



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:33 PM UTC

PDB ID : 8JMJ / pdb_00008jnj
Title : Structure of Helicobacter pylori Soj-DNA-Spo0J complex
Authors : Wu, C.T.; Chu, C.H.; Sun, Y.J.
Deposited on : 2023-06-05
Resolution : 2.57 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

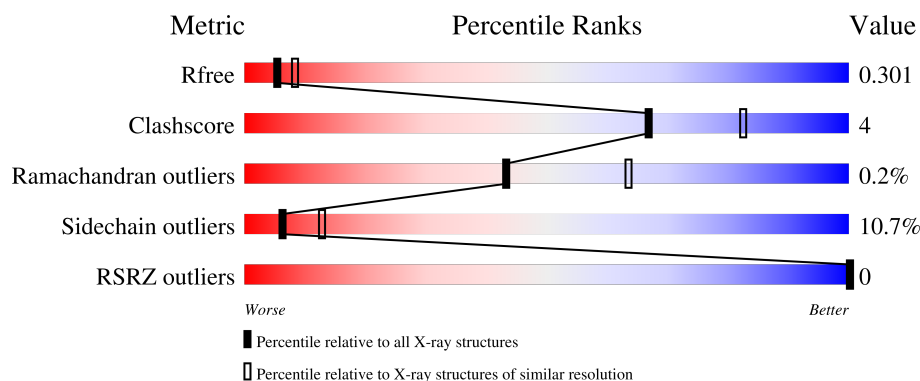
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	264	
1	B	264	
1	C	264	
1	D	264	
2	E	24	

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Mol	Chain	Length	Quality of chain
3	F	24	83% 12%
4	K	10	50% 10% 20% 20%
4	L	10	70% 30%
4	M	10	40% 30% 30%
4	N	10	60% 20% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9555 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 SpoOJ regulator (Soj).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2050	1327	337	378	8			
1	B	264	Total	C	N	O	S	0	0	0
			2050	1327	337	378	8			
1	C	264	Total	C	N	O	S	0	0	0
			2050	1327	337	378	8			
1	D	264	Total	C	N	O	S	0	0	0
			2050	1327	337	378	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	ASP	engineered mutation	UNP O25759
B	41	ALA	ASP	engineered mutation	UNP O25759
C	41	ALA	ASP	engineered mutation	UNP O25759
D	41	ALA	ASP	engineered mutation	UNP O25759

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*CP*CP*TP*GP*TP*TP*TP*CP*AP*CP*GP*TP*GP*GP*AP*AP*CP*AP*CP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			483	231	81	147	24			

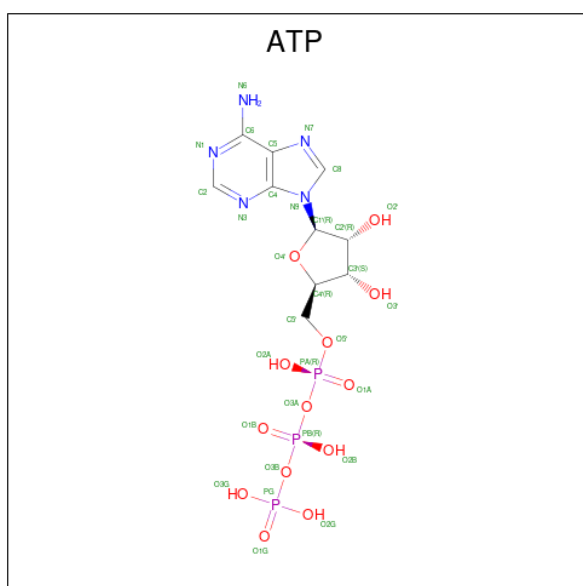
- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*GP*GP*TP*GP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*CP*AP*GP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	24	Total	C	N	O	P	0	0	0
			501	236	100	141	24			

- Molecule 4 is a protein called Probable chromosome-partitioning protein ParB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	10	Total	C	N	O	0	0	0
			62	37	15	10			
4	K	10	Total	C	N	O	0	0	0
			67	42	15	10			
4	M	10	Total	C	N	O	0	0	0
			62	37	15	10			
4	N	8	Total	C	N	O	0	0	0
			52	31	13	8			

