



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 12:17 PM EDT

PDB ID : 3CR7  
Title : Crystal structure of N-terminal truncation of APS Kinase from *Penicillium chrysogenum*: Ternary structure with ADP and PAPS  
Authors : Gay, S.C.; Segel, I.H.; Fisher, A.J.  
Deposited on : 2008-04-04  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

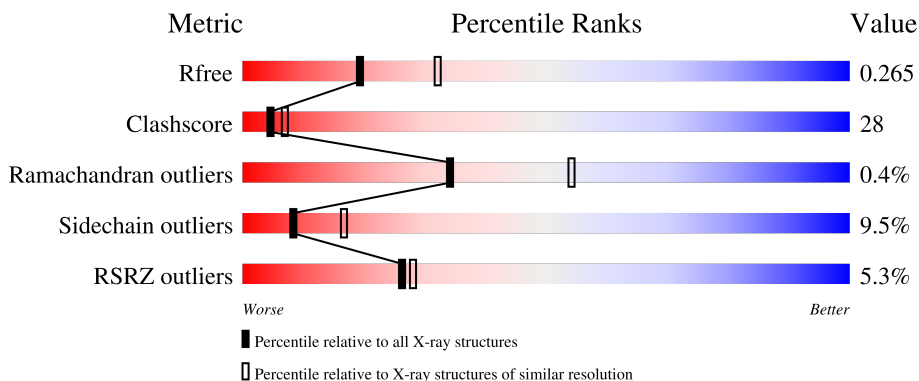
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of 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	197	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>
1	B	197	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	C	197	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div>
1	D	197	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></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
3	ADP	D	2006	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6230 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 Adenylyl-sulfate kinase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	179	1388	882	243	263	0	0	0
1	B	181	1407	889	249	269	0	0	0
1	C	178	1370	869	236	265	0	1	0
1	D	183	1397	883	243	271	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	LEU	-	expression tag	UNP Q12657
A	213	GLU	-	expression tag	UNP Q12657
A	214	HIS	-	expression tag	UNP Q12657
A	215	HIS	-	expression tag	UNP Q12657
A	216	HIS	-	expression tag	UNP Q12657
A	217	HIS	-	expression tag	UNP Q12657
A	218	HIS	-	expression tag	UNP Q12657
A	219	HIS	-	expression tag	UNP Q12657
B	212	LEU	-	expression tag	UNP Q12657
B	213	GLU	-	expression tag	UNP Q12657
B	214	HIS	-	expression tag	UNP Q12657
B	215	HIS	-	expression tag	UNP Q12657
B	216	HIS	-	expression tag	UNP Q12657
B	217	HIS	-	expression tag	UNP Q12657
B	218	HIS	-	expression tag	UNP Q12657
B	219	HIS	-	expression tag	UNP Q12657
C	212	LEU	-	expression tag	UNP Q12657
C	213	GLU	-	expression tag	UNP Q12657
C	214	HIS	-	expression tag	UNP Q12657
C	215	HIS	-	expression tag	UNP Q12657
C	216	HIS	-	expression tag	UNP Q12657

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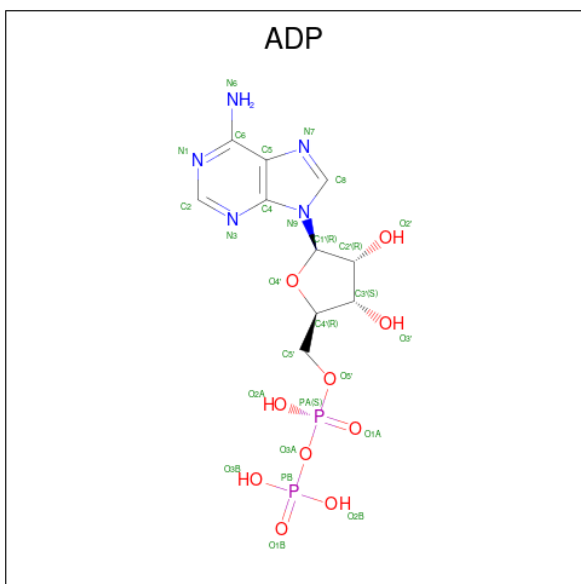
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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	HIS	-	expression tag	UNP Q12657
C	218	HIS	-	expression tag	UNP Q12657
C	219	HIS	-	expression tag	UNP Q12657
D	212	LEU	-	expression tag	UNP Q12657
D	213	GLU	-	expression tag	UNP Q12657
D	214	HIS	-	expression tag	UNP Q12657
D	215	HIS	-	expression tag	UNP Q12657
D	216	HIS	-	expression tag	UNP Q12657
D	217	HIS	-	expression tag	UNP Q12657
D	218	HIS	-	expression tag	UNP Q12657
D	219	HIS	-	expression tag	UNP Q12657

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

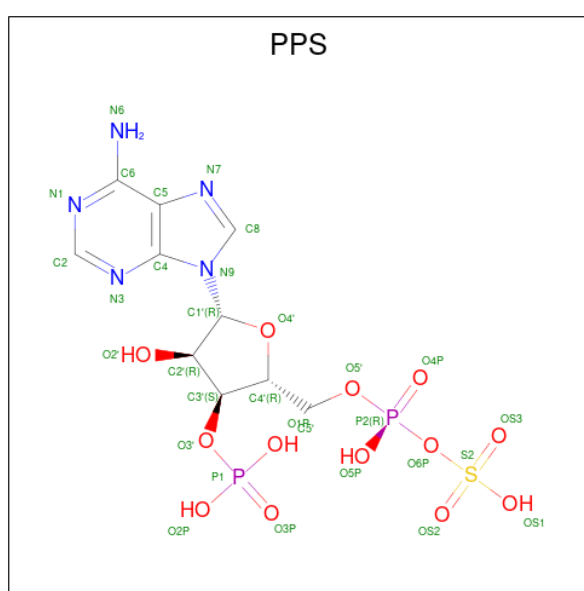
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 4 is 3'-PHOSPHATE-ADENOSINE-5'-PHOSPHATE SULFATE (three-letter code: PPS) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>13</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	Total 31	C 10	N 5	O 13	P 2	S 1	0	0
4	C	1	Total 31	C 10	N 5	O 13	P 2	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	131	Total 131 O 131	0	0
5	B	121	Total 121 O 121	0	0
5	C	105	Total 105 O 105	0	0

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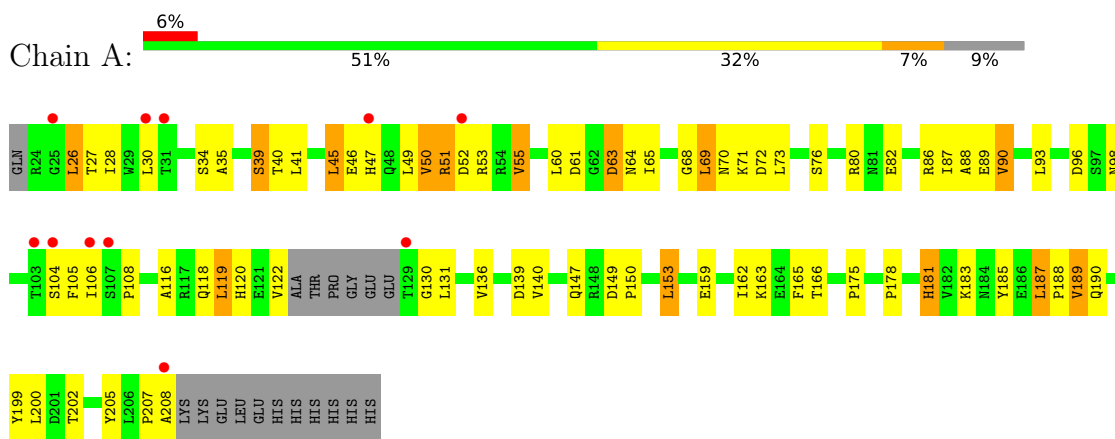
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	D	138	Total 138	O 138	0	0

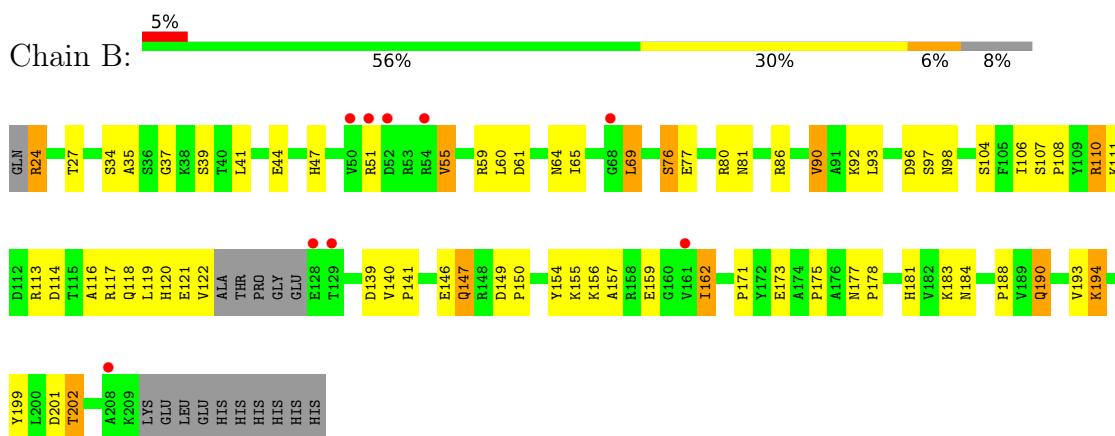
### 3 Residue-property plots [i](#)

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.

