137 (96%)	5 (4%)	36	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	93/104 (89%)	91 (98%)	2 (2%)	52	55
2	F	88/104 (85%)	85 (97%)	3 (3%)	37	38
2	G	89/104 (86%)	88 (99%)	1 (1%)	73	79
2	H	89/104 (86%)	87 (98%)	2 (2%)	52	55
All	All	960/1072 (90%)	939 (98%)	21 (2%)	52	55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	64	LYS
1	A	128	GLU
1	A	171	ILE
1	B	64	LYS
1	B	99	GLU
1	B	171	ILE
1	C	171	ILE
1	D	49	GLU
1	D	50	VAL
1	D	59	VAL
1	D	156	LYS
1	D	171	ILE
2	E	124	ASP
2	E	136	ARG
2	F	25	ASN
2	F	33	ILE
2	F	124	ASP
2	G	124	ASP
2	H	91	SER
2	H	124	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	ADP	C	1001	4	24,29,29	0.99	1 (4%)	29,45,45	1.46	4 (13%)
3	ADP	A	1001	4	24,29,29	0.98	2 (8%)	29,45,45	1.28	3 (10%)
3	ADP	B	1001	4	24,29,29	1.04	1 (4%)	29,45,45	1.39	4 (13%)
3	ADP	D	1001	4	24,29,29	0.97	1 (4%)	29,45,45	1.47	5 (17%)

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	ADP	C	1001	4	-	0/12/32/32	0/3/3/3
3	ADP	A	1001	4	-	0/12/32/32	0/3/3/3
3	ADP	B	1001	4	-	0/12/32/32	0/3/3/3
3	ADP	D	1001	4	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	ADP	C5-C4	2.71	1.48	1.40
3	C	1001	ADP	C5-C4	2.58	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1001	ADP	C5-C4	2.48	1.47	1.40
3	A	1001	ADP	O4'-C1'	2.25	1.44	1.41
3	A	1001	ADP	C5-C4	2.22	1.46	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	ADP	C4-C5-N7	-3.29	105.97	109.40
3	C	1001	ADP	N3-C2-N1	-3.28	123.55	128.68
3	B	1001	ADP	N3-C2-N1	-3.24	123.62	128.68
3	D	1001	ADP	C4-C5-N7	-3.22	106.05	109.40
3	D	1001	ADP	PA-O3A-PB	-3.18	121.90	132.83
3	D	1001	ADP	N3-C2-N1	-3.17	123.73	128.68
3	A	1001	ADP	N3-C2-N1	-3.11	123.81	128.68
3	C	1001	ADP	PA-O3A-PB	-2.91	122.84	132.83
3	C	1001	ADP	C4-C5-N7	-2.86	106.42	109.40
3	A	1001	ADP	C4-C5-N7	-2.78	106.50	109.40
3	C	1001	ADP	C3'-C2'-C1'	2.60	104.89	100.98
3	B	1001	ADP	PA-O3A-PB	-2.29	124.98	132.83
3	A	1001	ADP	PA-O3A-PB	-2.26	125.06	132.83
3	D	1001	ADP	O3B-PB-O2B	2.25	116.25	107.64
3	D	1001	ADP	C3'-C2'-C1'	2.17	104.25	100.98
3	B	1001	ADP	C2-N1-C6	2.07	122.30	118.75

There are no chirality outliers.

There are no torsion outliers.