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

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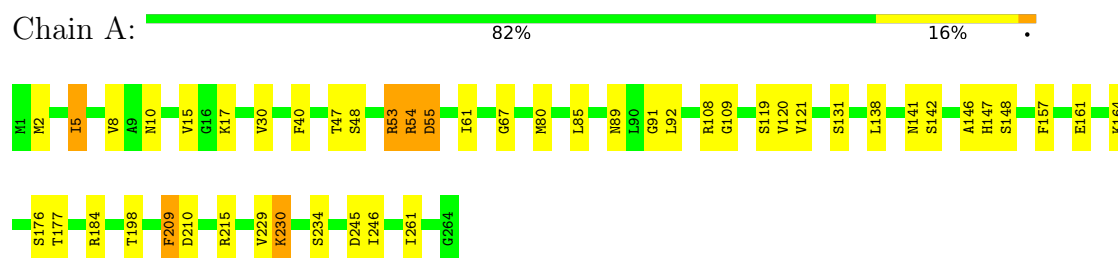
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	Mg 1	0	0
6	D	1	Total 1	Mg 1	0	0

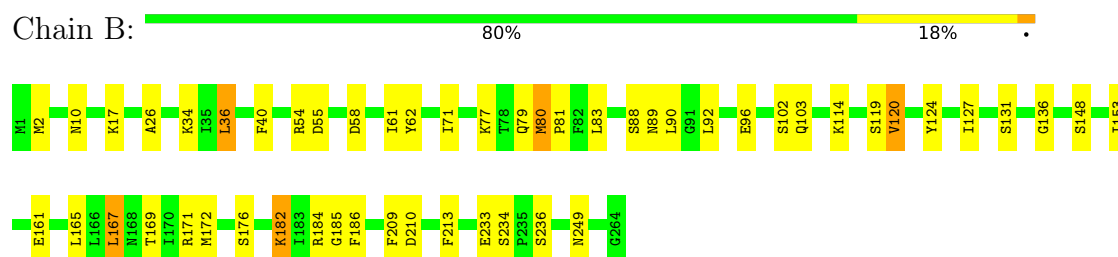
3 Residue-property plots [i](#)

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.

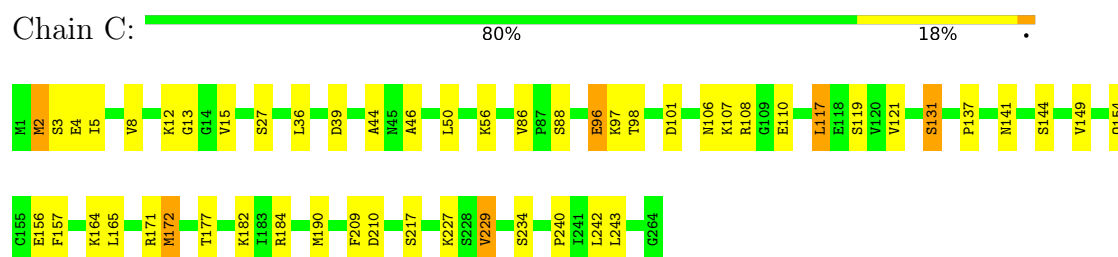
• Molecule 1: SpoOJ regulator (Soj)



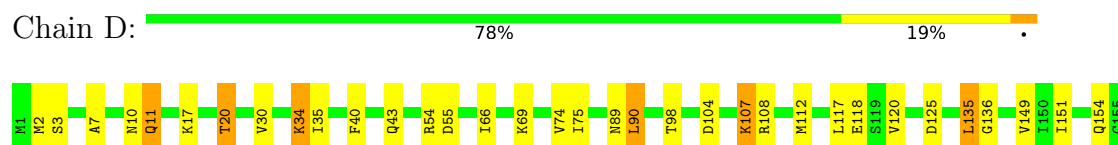
• Molecule 1: SpoOJ regulator (Soj)



• Molecule 1: SpoOJ regulator (Soj)



• Molecule 1: SpoOJ regulator (Soj)





- Molecule 2: DNA (5'-D(P*TP*CP*CP*CP*TP*GP*TP*TP*TP*CP*AP*CP*GP*TP*GP*G P*AP*AP*CP*AP*CP*CP*CP*T)-3')

Chain E: 96% .