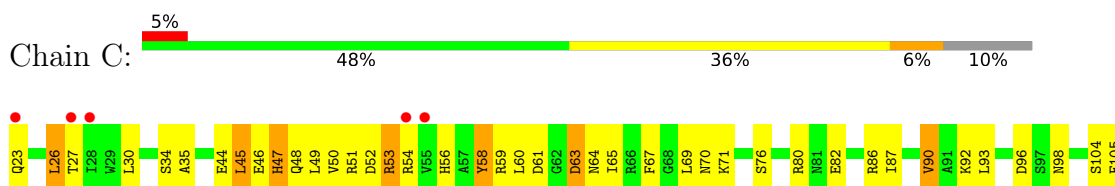
- Molecule 1: Adenylyl-sulfate kinase



- Molecule 1: Adenylyl-sulfate kinase



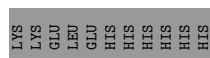
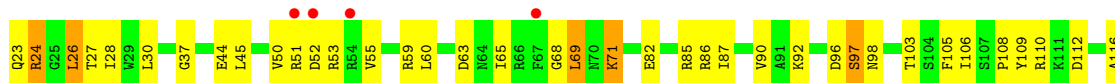
- Molecule 1: Adenylyl-sulfate kinase







● Molecule 1: Adenylyl-sulfate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.58Å 82.59Å 139.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.71 – 2.50 31.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (31.71-2.50) 99.4 (31.72-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.51Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.198 , 0.279 0.239 , 0.265	Depositor DCC
$R_{free}$ test set	1280 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1286e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPS, ADP, CL

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	0.47	0/1415	0.69	0/1921
1	B	0.51	1/1432 (0.1%)	0.65	0/1942
1	C	0.52	1/1398 (0.1%)	0.69	2/1898 (0.1%)
1	D	0.49	0/1425	0.66	0/1940
All	All	0.50	2/5670 (0.0%)	0.68	2/7701 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	58	TYR	C-O	-11.44	1.01	1.23
1	B	147	GLN	CB-CG	-5.26	1.38	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	TYR	O-C-N	-6.04	113.04	122.70
1	C	58	TYR	CA-C-O	5.58	131.82	120.10

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	1388	0	1357	91	0
1	B	1407	0	1383	61	1
1	C	1370	0	1317	89	0
1	D	1397	0	1344	73	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	4	0
3	C	27	0	12	3	0
3	D	27	0	12	11	0
4	A	31	0	12	4	0
4	C	31	0	12	1	0
5	A	131	0	0	14	0
5	B	121	0	0	7	0
5	C	105	0	0	11	0
5	D	138	0	0	11	0
All	All	6230	0	5473	317	1

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 28.