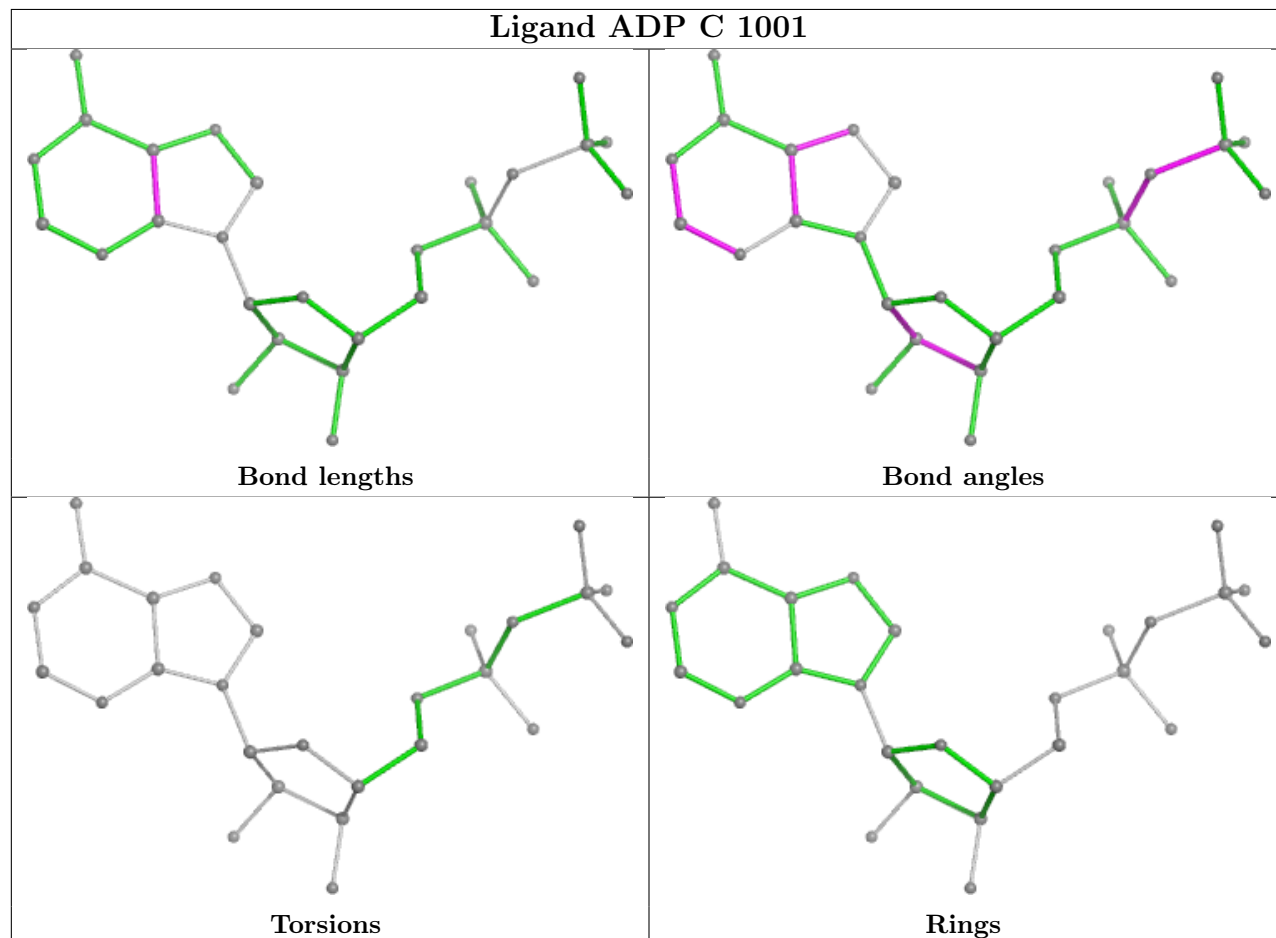
There are no ring outliers.