- Molecule 3: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*TP*TP*CP*CP*AP*CP*GP*TP*GP*A P*AP*AP*CP*AP*GP*GP*GP*A)-3')

Chain F: 83% 12% .



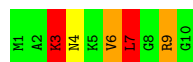
- Molecule 4: Probable chromosome-partitioning protein ParB

Chain L: 70% 30%



- Molecule 4: Probable chromosome-partitioning protein ParB

Chain K: 50% 10% 20% 20%



- Molecule 4: Probable chromosome-partitioning protein ParB

Chain M: 40% 30% 30%



- Molecule 4: Probable chromosome-partitioning protein ParB

Chain N: 60% 20% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.18Å 75.19Å 81.12Å 71.34° 71.46° 67.70°	Depositor
Resolution (Å)	28.57 – 2.57 28.57 – 2.57	Depositor EDS
% Data completeness (in resolution range)	90.7 (28.57-2.57) 90.3 (28.57-2.57)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.57Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.224 , 0.302 0.226 , 0.301	Depositor DCC
R_{free} test set	2009 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 14.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9555	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.68	0/2088	1.14	10/2822 (0.4%)
1	B	0.74	1/2088 (0.0%)	1.21	8/2822 (0.3%)
1	C	0.73	0/2088	1.14	9/2822 (0.3%)
1	D	0.77	0/2088	1.19	10/2822 (0.4%)
2	E	0.34	0/538	0.99	0/826
3	F	0.34	0/564	1.03	2/870 (0.2%)
4	K	1.13	0/66	2.11	4/85 (4.7%)
4	L	0.88	0/61	1.77	2/78 (2.6%)
4	M	0.97	0/61	2.23	6/78 (7.7%)
4	N	0.91	0/51	1.70	1/64 (1.6%)
All	All	0.71	1/9693 (0.0%)	1.17	52/13289 (0.4%)

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
4	K	0	1
4	L	0	1
4	M	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	ALA	CA-CB	-5.46	1.44	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	7	LEU	N-CA-C	8.54	123.44	112.34
1	A	261	ILE	N-CA-C	-8.25	103.83	111.67
1	D	209	PHE	N-CA-C	7.83	123.80	113.30
1	B	210	ASP	N-CA-C	7.57	120.49	111.33
3	F	6	DG	C4'-C3'-O3'	7.52	121.27	110.00
4	K	6	VAL	CA-C-N	7.42	135.70	121.54
4	K	6	VAL	C-N-CA	7.42	135.70	121.54
1	C	209	PHE	N-CA-C	7.39	122.42	112.88
4	N	8	GLY	N-CA-C	-7.34	101.99	112.55
1	D	108	ARG	N-CA-C	7.29	119.86	111.11
1	A	209	PHE	N-CA-C	7.25	123.01	113.30