All (317) 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:D:23:GLN:O	1:D:98:ASN:ND2	1.73	1.19
1:C:110[B]:ARG:NH1	1:C:176:ALA:H	1.48	1.11
1:D:51:ARG:HG2	1:D:52:ASP:OD1	1.47	1.11
1:A:51:ARG:HG2	1:A:52:ASP:OD1	1.57	1.02
1:C:110[B]:ARG:HH12	1:C:176:ALA:N	1.56	1.01
1:B:114:ASP:OD1	1:B:118:GLN:OE1	1.78	1.00
1:B:171:PRO:HG3	1:C:162:ILE:HG22	1.43	0.99
1:C:110[B]:ARG:HH12	1:C:176:ALA:H	1.00	0.96
1:C:64:ASN:HB3	1:C:65:ILE:HD12	1.43	0.95
1:A:51:ARG:HG2	1:A:51:ARG:HH11	1.27	0.95
1:B:47:HIS:O	1:B:51:ARG:HB2	1.71	0.91
1:C:59:ARG:CB	5:C:2101:HOH:O	2.19	0.91
1:A:47:HIS:HD2	5:A:2099:HOH:O	1.55	0.90
1:C:158:ARG:HG3	1:C:158:ARG:HH11	1.37	0.89
1:D:175:PRO:HB2	1:D:178:PRO:HG3	1.52	0.89
1:B:77:GLU:HG2	1:B:80:ARG:HH21	1.36	0.88
4:A:2002:PPS:N6	5:A:2109:HOH:O	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:CG1	1:A:55:VAL:O	2.23	0.87
1:C:110[B]:ARG:NH1	1:C:176:ALA:N	2.20	0.86
1:C:146:GLU:OE1	1:C:158:ARG:CZ	2.23	0.85
1:C:158:ARG:HH11	1:C:158:ARG:CG	1.89	0.85
1:A:208:ALA:HB3	5:A:2069:HOH:O	1.75	0.84
1:A:47:HIS:CD2	5:A:2099:HOH:O	2.30	0.84
1:A:52:ASP:O	1:A:53:ARG:HD3	1.77	0.84
1:D:175:PRO:CB	1:D:178:PRO:HG3	2.06	0.84
1:C:110[B]:ARG:HH12	1:C:176:ALA:CB	1.92	0.83
1:C:27:THR:OG1	1:C:120:HIS:CE1	2.31	0.82
1:B:60:LEU:HA	1:B:64:ASN:HD22	1.44	0.82
1:A:46:GLU:O	1:A:50:VAL:HG22	1.81	0.81
1:B:155:LYS:O	1:B:159:GLU:HG3	1.81	0.81
1:B:175:PRO:HB2	1:B:178:PRO:HG3	1.61	0.81
1:C:64:ASN:HB3	1:C:65:ILE:CD1	2.11	0.80
1:C:50:VAL:HG23	1:C:50:VAL:O	1.80	0.80
1:A:187:LEU:HD23	1:A:188:PRO:N	1.96	0.79
1:C:27:THR:OG1	1:C:120:HIS:HE1	1.65	0.79
1:C:158:ARG:HG3	1:C:158:ARG:NH1	1.94	0.79
1:B:121:GLU:O	1:B:122:VAL:HG23	1.83	0.79
1:D:122:VAL:CG2	1:D:123:ALA:N	2.45	0.79
1:A:51:ARG:HG2	1:A:51:ARG:NH1	1.96	0.79
1:C:204:GLY:HA2	5:C:2015:HOH:O	1.82	0.78
1:A:51:ARG:CG	1:A:52:ASP:OD1	2.32	0.77
1:B:175:PRO:HA	5:B:2087:HOH:O	1.84	0.76
1:A:30:LEU:HD23	1:A:136:VAL:HB	1.68	0.75
1:C:23:GLN:O	1:C:98:ASN:ND2	2.20	0.75
1:D:207:PRO:O	1:D:208:ALA:HB3	1.87	0.74
1:A:116:ALA:O	1:A:119:LEU:HD23	1.87	0.74
1:D:175:PRO:HB2	1:D:178:PRO:CG	2.17	0.74
1:D:190[A]:GLN:NE2	1:D:190[A]:GLN:H	1.86	0.74
1:A:163:LYS:O	5:A:2109:HOH:O	2.04	0.73
1:A:50:VAL:HG13	1:A:55:VAL:O	1.88	0.73
1:B:59:ARG:O	1:B:64:ASN:ND2	2.22	0.73
1:C:53:ARG:HB3	5:C:2018:HOH:O	1.88	0.73
1:D:186:GLU:CB	5:D:2141:HOH:O	2.38	0.71
1:C:67:PHE:O	1:C:71:LYS:HE3	1.89	0.71
1:B:92:LYS:NZ	1:B:119:LEU:O	2.21	0.70
1:A:50:VAL:HG12	1:A:55:VAL:O	1.92	0.70
1:C:60:LEU:HA	1:C:64:ASN:HD22	1.56	0.70
1:C:76:SER:O	1:C:80:ARG:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:C	1:A:53:ARG:HD3	2.12	0.69
1:C:110[B]:ARG:HH12	1:C:176:ALA:CA	2.06	0.68
1:B:76:SER:OG	5:B:2116:HOH:O	2.12	0.67
1:C:35:ALA:HA	3:C:2004:ADP:H5'1	1.76	0.67
1:D:28:ILE:HD13	1:D:45:LEU:HD21	1.77	0.67
1:C:67:PHE:O	1:C:71:LYS:CE	2.42	0.67
1:C:122:VAL:HG12	1:C:122:VAL:O	1.93	0.67
1:C:60:LEU:HD22	1:C:65:ILE:HD11	1.77	0.67
1:C:177:ASN:CB	5:C:2109:HOH:O	2.44	0.66
1:D:44:GLU:HA	1:D:44:GLU:OE1	1.94	0.66
1:A:53:ARG:HB3	1:A:207:PRO:HG2	1.77	0.65
3:D:2006:ADP:H2'	5:D:2111:HOH:O	1.96	0.65
1:D:118:GLN:O	1:D:122:VAL:HG13	1.95	0.65
1:A:35:ALA:HA	3:A:2001:ADP:H5'1	1.77	0.65
1:B:86:ARG:O	1:B:90:VAL:HG13	1.97	0.65
1:A:175:PRO:HB2	1:A:178:PRO:HG3	1.80	0.64
1:B:156:LYS:HB3	1:B:162:ILE:HG22	1.78	0.64
1:D:65:ILE:HD12	1:D:105:PHE:HZ	1.61	0.64
1:C:110[A]:ARG:NH2	5:C:2078:HOH:O	2.10	0.64
1:C:46:GLU:O	1:C:50:VAL:HG13	1.99	0.63
1:C:47:HIS:C	1:C:47:HIS:ND1	2.51	0.63
1:D:184:ASN:HD21	3:D:2006:ADP:HN61	1.46	0.63
1:D:122:VAL:HG23	1:D:123:ALA:N	2.13	0.62
1:C:139:ASP:OD2	5:C:2092:HOH:O	2.16	0.62
1:D:23:GLN:O	1:D:98:ASN:CG	2.37	0.62
1:C:51:ARG:C	1:C:52:ASP:OD1	2.38	0.62
1:A:181:HIS:CD2	5:A:2072:HOH:O	2.53	0.62
1:A:130:GLY:HA2	5:A:2090:HOH:O	2.00	0.61
1:B:106:ILE:HG22	1:B:108:PRO:HG3	1.82	0.60
1:D:109:TYR:O	1:D:112:ASP:HB2	2.01	0.60
1:C:92:LYS:HD2	1:C:119:LEU:HD12	1.83	0.60
1:D:53:ARG:NH2	1:D:201:ASP:OD2	2.32	0.60
1:C:110[B]:ARG:CZ	1:C:176:ALA:H	2.11	0.60
1:A:51:ARG:C	1:A:52:ASP:OD1	2.40	0.60
1:A:45:LEU:HD22	1:A:49:LEU:HD12	1.83	0.60
1:C:110[B]:ARG:NH1	1:C:176:ALA:CB	2.64	0.60
1:B:60:LEU:HA	1:B:64:ASN:ND2	2.16	0.59
1:B:97:SER:O	1:B:98:ASN:HB2	2.02	0.59
1:A:63:ASP:OD2	1:A:63:ASP:N	2.34	0.59
1:C:90:VAL:HA	1:C:93:LEU:HD12	1.84	0.59
1:C:82:GLU:OE2	1:C:86:ARG:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLU:OE1	1:C:158:ARG:NH2	2.36	0.59
4:C:2005:PPS:N3	4:C:2005:PPS:H2'	2.16	0.59
1:B:77:GLU:HG2	1:B:80:ARG:NH2	2.13	0.58
1:B:77:GLU:CG	1:B:80:ARG:HH21	2.11	0.58
1:B:184:ASN:HD21	3:B:2003:ADP:HN61	1.50	0.58
1:C:150:PRO:HG3	3:C:2004:ADP:H4'	1.86	0.58
1:A:159:GLU:OE1	5:A:2106:HOH:O	2.17	0.58
1:C:115:THR:O	1:C:119:LEU:HD23	2.03	0.58
1:B:139:ASP:OD2	1:B:181:HIS:HE1	1.87	0.58
1:C:47:HIS:ND1	1:C:48:GLN:N	2.52	0.58
4:A:2002:PPS:H4'	4:A:2002:PPS:O3P	2.04	0.58
1:A:187:LEU:O	3:A:2001:ADP:N6	2.35	0.57
1:D:122:VAL:HG22	1:D:123:ALA:N	2.19	0.57
1:D:207:PRO:O	1:D:208:ALA:CB	2.53	0.57
1:D:118:GLN:O	1:D:122:VAL:CG1	2.52	0.57
1:A:90:VAL:HA	1:A:93:LEU:HD12	1.87	0.57
1:C:183:LYS:O	1:C:187:LEU:HD12	2.05	0.57
1:A:181:HIS:HD2	5:A:2072:HOH:O	1.88	0.56
1:C:117:ARG:HH22	1:C:179:GLU:CD	2.07	0.56
1:B:81:ASN:HB3	5:B:2026:HOH:O	2.04	0.56
1:C:139:ASP:OD2	1:C:181:HIS:HE1	1.88	0.56
1:C:34:SER:O	1:C:35:ALA:HB3	2.06	0.56
1:A:130:GLY:CA	5:A:2090:HOH:O	2.51	0.56
1:A:60:LEU:HD22	1:A:65:ILE:HD11	1.86	0.56
1:D:82:GLU:O	1:D:86:ARG:HG3	2.05	0.56
1:B:175:PRO:CB	1:B:178:PRO:HG3	2.34	0.55
1:C:86:ARG:O	1:C:90:VAL:HG13	2.07	0.55
1:D:68:GLY:O	1:D:71:LYS:HG2	2.06	0.55
1:A:52:ASP:O	1:A:53:ARG:CD	2.52	0.54
1:A:86:ARG:O	1:A:90:VAL:HG13	2.07	0.54
1:A:207:PRO:O	1:A:208:ALA:C	2.44	0.54
1:A:45:LEU:O	1:A:45:LEU:CD2	2.56	0.54
1:D:52:ASP:O	1:D:53:ARG:HD3	2.07	0.54
1:B:24:ARG:HA	1:B:98:ASN:OD1	2.07	0.54
1:D:188:PRO:O	1:D:191:ASP:HB2	2.07	0.54
1:A:187:LEU:HD23	1:A:188:PRO:CD	2.38	0.54
1:D:30:LEU:HD23	1:D:136:VAL:HB	1.89	0.54
1:B:188:PRO:HB3	1:B:190:GLN:OE1	2.07	0.53
1:C:59:ARG:O	1:C:64:ASN:ND2	2.41	0.53
1:C:44:GLU:HB3	1:C:193:VAL:HG21	1.90	0.53
1:C:206:LEU:C	5:C:2059:HOH:O	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:OE1	5:B:2108:HOH:O	2.19	0.53
1:C:56:HIS:CB	5:C:2019:HOH:O	2.56	0.53
1:C:87:ILE:HD13	1:C:105:PHE:CE1	2.44	0.53
1:D:96:ASP:C	1:D:98:ASN:H	2.11	0.53
1:D:146:GLU:HG2	1:D:154:TYR:CD2	2.44	0.53
1:C:63:ASP:OD2	1:C:63:ASP:N	2.40	0.52
1:C:194:LYS:HG2	1:C:198:ASP:OD2	2.09	0.52
1:A:82:GLU:OE2	1:A:86:ARG:HD2	2.10	0.52
1:A:147:GLN:HA	1:A:147:GLN:OE1	2.10	0.52
1:B:64:ASN:HB3	1:B:65:ILE:HG12	1.92	0.52
1:D:175:PRO:HB3	1:D:178:PRO:HG3	1.91	0.52
1:A:34:SER:O	1:A:35:ALA:HB3	2.11	0.51
1:B:106:ILE:CG2	1:B:108:PRO:HG3	2.40	0.51
1:A:139:ASP:OD2	1:A:181:HIS:HE1	1.94	0.51
1:A:46:GLU:O	1:A:50:VAL:CG2	2.54	0.51
1:C:117:ARG:NH2	1:C:179:GLU:OE1	2.34	0.51
1:D:65:ILE:HD12	1:D:105:PHE:CZ	2.43	0.51
1:A:51:ARG:NH1	1:A:52:ASP:OD2	2.44	0.51
1:B:37:GLY:O	1:B:41:LEU:HG	2.10	0.51
1:B:194:LYS:HE3	5:B:2023:HOH:O	2.10	0.51
1:A:45:LEU:O	1:A:45:LEU:HD23	2.11	0.51
1:A:76:SER:O	1:A:80:ARG:HG3	2.11	0.51
1:D:60:LEU:HB3	1:D:65:ILE:HD11	1.93	0.51
1:A:80:ARG:NH2	1:A:166:THR:OG1	2.44	0.50
1:B:117:ARG:O	1:B:121:GLU:HG3	2.11	0.50
1:B:139:ASP:OD2	1:B:181:HIS:CE1	2.65	0.50
1:D:143:GLU:CB	5:D:2073:HOH:O	2.60	0.50
1:C:150:PRO:CG	3:C:2004:ADP:H4'	2.41	0.50
1:A:162:ILE:HG12	1:D:171:PRO:HG3	1.92	0.50
1:C:146:GLU:OE1	1:C:158:ARG:NH1	2.44	0.50
1:C:154:TYR:O	1:C:158:ARG:HG2	2.11	0.50
1:A:70:ASN:ND2	1:A:86:ARG:HE	2.10	0.50
1:B:175:PRO:HB2	1:B:178:PRO:CG	2.35	0.50
1:C:182:VAL:HG21	1:C:196:ILE:HD11	1.94	0.50
1:A:52:ASP:OD1	1:A:52:ASP:N	2.45	0.49
1:B:190:GLN:H	1:B:190:GLN:CD	2.16	0.49
1:D:117:ARG:O	1:D:121:GLU:HG3	2.12	0.49
1:D:92:LYS:NZ	1:D:123:ALA:HB2	2.28	0.49
1:D:27:THR:OG1	1:D:120:HIS:HE1	1.96	0.49
1:B:190:GLN:H	1:B:190:GLN:NE2	2.10	0.49
1:B:37:GLY:HA2	3:B:2003:ADP:PA	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ASN:HD21	3:D:2006:ADP:N6	2.11	0.49
1:A:89:GLU:O	1:A:93:LEU:HG	2.12	0.49
1:C:61:ASP:HB3	1:C:104:SER:HB3	1.94	0.49
1:C:86:ARG:HG2	1:D:69:LEU:CD2	2.43	0.49
1:C:106:ILE:HG22	1:C:108:PRO:HG3	1.95	0.49
1:C:206:LEU:CB	5:C:2053:HOH:O	2.61	0.49
1:D:37:GLY:HA2	3:D:2006:ADP:O1A	2.13	0.49
4:A:2002:PPS:P1	4:A:2002:PPS:HO2'	2.36	0.48
1:A:120:HIS:O	1:A:131:LEU:HB2	2.12	0.48
1:A:64:ASN:CB	1:A:65:ILE:HD12	2.42	0.48
1:B:55:VAL:O	1:B:55:VAL:CG1	2.61	0.48
1:A:28:ILE:HD11	1:A:200:LEU:HD11	1.96	0.48
1:A:187:LEU:HD23	1:A:187:LEU:C	2.33	0.48
1:B:90:VAL:HA	1:B:93:LEU:HD12	1.95	0.48
1:B:183:LYS:HE2	5:B:2014:HOH:O	2.13	0.48
1:A:187:LEU:C	1:A:187:LEU:CD2	2.82	0.47
3:D:2006:ADP:C2'	5:D:2111:HOH:O	2.57	0.47
1:A:45:LEU:CD2	1:A:45:LEU:C	2.82	0.47
5:C:2006:HOH:O	1:D:71:LYS:HE3	2.13	0.47
1:B:149:ASP:N	1:B:150:PRO:HD3	2.29	0.47
1:C:110[B]:ARG:NH1	1:C:176:ALA:HB2	2.30	0.47
1:A:118:GLN:O	1:A:122:VAL:HG13	2.14	0.47
3:D:2006:ADP:C8	3:D:2006:ADP:H3'	2.49	0.47
1:A:188:PRO:C	1:A:190:GLN:N	2.67	0.47
1:B:201:ASP:HA	5:B:2034:HOH:O	2.14	0.47
1:D:27:THR:OG1	1:D:120:HIS:CE1	2.68	0.47
1:C:45:LEU:CD2	1:C:49:LEU:HD22	2.44	0.47
3:D:2006:ADP:C3'	5:D:2111:HOH:O	2.62	0.47
1:A:88:ALA:HB1	1:A:119:LEU:HD21	1.95	0.47
1:B:34:SER:O	1:B:35:ALA:HB3	2.14	0.47
1:D:122:VAL:HG22	1:D:123:ALA:H	1.79	0.47
1:D:139:ASP:OD2	1:D:181:HIS:HE1	1.98	0.46
1:D:106:ILE:HG22	1:D:108:PRO:HG3	1.96	0.46
1:B:156:LYS:CB	1:B:162:ILE:HG22	2.45	0.46
1:B:184:ASN:ND2	3:B:2003:ADP:HN61	2.11	0.46
1:C:45:LEU:HD21	1:C:49:LEU:HD22	1.97	0.46
1:C:45:LEU:O	1:C:49:LEU:HB2	2.16	0.46
1:D:184:ASN:ND2	3:D:2006:ADP:N6	2.63	0.46
1:A:64:ASN:HB3	1:A:65:ILE:HD12	1.98	0.46
1:A:188:PRO:O	1:A:190:GLN:N	2.48	0.46
1:C:70:ASN:HD21	1:C:86:ARG:HE	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:C	1:A:98:ASN:H	2.20	0.46
1:C:61:ASP:HA	1:C:105:PHE:CZ	2.50	0.46
1:D:142:VAL:O	1:D:146:GLU:HG3	2.16	0.45
1:A:153:LEU:HB3	1:A:165:PHE:CE2	2.51	0.45
1:C:199:TYR:CD1	1:C:199:TYR:C	2.88	0.45
1:A:149:ASP:N	1:A:150:PRO:HD3	2.31	0.45
1:B:171:PRO:CG	1:C:162:ILE:HG22	2.30	0.45
1:D:65:ILE:HD13	1:D:87:ILE:HG12	1.98	0.45
1:B:61:ASP:H	1:B:64:ASN:HB2	1.82	0.45
1:D:154:TYR:O	1:D:158:ARG:HG2	2.17	0.45
1:B:110:ARG:HG2	1:B:173:GLU:OE1	2.16	0.45
1:D:106:ILE:CG2	1:D:108:PRO:HG3	2.47	0.45
1:A:26:LEU:N	1:A:26:LEU:HD23	2.31	0.45
1:B:27:THR:OG1	1:B:120:HIS:HE1	1.99	0.45
1:C:149:ASP:N	1:C:150:PRO:HD3	2.32	0.45
1:B:157:ALA:HA	1:B:162:ILE:HG23	1.99	0.45
1:D:190[A]:GLN:H	1:D:190[A]:GLN:HE21	1.63	0.44
1:D:85:ARG:NH1	5:D:2120:HOH:O	2.36	0.44
1:A:39:SER:OG	3:A:2001:ADP:O2B	2.35	0.44
1:C:45:LEU:O	1:C:49:LEU:CB	2.66	0.44
1:D:50:VAL:HG22	1:D:55:VAL:O	2.17	0.44
1:D:86:ARG:O	1:D:90:VAL:HG13	2.17	0.44
1:A:187:LEU:CD2	1:A:188:PRO:O	2.66	0.44
1:A:61:ASP:HA	1:A:105:PHE:CZ	2.52	0.44
3:D:2006:ADP:C8	3:D:2006:ADP:C3'	3.01	0.44
1:B:24:ARG:NH2	1:B:96:ASP:OD1	2.51	0.44
1:D:119:LEU:HA	1:D:122:VAL:HG13	2.00	0.44
1:D:188:PRO:O	1:D:189:VAL:C	2.56	0.44
1:A:73:LEU:CD2	5:A:2088:HOH:O	2.65	0.43
1:C:194:LYS:HB2	1:C:194:LYS:HE3	1.31	0.43
1:A:87:ILE:HD13	1:A:105:PHE:CE1	2.53	0.43
1:B:146:GLU:HG2	1:B:154:TYR:CD2	2.52	0.43
1:C:110[A]:ARG:NH1	1:C:174:ALA:O	2.51	0.43
1:C:180:VAL:HG11	1:C:196:ILE:HD13	2.00	0.43
1:B:107:SER:N	1:B:108:PRO:HD3	2.33	0.43
1:B:194:LYS:HA	1:B:194:LYS:HD3	1.71	0.43
1:C:201:ASP:O	1:C:202:THR:C	2.57	0.43
1:C:131:LEU:HA	1:C:132:PRO:HD3	1.88	0.43
1:C:155:LYS:O	1:C:159:GLU:HG3	2.18	0.43
1:A:130:GLY:HA3	5:A:2090:HOH:O	2.18	0.43
1:C:58:TYR:CG	1:D:97:SER:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLY:O	1:A:71:LYS:HB2	2.19	0.43
1:C:87:ILE:HD13	1:C:105:PHE:CD1	2.54	0.43
1:A:104:SER:O	1:A:104:SER:OG	2.31	0.43
1:B:44:GLU:HB3	1:B:193:VAL:HG21	2.00	0.43
1:B:199:TYR:O	1:B:202:THR:HB	2.19	0.43
1:C:45:LEU:CD2	1:C:45:LEU:C	2.87	0.43
1:D:184:ASN:ND2	3:D:2006:ADP:HN61	2.12	0.43
1:A:183:LYS:O	1:A:187:LEU:HD12	2.19	0.42
1:D:208:ALA:HA	5:D:2015:HOH:O	2.18	0.42
1:A:106:ILE:HG22	1:A:108:PRO:HG3	2.01	0.42
1:A:200:LEU:HD22	1:A:205:TYR:HD1	1.84	0.42
1:D:123:ALA:HB3	5:D:2092:HOH:O	2.19	0.42
1:C:58:TYR:HB2	1:D:97:SER:HB2	2.01	0.42
1:D:110:ARG:HG2	1:D:173:GLU:OE1	2.19	0.42
1:A:40:THR:HB	5:A:2085:HOH:O	2.19	0.42
1:A:86:ARG:HG2	1:B:69:LEU:HD21	2.01	0.42
1:A:187:LEU:HA	1:A:188:PRO:HD3	1.89	0.42
1:A:51:ARG:CB	1:A:52:ASP:OD1	2.67	0.42
1:D:60:LEU:HB2	1:D:103:THR:HG22	2.00	0.42
1:B:116:ALA:O	1:B:120:HIS:HD2	2.03	0.42
1:B:140:VAL:HA	1:B:141:PRO:HD3	1.89	0.42
1:D:53:ARG:HB3	1:D:207:PRO:HG2	2.02	0.42
1:D:116:ALA:O	1:D:120:HIS:HD2	2.03	0.42
1:A:188:PRO:O	1:A:189:VAL:C	2.59	0.41
1:D:26:LEU:HB2	1:D:132:PRO:HB2	2.00	0.41
1:D:148:ARG:HD3	3:D:2006:ADP:O4'	2.20	0.41
1:A:71:LYS:HE3	1:A:71:LYS:HB3	1.60	0.41
1:A:116:ALA:O	1:A:120:HIS:HD2	2.03	0.41
1:D:92:LYS:HZ3	1:D:123:ALA:HB2	1.85	0.41
1:A:27:THR:OG1	1:A:120:HIS:HE1	2.03	0.41
1:A:65:ILE:HG21	1:A:87:ILE:HD11	2.02	0.41
1:C:178:PRO:C	1:C:180:VAL:N	2.72	0.41
1:B:37:GLY:HA2	3:B:2003:ADP:O1A	2.20	0.41
1:C:26:LEU:HB2	1:C:132:PRO:HB2	2.02	0.41
1:D:149:ASP:OD2	1:D:154:TYR:HB2	2.19	0.41
1:A:72:ASP:OD1	1:A:86:ARG:NH2	2.54	0.41
1:A:45:LEU:HD22	1:A:45:LEU:O	2.21	0.41
1:A:199:TYR:CD1	1:A:199:TYR:C	2.93	0.41
1:B:147:GLN:O	1:B:147:GLN:HG2	2.20	0.41
4:A:2002:PPS:P1	4:A:2002:PPS:O2'	2.78	0.41
1:C:187:LEU:HD23	1:C:188:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:HD2	5:D:2049:HOH:O	2.20	0.41
1:A:140:VAL:HG12	1:A:185:TYR:HD1	1.86	0.41
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.91	0.41
1:D:28:ILE:CD1	1:D:45:LEU:HD21	2.50	0.41
1:B:107:SER:O	1:B:113:ARG:NH1	2.51	0.40
1:C:30:LEU:HD23	1:C:136:VAL:HB	2.03	0.40
1:D:110:ARG:CD	5:D:2049:HOH:O	2.68	0.40
1:D:164:GLU:HB3	5:D:2051:HOH:O	2.20	0.40
1:A:41:LEU:O	1:A:45:LEU:N	2.49	0.40
1:C:206:LEU:CA	5:C:2053:HOH:O	2.69	0.40
1:A:73:LEU:HD23	5:A:2088:HOH:O	2.21	0.40
1:C:96:ASP:OD1	1:C:96:ASP:O	2.39	0.40
1:D:24:ARG:NH2	1:D:127:GLU:OE2	2.54	0.40