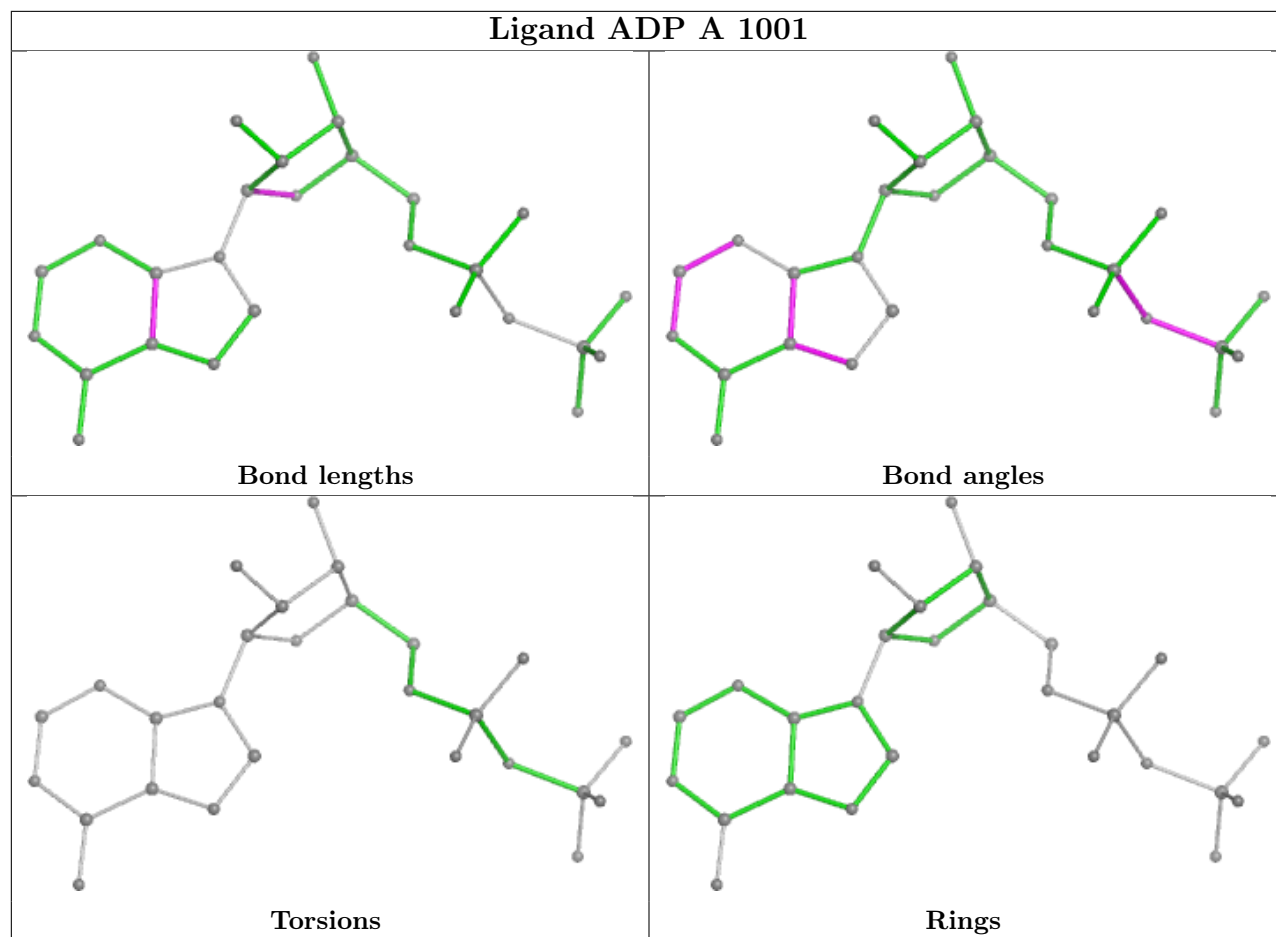
3 monomers are involved in 3 short contacts:

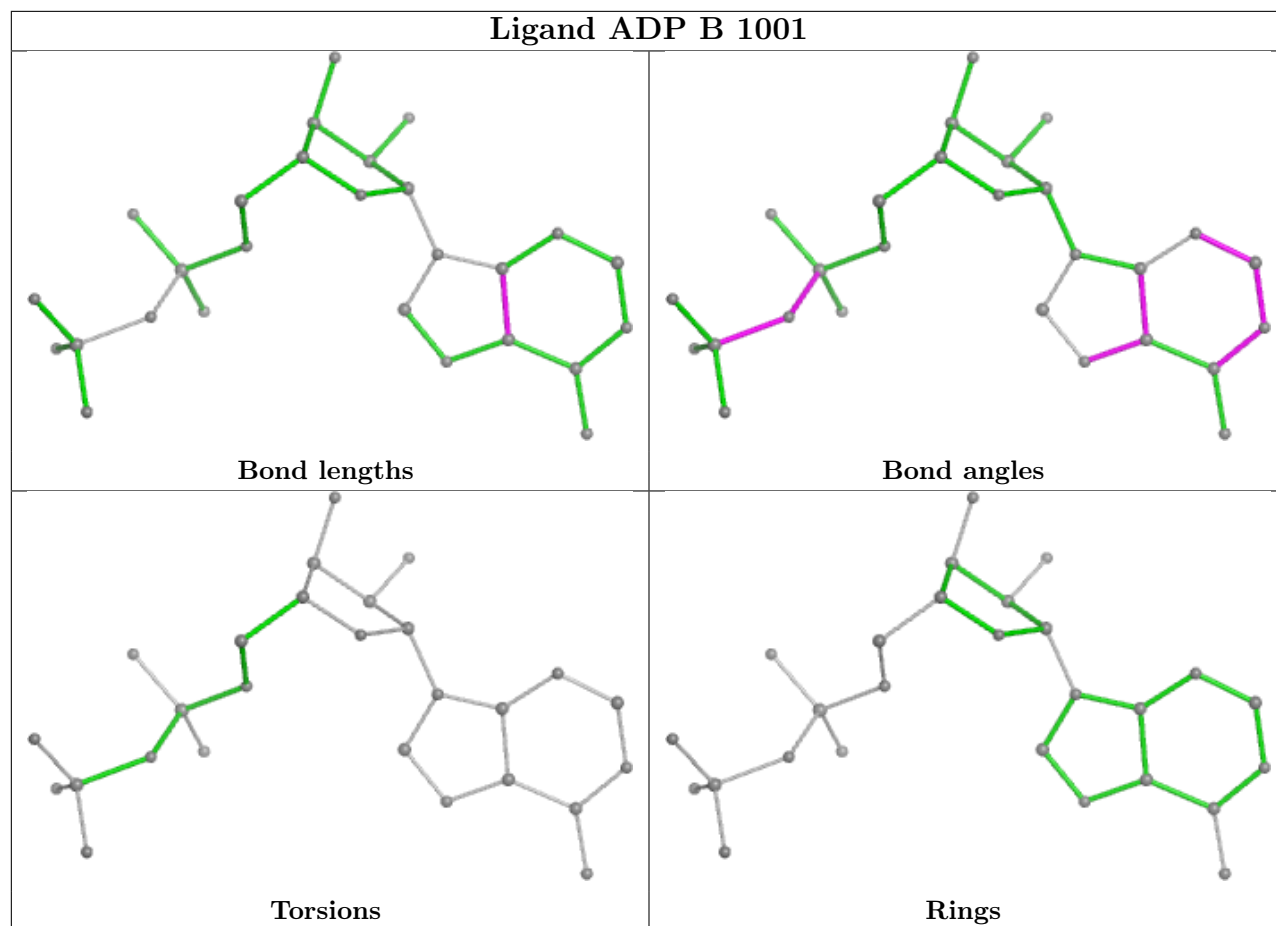
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	ADP	1	0
3	B	1001	ADP	1	0
3	D	1001	ADP	1	0

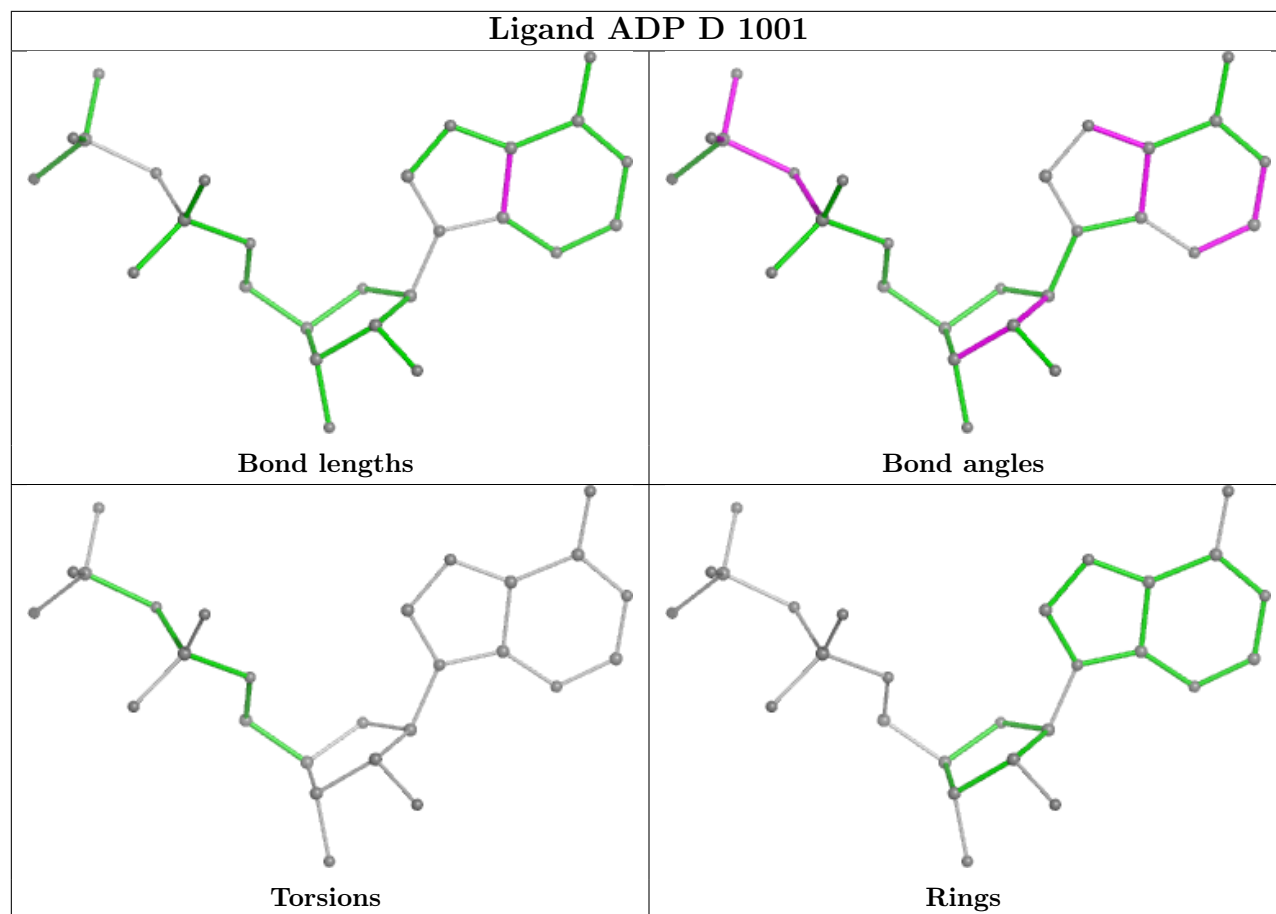
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	178:GLY	C	179:GLY	N	3.03