1	D	120	VAL	N-CA-C	7.22	119.98	112.83
1	A	120	VAL	N-CA-C	7.19	119.94	112.83
1	B	209	PHE	N-CA-C	7.15	122.88	113.30
1	B	136	GLY	CA-C-N	7.10	126.62	119.24
1	B	136	GLY	C-N-CA	7.10	126.62	119.24
4	M	2	ALA	N-CA-C	7.08	122.09	113.17
4	K	4	ASN	N-CA-C	6.95	121.34	112.86
4	L	6	VAL	N-CA-C	6.94	120.75	111.17
4	K	7	LEU	N-CA-C	6.78	125.25	110.80
1	C	157	PHE	N-CA-C	6.57	119.27	111.71
1	B	234	SER	N-CA-C	6.52	122.51	113.45
1	C	154	GLN	N-CA-C	-6.33	99.70	109.76
1	D	157	PHE	N-CA-C	6.20	118.84	111.71
4	L	2	ALA	N-CA-C	5.89	117.81	110.91
1	A	55	ASP	N-CA-C	-5.75	106.25	113.72
1	C	106	ASN	N-CA-C	5.71	117.58	111.36
1	A	67	GLY	N-CA-C	-5.66	106.84	115.00
1	A	157	PHE	N-CA-C	5.66	118.22	111.71
1	B	120	VAL	N-CA-C	5.64	118.41	112.83
1	D	20	THR	N-CA-CB	5.63	118.49	110.16
1	C	15	VAL	N-CA-C	5.54	117.50	112.29
1	D	234	SER	N-CA-C	5.54	121.15	113.45
1	C	234	SER	N-CA-C	5.51	120.41	113.25
1	D	136	GLY	CA-C-N	5.45	125.79	119.47
1	D	136	GLY	C-N-CA	5.45	125.79	119.47
4	M	5	LYS	N-CA-C	5.45	122.40	110.80
3	F	6	DG	O4'-C1'-N9	5.41	116.51	108.40
1	D	75	ILE	N-CA-C	5.38	115.94	108.84
1	A	53	ARG	N-CA-C	-5.37	102.53	110.48
1	D	210	ASP	N-CA-C	5.31	117.76	111.33
1	C	156	GLU	N-CA-C	-5.30	101.06	108.96
1	C	210	ASP	N-CA-C	5.27	118.50	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	8	GLY	CA-C-N	5.26	131.16	121.70
4	M	8	GLY	C-N-CA	5.26	131.16	121.70
1	A	109	GLY	N-CA-C	5.19	120.16	114.40
1	A	234	SER	N-CA-C	5.19	121.27	109.81
1	B	185	GLY	N-CA-C	5.19	117.99	111.09
4	M	6	VAL	N-CA-C	5.17	120.09	109.34
1	B	103	GLN	N-CA-C	-5.16	106.99	113.28
1	A	15	VAL	N-CA-C	5.14	117.92	112.83
1	C	13	GLY	N-CA-C	5.02	118.37	111.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	ARG	Peptide
4	K	7	LEU	Peptide
4	L	8	GLY	Peptide
4	M	6	VAL	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	2050	0	2134	15	0
1	B	2050	0	2134	16	0
1	C	2050	0	2135	20	0
1	D	2050	0	2135	15	0
2	E	483	0	272	1	0
3	F	501	0	269	3	0
4	K	67	0	76	3	0
4	L	62	0	60	0	0
4	M	62	0	60	1	0
4	N	52	0	50	0	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
5	D	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	9555	0	9373	68	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 4.