All (1) 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)
1:B:147:GLN:NE2	1:D:147:GLN:NE2 2_564	1.70	0.50

## 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	175/197 (89%)	158 (90%)	16 (9%)	1 (1%)	25	43
1	B	177/197 (90%)	167 (94%)	10 (6%)	0	100	100
1	C	175/197 (89%)	157 (90%)	16 (9%)	2 (1%)	14	26
1	D	180/197 (91%)	165 (92%)	15 (8%)	0	100	100
All	All	707/788 (90%)	647 (92%)	57 (8%)	3 (0%)	34	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	THR
1	A	189	VAL
1	C	54	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	143/168 (85%)	129 (90%)	14 (10%)	8	15
1	B	146/168 (87%)	132 (90%)	14 (10%)	8	16
1	C	139/168 (83%)	126 (91%)	13 (9%)	8	17
1	D	142/168 (84%)	128 (90%)	14 (10%)	8	15
All	All	570/672 (85%)	515 (90%)	55 (10%)	8	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	39	SER
1	A	45	LEU
1	A	50	VAL
1	A	51	ARG
1	A	55	VAL
1	A	63	ASP
1	A	69	LEU
1	A	90	VAL
1	A	119	LEU
1	A	153	LEU
1	A	181	HIS
1	A	187	LEU
1	A	202	THR
1	B	24	ARG
1	B	39	SER
1	B	55	VAL
1	B	69	LEU
1	B	76	SER

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Mol	Chain	Res	Type
1	B	90	VAL
1	B	104	SER
1	B	110	ARG
1	B	111	LYS
1	B	162	ILE
1	B	177	ASN
1	B	190	GLN
1	B	194	LYS
1	B	202	THR
1	C	26	LEU
1	C	45	LEU
1	C	47	HIS
1	C	53	ARG
1	C	63	ASP
1	C	69	LEU
1	C	90	VAL
1	C	119	LEU
1	C	143	GLU
1	C	158	ARG
1	C	162	ILE
1	C	184	ASN
1	C	187	LEU
1	D	24	ARG
1	D	26	LEU
1	D	59	ARG
1	D	63	ASP
1	D	69	LEU
1	D	71	LYS
1	D	97	SER
1	D	118	GLN
1	D	122	VAL
1	D	164	GLU
1	D	177	ASN
1	D	185	TYR
1	D	190[A]	GLN
1	D	190[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	120	HIS
1	A	181	HIS
1	A	184	ASN
1	B	64	ASN
1	B	120	HIS
1	B	177	ASN
1	B	181	HIS
1	B	184	ASN
1	C	64	ASN
1	C	70	ASN
1	C	120	HIS
1	C	181	HIS
1	C	184	ASN
1	D	120	HIS
1	D	181	HIS
1	D	184	ASN