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	179/191 (93%)	0.31	8 (4%) 33 38	28, 49, 90, 122	0
1	B	174/191 (91%)	0.26	6 (3%) 45 51	28, 46, 83, 103	0
1	C	179/191 (93%)	0.70	26 (14%) 2 3	37, 66, 97, 129	0
1	D	165/191 (86%)	0.86	30 (18%) 1 1	31, 74, 119, 142	0
2	E	126/137 (91%)	0.56	8 (6%) 20 24	27, 41, 89, 122	0
2	F	118/137 (86%)	0.17	2 (1%) 70 74	32, 46, 91, 116	0
2	G	120/137 (87%)	0.14	5 (4%) 36 42	29, 43, 92, 120	0
2	H	119/137 (86%)	0.35	5 (4%) 36 42	26, 37, 78, 107	0
All	All	1180/1312 (89%)	0.44	90 (7%) 13 17	26, 50, 101, 142	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	TYR	5.9
1	D	59	VAL	5.4
2	H	136	ARG	5.3
1	D	58	PHE	5.2
1	D	24	LEU	5.2
1	A	44	VAL	4.7
1	A	155	VAL	4.6
1	D	34	PHE	4.5
2	E	136	ARG	4.3
1	D	37	GLU	4.1
1	D	1	MET	4.0
1	D	152	LYS	3.9
1	B	153	SER	3.9
1	B	48[A]	VAL	3.9
1	B	155	VAL	3.8
1	C	24	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	148	ILE	3.7
1	D	81	ASP	3.7
2	G	130	GLY	3.7
1	D	57	TYR	3.6
1	D	36	LEU	3.6
1	D	155	VAL	3.5
1	C	152	LYS	3.5
1	C	25	GLY	3.5
1	D	49	GLU	3.4
1	A	43	GLU	3.4
2	E	95	GLY	3.4
2	G	124	ASP	3.3
2	F	127	ARG	3.3
1	C	59	VAL	3.2
1	C	176	ARG	3.2
1	D	148	ILE	3.1
1	C	150	LEU	3.1
1	C	23	LYS	3.1
2	G	91	SER	3.1
1	C	26	TYR	2.9
1	C	153	SER	2.9
1	D	154	GLY	2.8
1	C	65	ASP	2.8
1	D	3	ILE	2.8
1	D	131	ILE	2.8
1	A	45	ASP	2.7
1	A	46	GLY	2.7
1	D	25	GLY	2.7
2	E	87	GLY	2.7
1	C	139	THR	2.7
2	H	91	SER	2.7
1	C	175	LEU	2.7
1	D	82	LEU	2.7
1	C	28	TYR	2.6
1	A	152	LYS	2.6
1	C	63	LEU	2.6
2	H	86	PRO	2.6
1	C	46	GLY	2.6
1	D	60	GLU	2.5
1	A	42	ARG	2.5
1	C	16	ILE	2.5
1	D	153	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	68	VAL	2.5
1	D	70	LEU	2.4
1	D	150	LEU	2.4
1	C	69	VAL	2.4
1	A	153	SER	2.4
1	D	129	ASN	2.4
1	C	60	GLU	2.4
2	E	91	SER	2.4
2	E	86	PRO	2.4
1	C	98	ARG	2.4
2	G	126	THR	2.3
1	D	27	GLU	2.3
1	B	151	ILE	2.3
2	E	96	PRO	2.2
1	C	156	LYS	2.2
1	C	82	LEU	2.2
1	B	152	LYS	2.2
1	D	156	LYS	2.2
1	C	2	LEU	2.2
1	D	56	ALA	2.2
1	B	150	LEU	2.1
2	F	90	LYS	2.1
1	D	149	GLY	2.1
2	G	127	ARG	2.1
1	C	1	MET	2.1
1	D	31	LEU	2.1
2	H	89	SER	2.0
2	H	96	PRO	2.0
1	C	57	TYR	2.0
2	E	88	GLY	2.0
1	C	12	GLY	2.0
2	E	124	ASP	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](#)