All (68) 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:7:ALA:HB3	1:D:149:VAL:HG22	1.83	0.60
1:A:210:ASP:O	1:A:215:ARG:NH2	2.34	0.59
1:B:36:LEU:HB3	1:B:127:ILE:HG12	1.85	0.57
1:C:39:ASP:O	1:C:88:SER:OG	2.23	0.56
1:D:174:GLN:NE2	1:D:181:LEU:O	2.36	0.56
1:C:97:LYS:NZ	1:C:101:ASP:OD2	2.41	0.54
1:C:5:ILE:HD13	1:C:117:LEU:HD23	1.90	0.54
1:C:2:MET:SD	1:C:2:MET:N	2.81	0.54
2:E:23:DC:N3	3:F:2:DG:N1	2.57	0.53
1:D:54:ARG:HE	1:D:89:ASN:HB2	1.75	0.52
1:A:10:ASN:H	1:A:17:LYS:HD3	1.76	0.51
1:D:10:ASN:H	1:D:17:LYS:HD3	1.75	0.50
1:A:48:SER:O	1:A:53:ARG:NH2	2.45	0.49
1:B:88:SER:OG	1:B:89:ASN:N	2.45	0.49
1:C:4:GLU:OE2	1:C:184:ARG:NH1	2.46	0.49
1:C:8:VAL:O	1:C:131:SER:OG	2.30	0.49
1:D:230:LYS:HA	1:D:233:GLU:HG2	1.94	0.49
1:C:110:GLU:O	1:C:144:SER:OG	2.30	0.48
1:C:36:LEU:HD11	1:C:86:VAL:HG23	1.95	0.48
1:A:8:VAL:O	1:A:131:SER:OG	2.32	0.48
1:B:62:TYR:HB2	1:B:92:LEU:HA	1.96	0.47
1:C:240:PRO:HD2	1:C:243:LEU:HD12	1.95	0.47
4:M:8:GLY:HA2	4:M:9:ARG:HG2	1.96	0.47
1:A:48:SER:HB3	1:A:53:ARG:HH21	1.80	0.46
1:C:172:MET:HE3	1:C:172:MET:HB2	1.86	0.46
1:A:176:SER:OG	1:A:177:THR:N	2.50	0.45
1:B:61:ILE:HG23	1:B:92:LEU:HD13	1.98	0.45
3:F:5:DT:H2'	3:F:6:DG:C8	2.51	0.45
1:D:196:ASN:HD21	3:F:13:DG:H3'	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:MET:HB2	1:B:83:LEU:HB3	1.99	0.45
1:C:39:ASP:HB2	1:C:46:ALA:HB3	1.99	0.44
4:K:3:LYS:H	4:K:3:LYS:HG2	1.52	0.44
1:D:154:GLN:HG2	1:D:156:GLU:HG3	1.98	0.44
1:B:10:ASN:H	1:B:17:LYS:HD3	1.82	0.44
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.89	0.43
1:D:11:GLN:HB3	1:D:135:LEU:HD13	2.00	0.43
1:D:107:LYS:HA	1:D:107:LYS:HD2	1.76	0.43
1:C:12:LYS:NZ	5:D:500:ATP:O2G	2.42	0.43
1:C:44:ALA:HB2	1:C:88:SER:HB2	2.00	0.43
1:A:47:THR:HG23	1:A:85:LEU:HD21	2.00	0.43
1:A:148:SER:HB2	1:A:184:ARG:HB2	2.00	0.43
1:C:96:GLU:HG3	1:C:137:PRO:HG2	2.01	0.43
1:A:5:ILE:HB	1:A:146:ALA:HA	2.01	0.42
1:A:230:LYS:NZ	1:A:245:ASP:OD1	2.42	0.42
1:B:186:PHE:HB2	1:B:213:PHE:HA	2.01	0.42
1:B:233:GLU:O	1:B:236:SER:OG	2.30	0.42
1:A:89:ASN:HD22	1:A:91:GLY:H	1.68	0.42
1:C:56:LYS:HD2	4:K:7:LEU:HD22	2.01	0.42
1:B:34:LYS:HG3	1:B:124:TYR:CD1	2.55	0.42
1:B:167:LEU:HD11	1:B:186:PHE:HZ	1.85	0.42
1:A:164:LYS:HD2	1:A:209:PHE:HZ	1.85	0.41
1:D:160:LEU:HG	1:D:204:GLU:HG2	2.02	0.41
1:B:80:MET:HE2	1:B:80:MET:HB3	1.76	0.41
1:B:148:SER:HB2	1:B:184:ARG:HB2	2.01	0.41
1:C:229:VAL:HG21	1:D:195:LEU:HD13	2.01	0.41
1:C:27:SER:HA	1:C:242:LEU:HD21	2.01	0.41
1:B:182:LYS:HE3	1:B:182:LYS:HB3	1.61	0.41
1:D:34:LYS:N	1:D:125:ASP:OD2	2.43	0.41
1:D:112:MET:HE2	1:D:112:MET:HB3	1.96	0.41
1:B:80:MET:HA	1:B:81:PRO:HD3	1.98	0.41
1:C:50:LEU:O	4:K:9:ARG:NH1	2.53	0.41
1:A:61:ILE:HG23	1:A:92:LEU:HD13	2.03	0.41
1:B:54:ARG:HG2	1:B:89:ASN:HD22	1.86	0.41
1:C:165:LEU:HD13	1:D:90:LEU:HD13	2.02	0.41
1:B:172:MET:O	1:B:176:SER:OG	2.32	0.40
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.87	0.40
1:A:2:MET:HE3	1:A:147:HIS:CE1	2.57	0.40
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