### 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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	D	2006	-	24,29,29	1.09	1 (4%)	29,45,45	1.76	8 (27%)
3	ADP	B	2003	-	24,29,29	1.02	1 (4%)	29,45,45	1.56	5 (17%)
3	ADP	C	2004	-	24,29,29	1.01	1 (4%)	29,45,45	1.40	4 (13%)
4	PPS	A	2002	-	29,33,33	5.49	19 (65%)	32,52,52	1.36	4 (12%)
3	ADP	A	2001	-	24,29,29	1.07	2 (8%)	29,45,45	1.38	4 (13%)
4	PPS	C	2005	-	29,33,33	5.66	19 (65%)	32,52,52	1.62	6 (18%)

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	D	2006	-	-	2/12/32/32	0/3/3/3
3	ADP	B	2003	-	-	3/12/32/32	0/3/3/3
3	ADP	C	2004	-	-	2/12/32/32	0/3/3/3
4	PPS	A	2002	-	-	3/11/37/37	0/3/3/3
3	ADP	A	2001	-	-	2/12/32/32	0/3/3/3
4	PPS	C	2005	-	-	4/11/37/37	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2002	PPS	C2-N3	15.63	1.57	1.32
4	C	2005	PPS	C2-N3	15.13	1.56	1.32
4	A	2002	PPS	C4-N3	12.07	1.52	1.35
4	C	2005	PPS	C4-N3	11.75	1.51	1.35
4	C	2005	PPS	P2-O6P	11.11	1.68	1.59
4	A	2002	PPS	P2-O6P	9.61	1.67	1.59
4	C	2005	PPS	C2-N1	9.61	1.51	1.33
4	C	2005	PPS	C8-N7	9.36	1.51	1.34
4	A	2002	PPS	C2-N1	9.26	1.51	1.33
4	A	2002	PPS	C8-N7	8.56	1.49	1.34
4	C	2005	PPS	OS3-S2	5.66	1.69	1.45
4	C	2005	PPS	OS2-S2	5.62	1.69	1.45
4	C	2005	PPS	P1-O3'	5.61	1.69	1.59
4	A	2002	PPS	OS3-S2	5.60	1.69	1.45
4	A	2002	PPS	OS2-S2	5.41	1.68	1.45
4	A	2002	PPS	P1-O3'	5.38	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2005	PPS	C5-C4	4.71	1.53	1.40
4	A	2002	PPS	P2-O4P	4.50	1.66	1.50
4	A	2002	PPS	C5-C4	4.48	1.52	1.40
4	C	2005	PPS	O4'-C1'	4.44	1.47	1.41
4	C	2005	PPS	P2-O4P	4.41	1.66	1.50
4	A	2002	PPS	O4'-C1'	4.21	1.47	1.41
4	C	2005	PPS	C6-N6	4.01	1.48	1.34
4	C	2005	PPS	C6-N1	3.69	1.53	1.37
4	C	2005	PPS	C6-C5	3.69	1.57	1.43
4	C	2005	PPS	P1-O1P	3.60	1.68	1.54
4	A	2002	PPS	P1-O2P	3.54	1.68	1.54
4	C	2005	PPS	P1-O2P	3.54	1.68	1.54
4	A	2002	PPS	P1-O1P	3.51	1.68	1.54
4	A	2002	PPS	C6-N1	3.50	1.52	1.37
4	A	2002	PPS	C6-N6	3.37	1.46	1.34
4	C	2005	PPS	C5-N7	3.36	1.51	1.39
4	A	2002	PPS	C6-C5	3.15	1.55	1.43
4	A	2002	PPS	C5-N7	3.13	1.51	1.39
3	D	2006	ADP	C5-C4	2.90	1.48	1.40
4	C	2005	PPS	OS1-S2	2.86	1.67	1.50
4	A	2002	PPS	OS1-S2	2.77	1.67	1.50
3	A	2001	ADP	C5-C4	2.75	1.48	1.40
3	B	2003	ADP	C5-C4	2.51	1.47	1.40
3	C	2004	ADP	C5-C4	2.48	1.47	1.40
3	A	2001	ADP	C2-N3	2.35	1.35	1.32
4	C	2005	PPS	P2-O5'	2.34	1.68	1.59
4	A	2002	PPS	P2-O5'	2.00	1.67	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2005	PPS	N3-C2-N1	-6.03	119.25	128.68
4	A	2002	PPS	N3-C2-N1	-5.41	120.22	128.68
3	D	2006	ADP	C2'-C3'-C4'	-4.20	94.49	102.64
3	B	2003	ADP	N3-C2-N1	-3.98	122.46	128.68
3	C	2004	ADP	N3-C2-N1	-3.67	122.94	128.68
3	A	2001	ADP	N3-C2-N1	-3.56	123.11	128.68
3	D	2006	ADP	N3-C2-N1	-3.21	123.66	128.68
3	D	2006	ADP	C4-C5-N7	-2.94	106.33	109.40
3	B	2003	ADP	C4-C5-N7	-2.91	106.36	109.40
3	D	2006	ADP	O4'-C1'-C2'	-2.91	102.67	106.93
4	C	2005	PPS	O5'-P2-O6P	2.66	110.74	102.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2004	ADP	C1'-N9-C4	-2.65	121.98	126.64
3	D	2006	ADP	O2'-C2'-C3'	-2.63	103.33	111.82
4	C	2005	PPS	C1'-N9-C4	-2.54	122.18	126.64
4	A	2002	PPS	C3'-C2'-C1'	2.54	105.51	99.89
3	B	2003	ADP	C2-N1-C6	2.51	123.04	118.75
3	B	2003	ADP	C1'-N9-C4	-2.45	122.33	126.64
4	C	2005	PPS	C3'-C2'-C1'	2.44	105.29	99.89
3	D	2006	ADP	C1'-N9-C4	-2.38	122.46	126.64
3	A	2001	ADP	C3'-C2'-C1'	2.33	104.49	100.98
3	C	2004	ADP	C2-N1-C6	2.31	122.70	118.75
4	A	2002	PPS	O4'-C1'-C2'	2.23	110.18	106.93
3	C	2004	ADP	O2A-PA-O1A	2.22	123.21	112.24
3	B	2003	ADP	O2B-PB-O3A	2.20	112.02	104.64
3	D	2006	ADP	O3'-C3'-C4'	2.12	117.19	111.05
3	A	2001	ADP	C2-N1-C6	2.09	122.33	118.75
3	A	2001	ADP	C4-C5-N7	-2.08	107.23	109.40
4	C	2005	PPS	O2'-C2'-C3'	-2.05	105.36	111.17
4	C	2005	PPS	C4-C5-N7	-2.02	107.30	109.40
4	A	2002	PPS	C2'-C3'-C4'	2.01	106.78	103.22
3	D	2006	ADP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

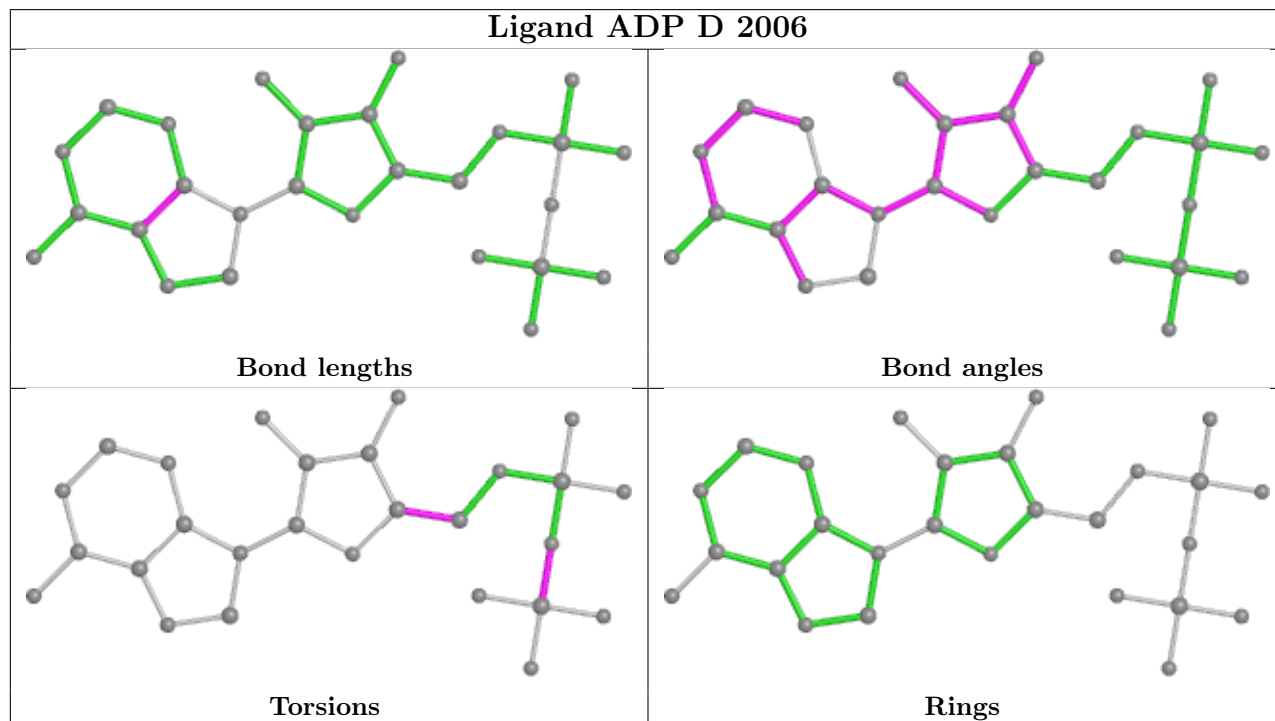
Mol	Chain	Res	Type	Atoms
3	A	2001	ADP	PA-O3A-PB-O2B
3	B	2003	ADP	PA-O3A-PB-O2B
3	C	2004	ADP	PA-O3A-PB-O2B
4	C	2005	PPS	C3'-C4'-C5'-O5'
4	C	2005	PPS	C4'-C3'-O3'-P1
4	A	2002	PPS	C4'-C3'-O3'-P1
4	C	2005	PPS	O4'-C4'-C5'-O5'
4	A	2002	PPS	C2'-C3'-O3'-P1
3	D	2006	ADP	PA-O3A-PB-O1B
3	B	2003	ADP	PA-O3A-PB-O1B
3	C	2004	ADP	PA-O3A-PB-O1B
3	A	2001	ADP	PA-O3A-PB-O3B
3	B	2003	ADP	PA-O3A-PB-O3B
4	A	2002	PPS	C3'-O3'-P1-O1P
4	C	2005	PPS	C3'-O3'-P1-O2P
3	D	2006	ADP	O4'-C4'-C5'-O5'