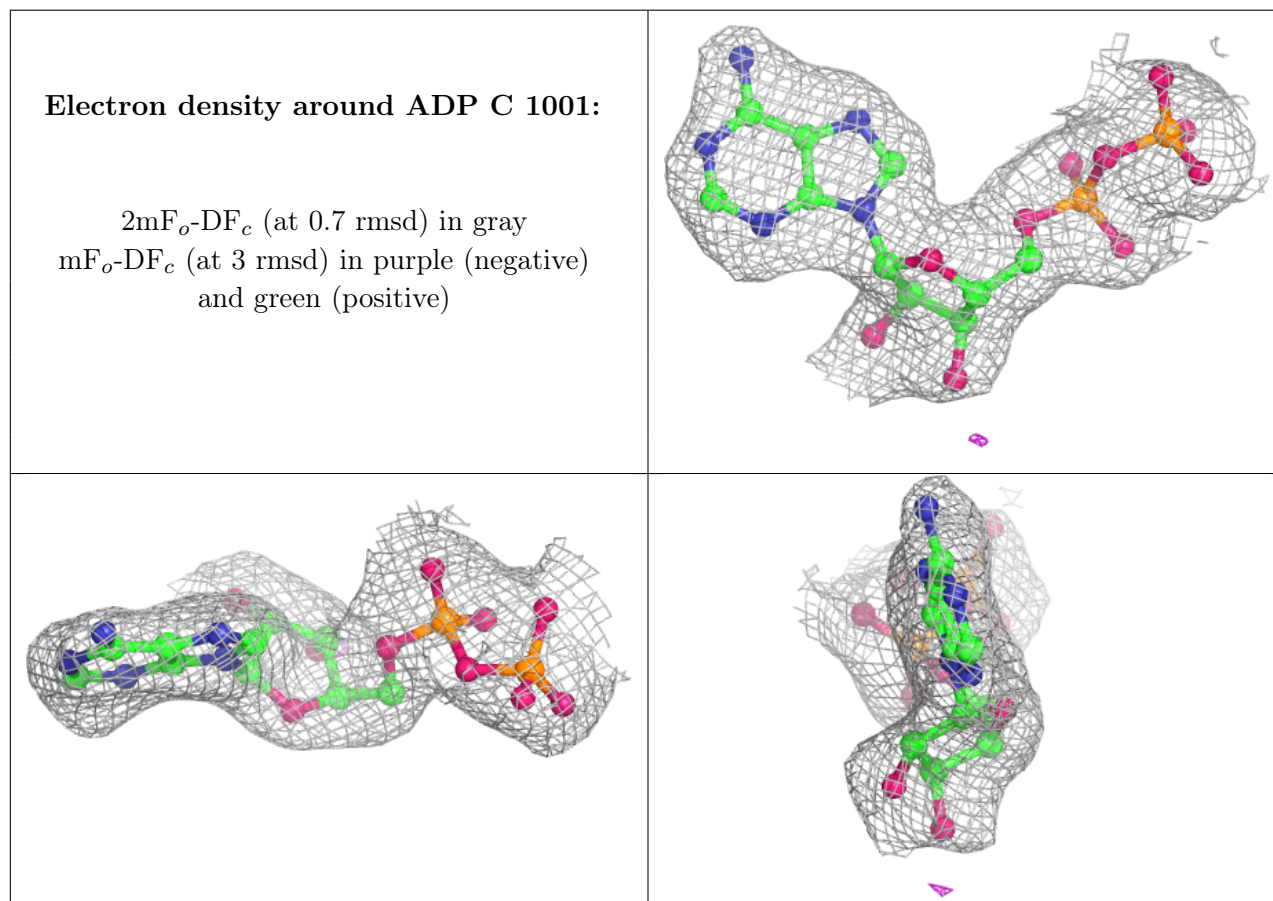
There are no monosaccharides in this entry.