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	262/264 (99%)	254 (97%)	8 (3%)	0	100	100
1	B	262/264 (99%)	256 (98%)	6 (2%)	0	100	100
1	C	262/264 (99%)	250 (95%)	12 (5%)	0	100	100
1	D	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
4	K	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
4	L	8/10 (80%)	4 (50%)	4 (50%)	0	100	100
4	M	8/10 (80%)	4 (50%)	4 (50%)	0	100	100
4	N	6/10 (60%)	4 (67%)	2 (33%)	0	100	100
All	All	1078/1096 (98%)	1033 (96%)	43 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	3	LYS
4	K	7	LEU

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	227/227 (100%)	211 (93%)	16 (7%)	14	29
1	B	227/227 (100%)	203 (89%)	24 (11%)	6	13
1	C	227/227 (100%)	206 (91%)	21 (9%)	8	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	227/227 (100%)	195 (86%)	32 (14%)	3	6
4	K	5/7 (71%)	1 (20%)	4 (80%)	0	0
4	L	3/7 (43%)	3 (100%)	0	100	100
4	M	3/7 (43%)	2 (67%)	1 (33%)	0	0
4	N	3/7 (43%)	2 (67%)	1 (33%)	0	0
All	All	922/936 (98%)	823 (89%)	99 (11%)	6	13

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	30	VAL
1	A	40	PHE
1	A	54	ARG
1	A	55	ASP
1	A	80	MET
1	A	108	ARG
1	A	119	SER
1	A	121	VAL
1	A	141	ASN
1	A	142	SER
1	A	161	GLU
1	A	198	THR
1	A	229	VAL
1	A	230	LYS
1	A	246	ILE
1	B	2	MET
1	B	36	LEU
1	B	40	PHE
1	B	55	ASP
1	B	58	ASP
1	B	71	ILE
1	B	77	LYS
1	B	79	GLN
1	B	80	MET
1	B	90	LEU
1	B	96	GLU
1	B	102	SER
1	B	114	LYS
1	B	119	SER

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Mol	Chain	Res	Type
1	B	120	VAL
1	B	131	SER
1	B	153	ILE
1	B	161	GLU
1	B	165	LEU
1	B	167	LEU
1	B	169	THR
1	B	171	ARG
1	B	182	LYS
1	B	249	ASN
1	C	2	MET
1	C	3	SER
1	C	96	GLU
1	C	98	THR
1	C	107	LYS
1	C	108	ARG
1	C	117	LEU
1	C	119	SER
1	C	121	VAL
1	C	131	SER
1	C	141	ASN
1	C	149	VAL
1	C	164	LYS
1	C	171	ARG
1	C	172	MET
1	C	177	THR
1	C	182	LYS
1	C	190	MET
1	C	217	SER
1	C	227	LYS
1	C	229	VAL
1	D	2	MET
1	D	3	SER
1	D	11	GLN
1	D	20	THR
1	D	30	VAL
1	D	34	LYS
1	D	35	ILE
1	D	40	PHE
1	D	43	GLN
1	D	55	ASP
1	D	66	ILE

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Mol	Chain	Res	Type
1	D	69	LYS
1	D	74	VAL
1	D	90	LEU
1	D	98	THR
1	D	104	ASP
1	D	107	LYS
1	D	118	GLU
1	D	135	LEU
1	D	151	ILE
1	D	160	LEU
1	D	165	LEU
1	D	167	LEU
1	D	169	THR
1	D	176	SER
1	D	177	THR
1	D	190	MET
1	D	192	VAL
1	D	211	SER
1	D	219	THR
1	D	230	LYS
1	D	263	GLN
4	K	3	LYS
4	K	6	VAL
4	K	7	LEU
4	K	9	ARG
4	M	9	ARG
4	N	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	89	ASN
1	A	103	GLN
1	B	103	GLN
1	B	255	GLN
1	C	31	HIS
1	C	73	GLN
1	C	255	GLN
1	C	263	GLN

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 oligosaccharides 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$
5	ATP	D	500	6	32,33,33	1.45	5 (15%)	48,52,52	1.92	14 (29%)
5	ATP	A	500	6	32,33,33	1.39	7 (21%)	48,52,52	2.03	17 (35%)
5	ATP	C	500	6	32,33,33	1.48	6 (18%)	48,52,52	1.91	16 (33%)
5	ATP	B	500	6	32,33,33	1.47	6 (18%)	48,52,52	1.92	13 (27%)