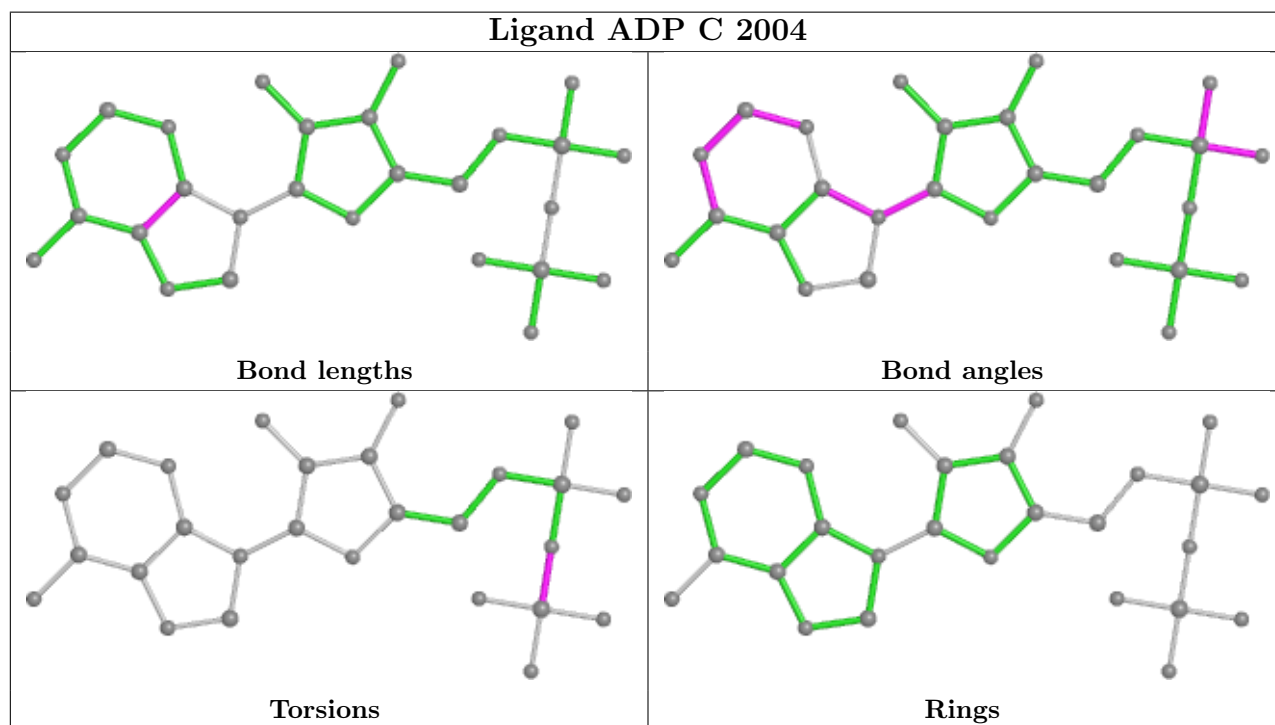
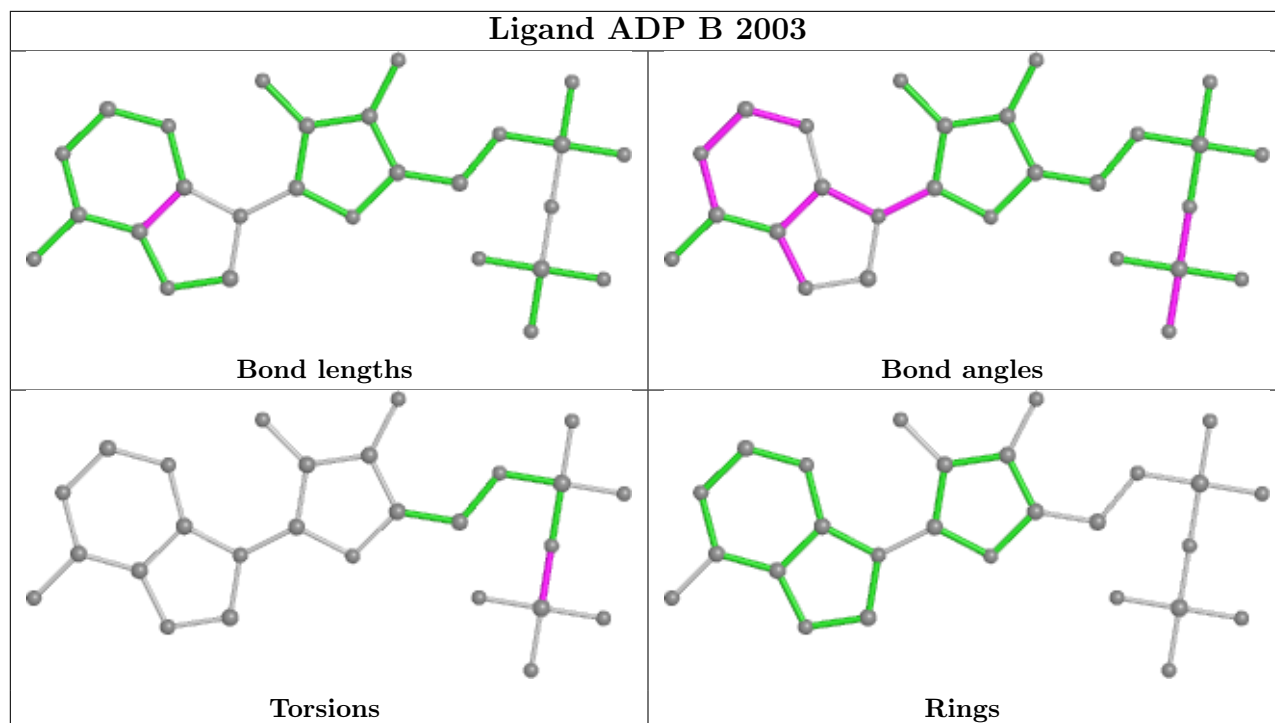
There are no ring outliers.

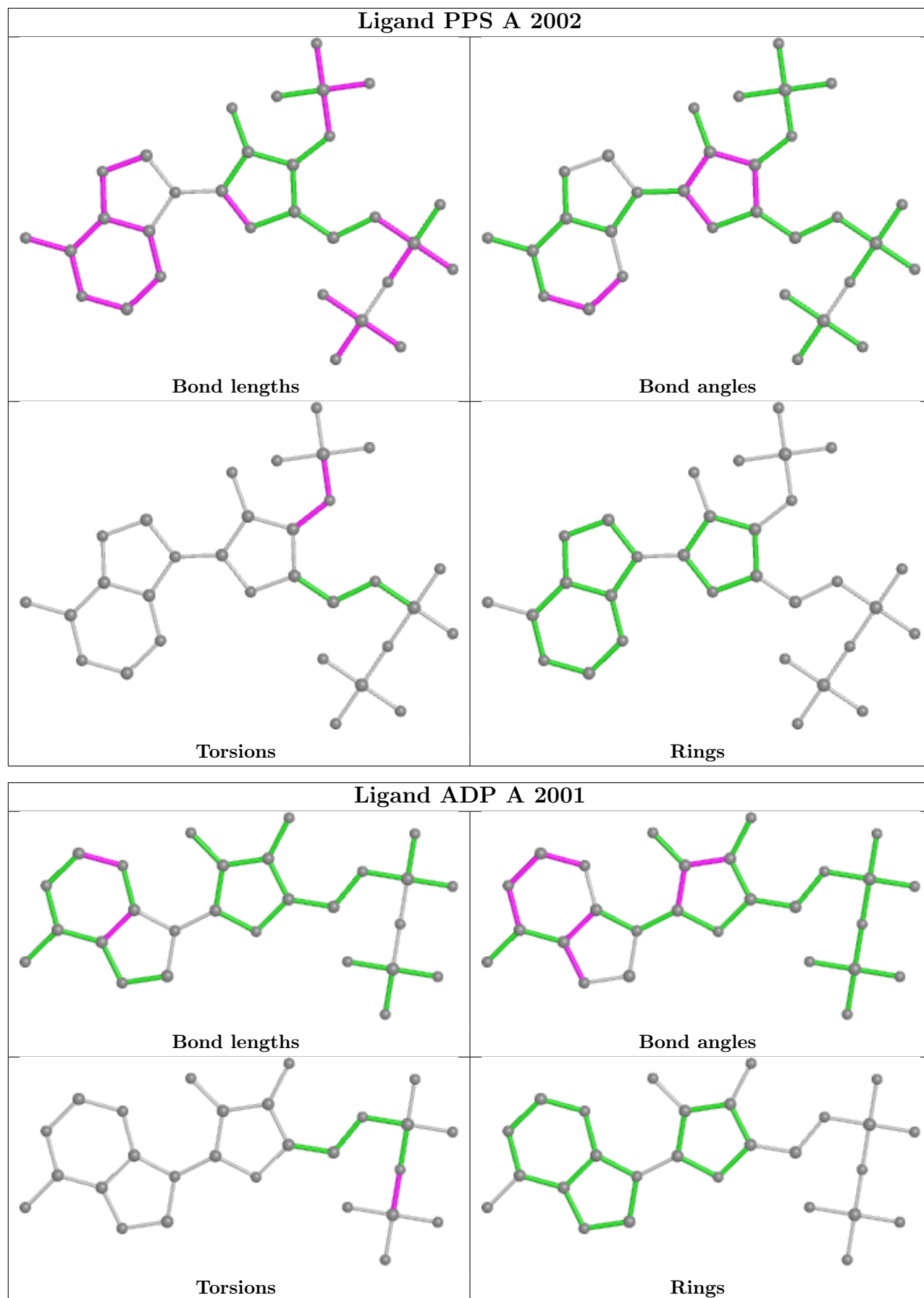
6 monomers are involved in 26 short contacts:

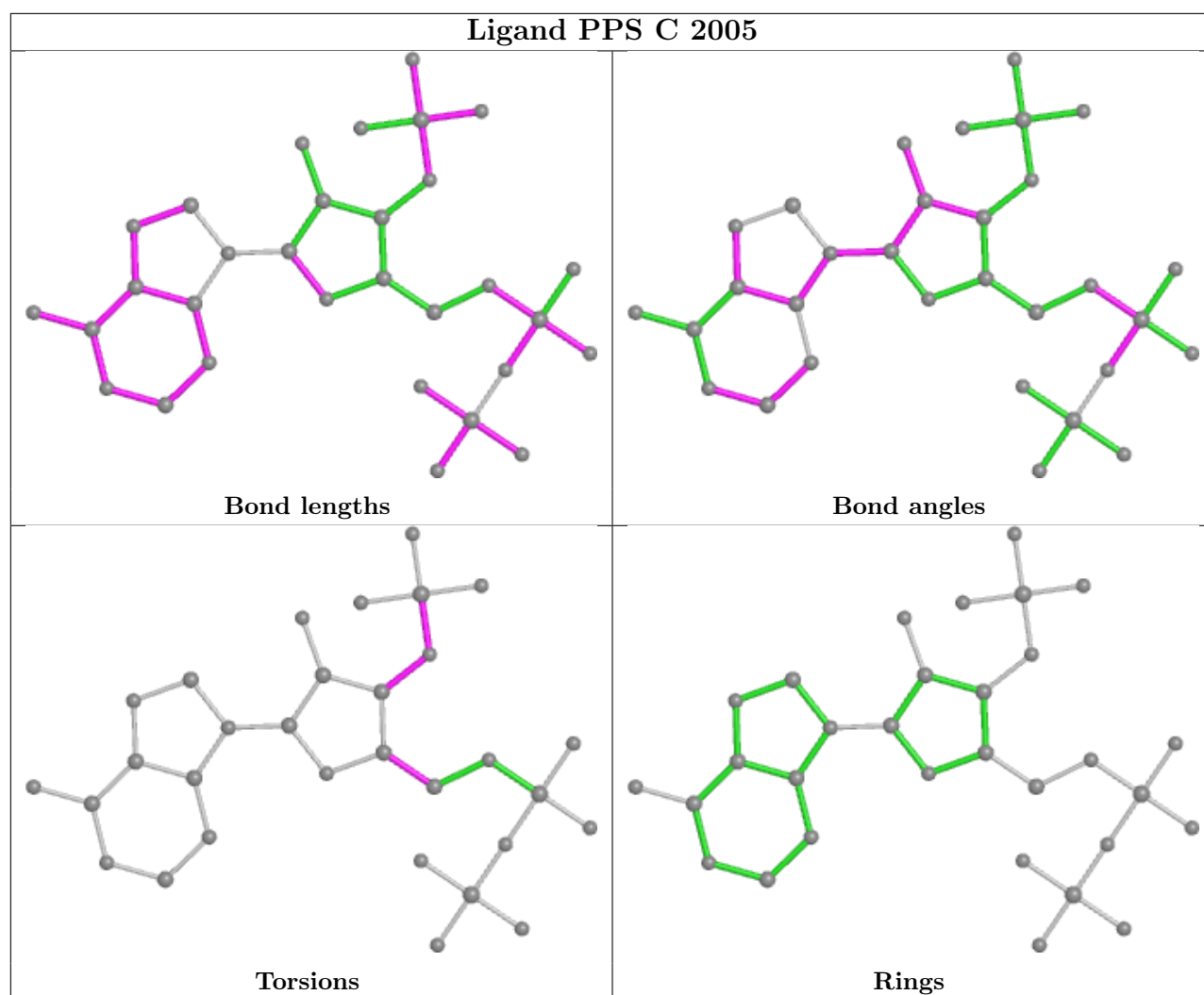
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2006	ADP	11	0
3	B	2003	ADP	4	0
3	C	2004	ADP	3	0
4	A	2002	PPS	4	0
3	A	2001	ADP	3	0
4	C	2005	PPS	1	0

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](#)

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	179/197 (90%)	0.40	11 (6%) 21 22	16, 35, 68, 130	6 (3%)
1	B	181/197 (91%)	0.13	9 (4%) 28 30	13, 33, 58, 90	4 (2%)
1	C	178/197 (90%)	0.27	10 (5%) 24 25	19, 36, 72, 114	1 (0%)
1	D	183/197 (92%)	0.03	8 (4%) 34 37	15, 31, 69, 100	1 (0%)
All	All	721/788 (91%)	0.21	38 (5%) 26 28	13, 34, 70, 130	12 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	129	THR	5.3
1	A	107	SER	3.6
1	D	52	ASP	3.2
1	B	208	ALA	3.1
1	C	28	ILE	3.1
1	C	55	VAL	3.0
1	C	204	GLY	3.0
1	A	129	THR	3.0
1	C	188	PRO	2.9
1	D	51	ARG	2.8
1	C	129	THR	2.8
1	A	52	ASP	2.8
1	B	128	GLU	2.8
1	B	50	VAL	2.8
1	C	54	ARG	2.6
1	C	197	ILE	2.6
1	D	129	THR	2.6
1	D	122	VAL	2.5
1	A	208	ALA	2.5
1	D	54	ARG	2.4
1	D	207	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	23	GLN	2.4
1	A	104	SER	2.4
1	D	161	VAL	2.4
1	A	31	THR	2.4
1	A	106	ILE	2.3
1	A	30	LEU	2.3
1	A	103	THR	2.2
1	B	51	ARG	2.2
1	B	161	VAL	2.2
1	B	54	ARG	2.2
1	D	67	PHE	2.2
1	A	25	GLY	2.1
1	A	47	HIS	2.1
1	B	68	GLY	2.1
1	B	52	ASP	2.1
1	C	27	THR	2.1
1	C	187	LEU	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
3	ADP	C	2004	27/27	0.94	0.14	13,39,89,263	0
3	ADP	A	2001	27/27	0.95	0.14	0,37,86,162	0
3	ADP	D	2006	27/27	0.96	0.15	5,22,72,118	0
4	PPS	A	2002	31/31	0.96	0.15	7,29,91,116	0
4	PPS	C	2005	31/31	0.96	0.18	0,28,94,247	0
2	CL	B	502	1/1	0.98	0.18	31,31,31,31	0

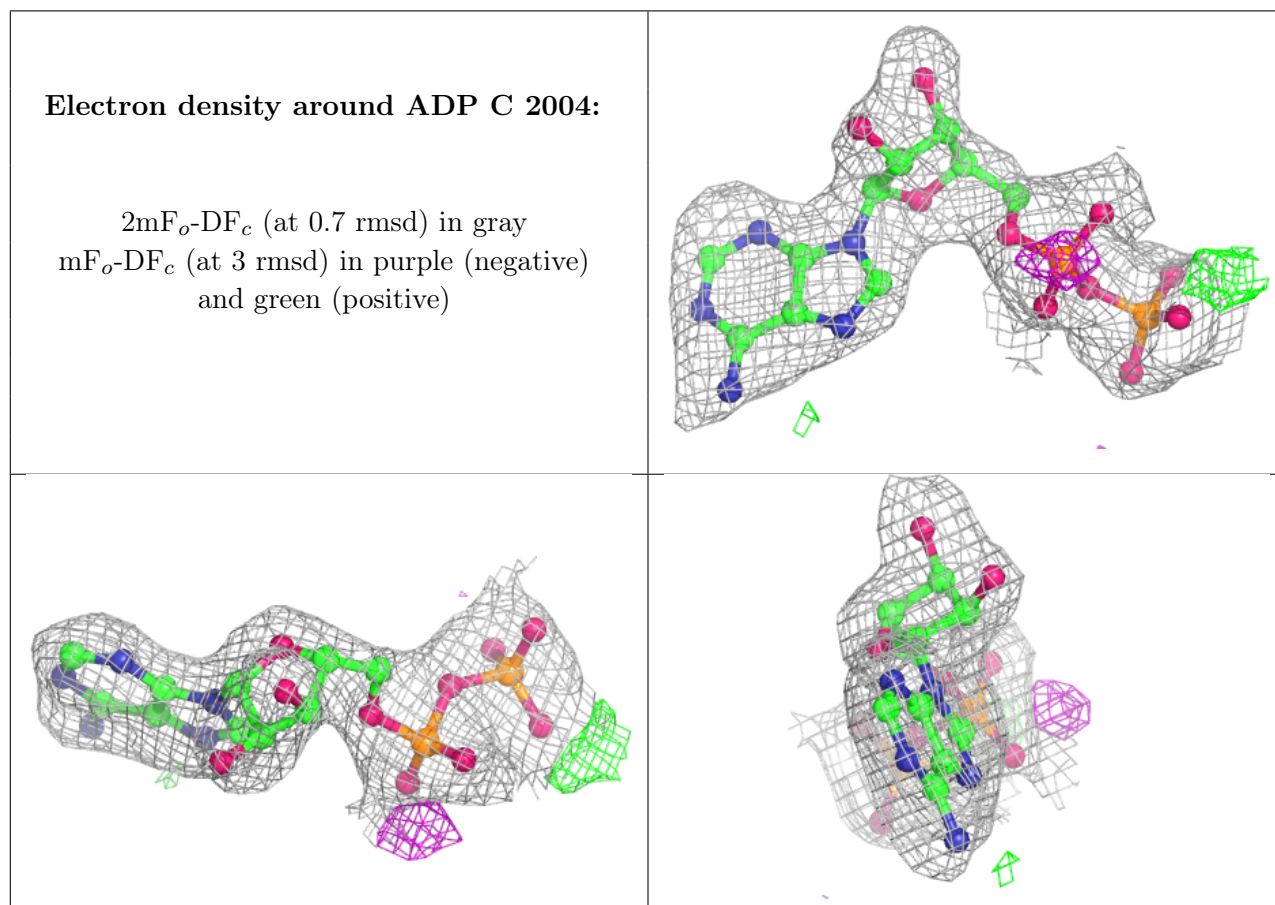
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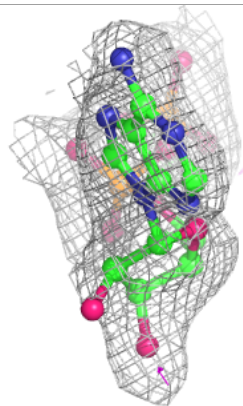
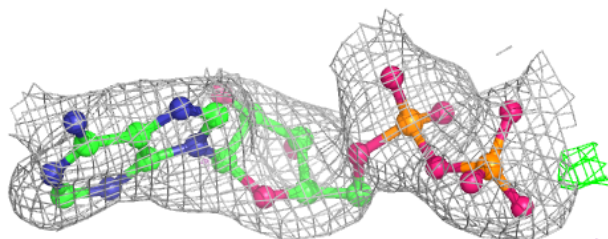
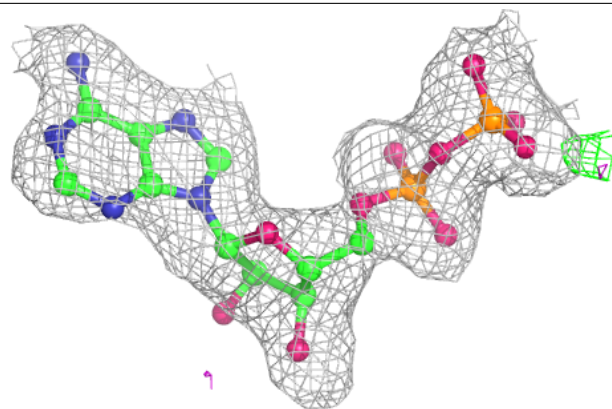
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	B	2003	27/27	0.98	0.12	4,25,50,57	0
2	CL	A	503	1/1	0.99	0.07	22,22,22,22	0
2	CL	C	501	1/1	0.99	0.13	21,21,21,21	0

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.