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, 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.

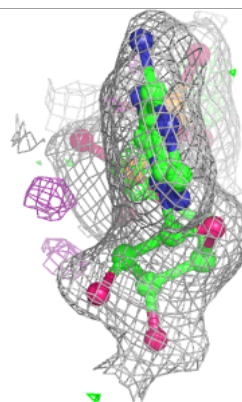
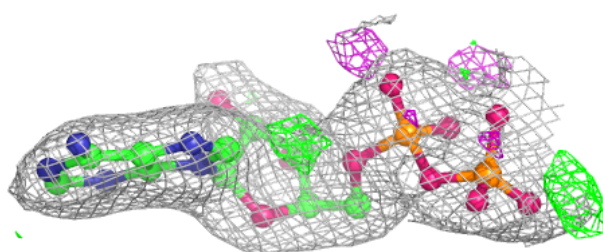
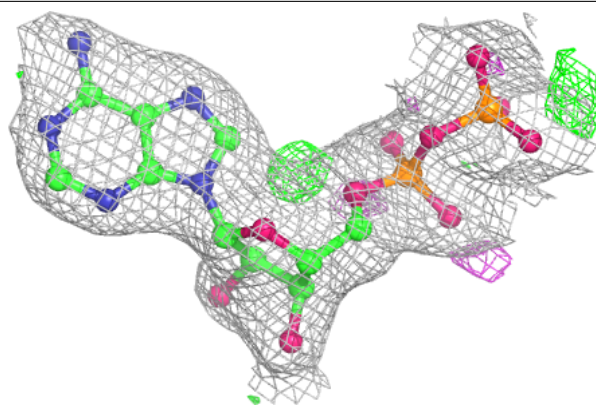
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	1002	1/1	0.92	0.09	37,37,37,37	0
4	MG	C	1002	1/1	0.95	0.04	53,53,53,53	0
3	ADP	C	1001	27/27	0.96	0.14	44,64,83,91	0
3	ADP	D	1001	27/27	0.96	0.11	43,53,76,84	0
3	ADP	A	1001	27/27	0.96	0.12	26,38,47,51	0
3	ADP	B	1001	27/27	0.96	0.12	30,39,50,58	0
4	MG	D	1002	1/1	0.96	0.07	69,69,69,69	0
4	MG	B	1002	1/1	0.98	0.07	35,35,35,35	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.

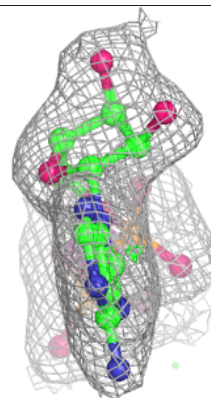
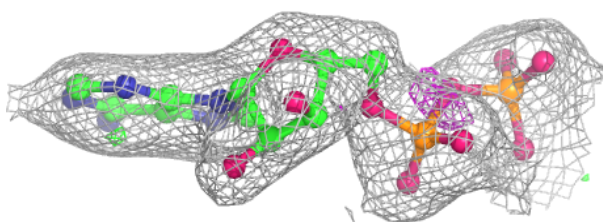
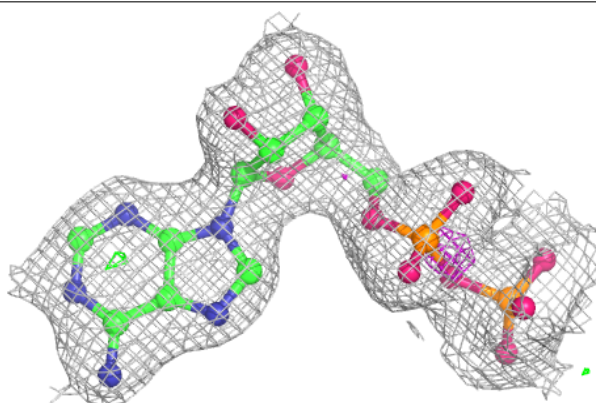


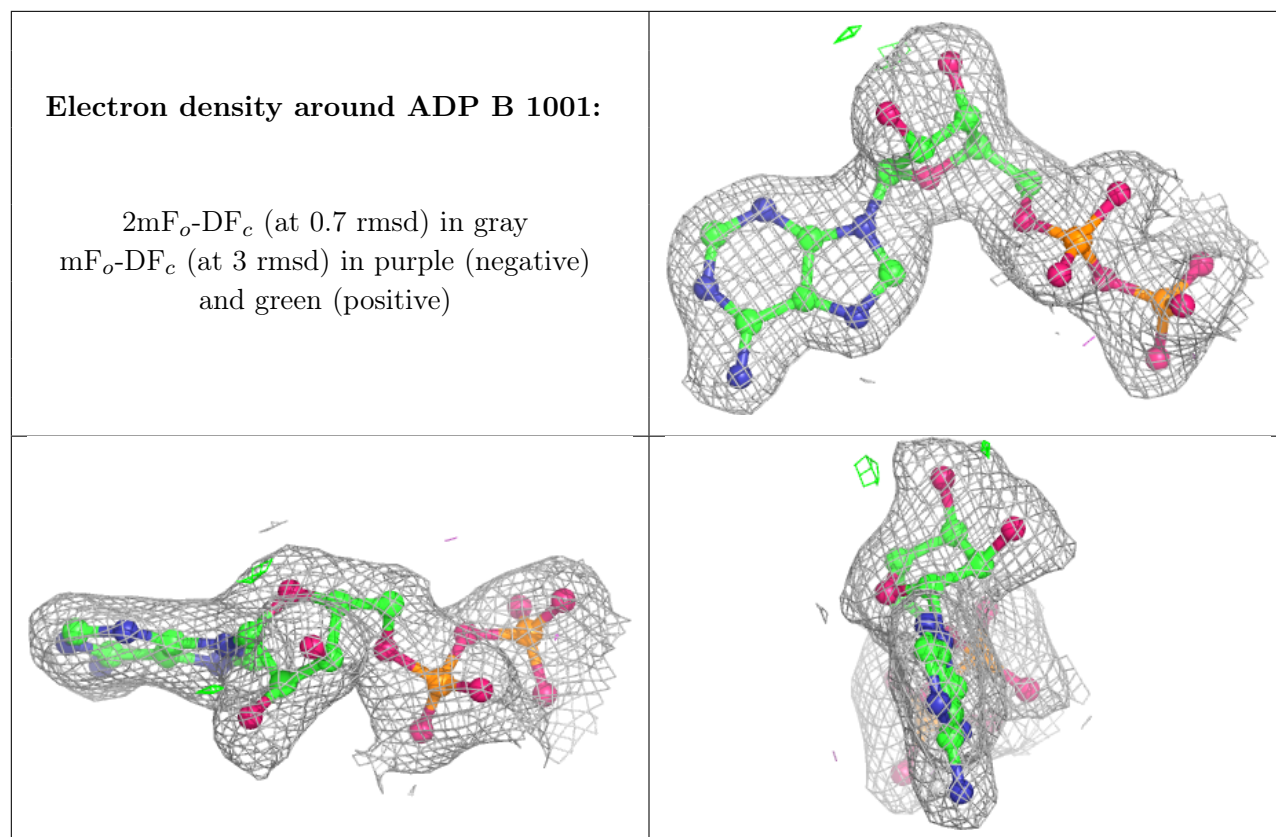
Electron density around ADP D 1001:

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

**Electron density around ADP A 1001:**

$2mF_o-DF_c$ (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.