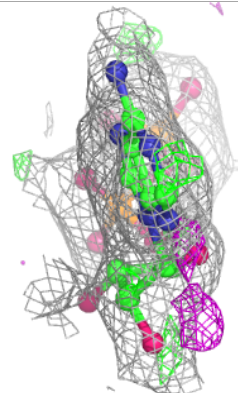
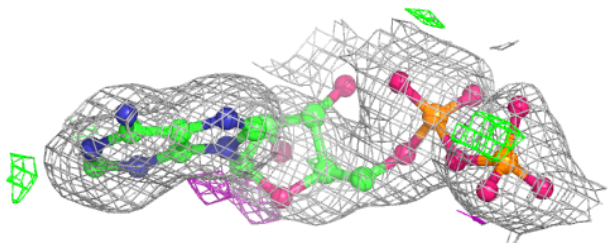
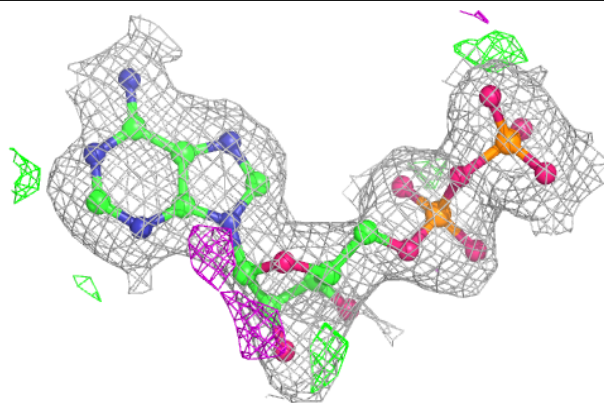


**Electron density around ADP A 2001:**

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

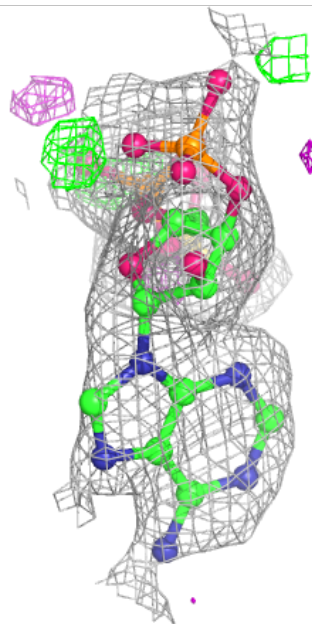
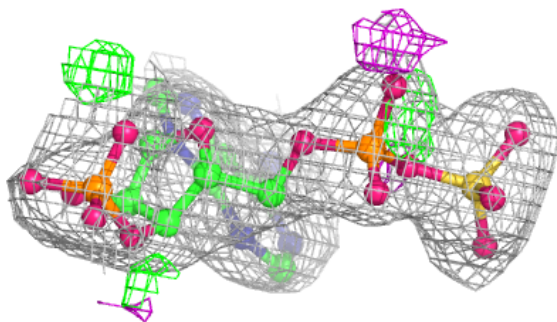
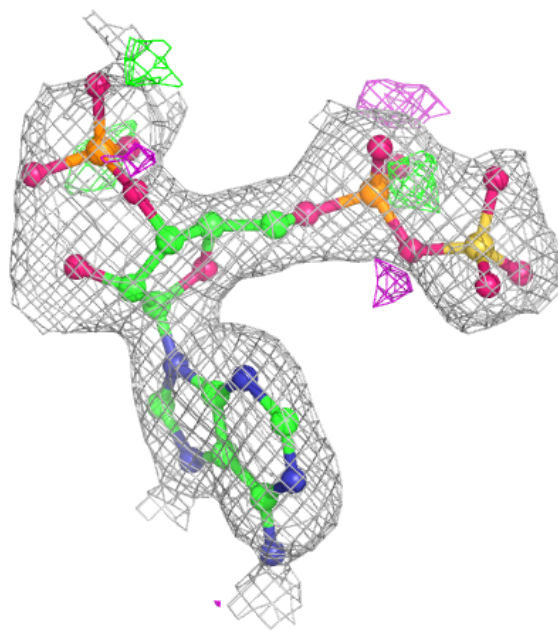
**Electron density around ADP D 2006:**

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



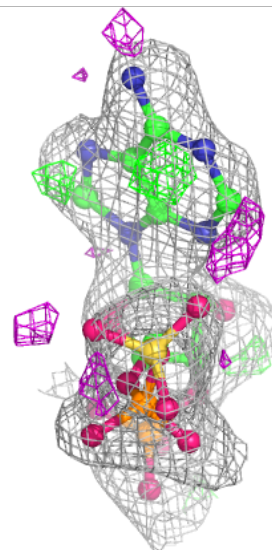
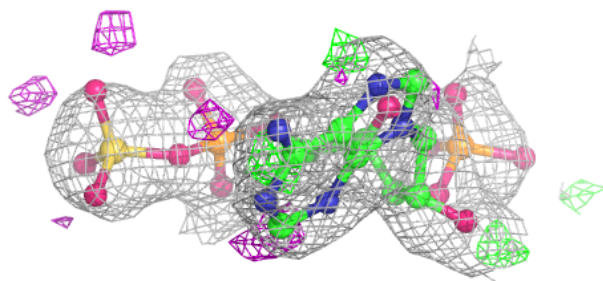
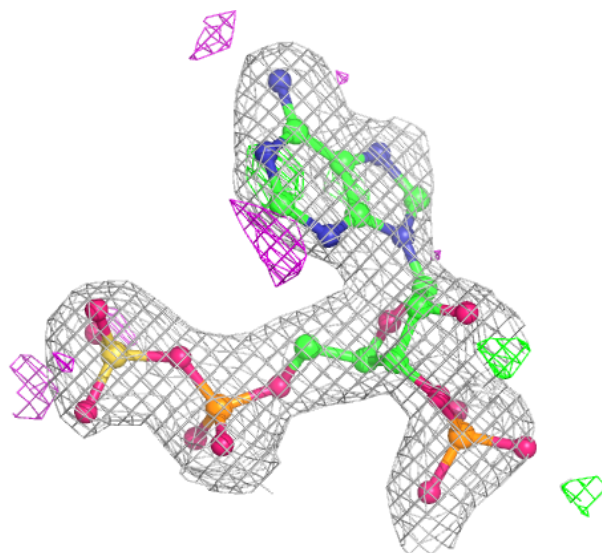
**Electron density around PPS A 2002:**

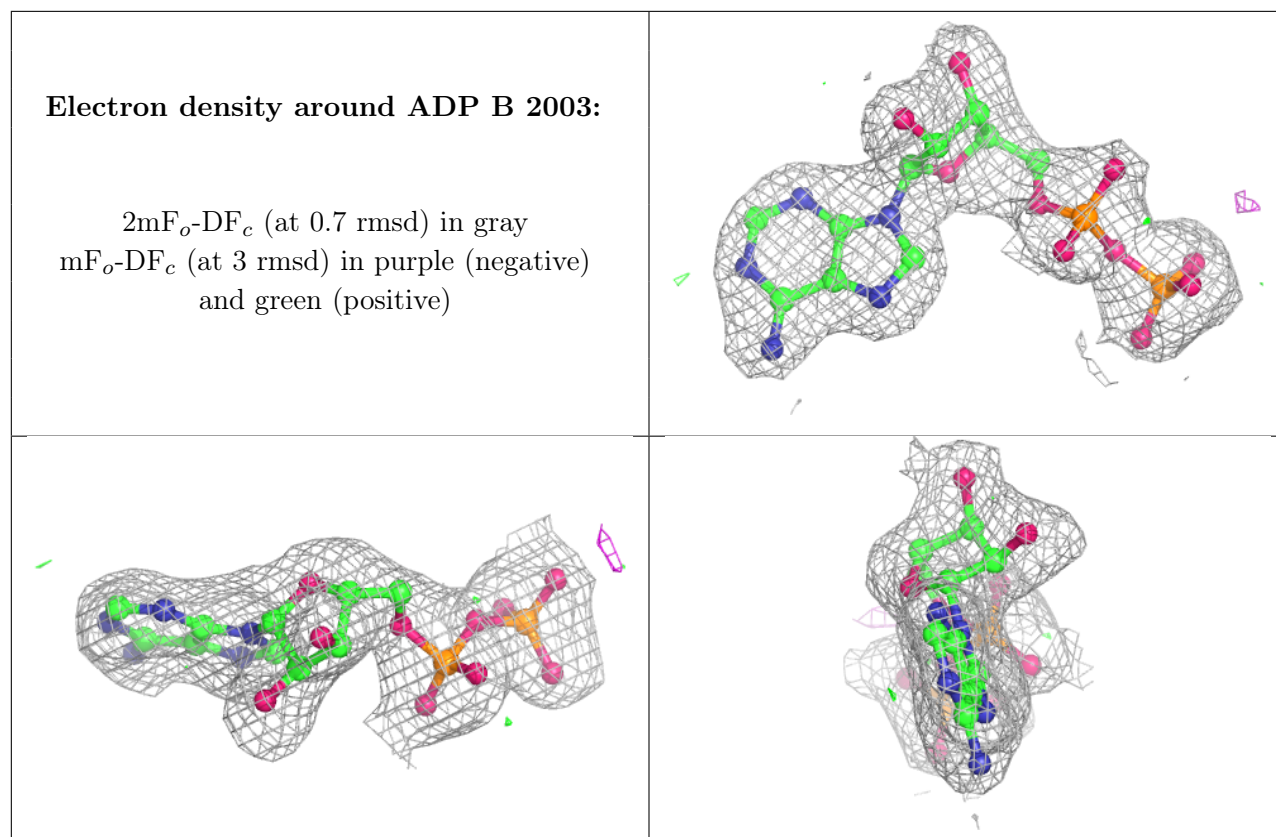
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PPS C 2005:**

$2mF_o-DF_c$  (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.