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
5	ATP	D	500	6	-	0/22/38/38	0/3/3/3
5	ATP	A	500	6	-	0/22/38/38	0/3/3/3
5	ATP	C	500	6	-	1/22/38/38	0/3/3/3
5	ATP	B	500	6	-	1/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	500	ATP	C5-C4	4.77	1.47	1.39
5	C	500	ATP	C5-C4	4.59	1.47	1.39
5	B	500	ATP	C5-C4	4.41	1.46	1.39
5	A	500	ATP	C5-C4	4.17	1.46	1.39
5	B	500	ATP	PB-O3B	3.05	1.62	1.59
5	D	500	ATP	C5-C6	2.84	1.48	1.41
5	A	500	ATP	C5-C6	2.83	1.48	1.41
5	C	500	ATP	C8-N7	2.82	1.37	1.31
5	D	500	ATP	PB-O3B	2.67	1.62	1.59
5	C	500	ATP	C5-C6	2.66	1.48	1.41
5	B	500	ATP	C5-C6	2.49	1.47	1.41
5	B	500	ATP	C8-N7	2.45	1.36	1.31
5	C	500	ATP	PA-O3A	2.45	1.62	1.59
5	A	500	ATP	C4-N9	-2.42	1.32	1.37
5	D	500	ATP	C8-N7	2.41	1.36	1.31
5	C	500	ATP	C8-N9	-2.38	1.33	1.37
5	C	500	ATP	C5-N7	-2.37	1.34	1.39
5	A	500	ATP	C8-N7	2.35	1.36	1.31
5	B	500	ATP	PA-O3A	2.26	1.61	1.59
5	B	500	ATP	C5-N7	-2.23	1.35	1.39
5	A	500	ATP	C5-N7	-2.20	1.35	1.39
5	D	500	ATP	C5-N7	-2.15	1.35	1.39
5	A	500	ATP	C8-N9	-2.09	1.34	1.37
5	A	500	ATP	PB-O3B	2.07	1.61	1.59

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	ATP	O4'-C1'-N9	-5.46	97.61	108.09
5	B	500	ATP	C5-C4-N3	-5.26	119.47	126.72
5	C	500	ATP	C5-C4-N3	-5.26	119.48	126.72
5	D	500	ATP	C5-C4-N3	-4.97	119.87	126.72
5	A	500	ATP	C5-C4-N3	-4.44	120.61	126.72
5	A	500	ATP	C4-C5-N7	-4.41	105.54	110.58
5	C	500	ATP	N3-C4-N9	4.32	134.52	127.17
5	D	500	ATP	N3-C4-N9	4.09	134.13	127.17
5	B	500	ATP	N3-C4-N9	4.00	133.97	127.17
5	D	500	ATP	C2'-C1'-N9	3.80	122.74	113.30
5	C	500	ATP	O4'-C1'-N9	-3.75	100.89	108.09
5	C	500	ATP	C4-N9-C8	3.73	109.65	105.74
5	C	500	ATP	C4-C5-N7	-3.72	106.33	110.58
5	B	500	ATP	C2-N3-C4	3.66	120.78	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	ATP	N3-C2-N1	-3.62	123.11	128.58
5	B	500	ATP	C2'-C1'-N9	3.52	122.05	113.30
5	D	500	ATP	C4-C5-N7	-3.46	106.63	110.58
5	D	500	ATP	C2-N3-C4	3.33	119.96	111.83
5	A	500	ATP	C2'-C1'-N9	3.21	121.27	113.30
5	B	500	ATP	C4-C5-N7	-3.19	106.94	110.58
5	B	500	ATP	O4'-C1'-N9	-3.16	102.02	108.09
5	D	500	ATP	N3-C2-N1	-3.12	123.86	128.58
5	B	500	ATP	O2B-PB-O3B	3.07	115.58	107.27
5	C	500	ATP	C2-N3-C4	2.97	119.10	111.83
5	A	500	ATP	N3-C4-N9	2.97	132.22	127.17
5	D	500	ATP	C4-N9-C8	2.97	108.85	105.74
5	A	500	ATP	C4-N9-C8	2.95	108.83	105.74
5	A	500	ATP	C6-C5-N7	2.93	137.73	132.09
5	A	500	ATP	C5-N7-C8	2.92	108.04	103.45
5	A	500	ATP	C2-N3-C4	2.82	118.72	111.83
5	C	500	ATP	C5-N7-C8	2.74	107.76	103.45
5	A	500	ATP	O3G-PG-O2G	2.72	117.99	107.80
5	B	500	ATP	C2'-C3'-C4'	2.65	107.72	102.61
5	B	500	ATP	C2-N1-C6	2.62	123.04	118.73
5	C	500	ATP	N9-C8-N7	-2.60	110.25	113.94
5	A	500	ATP	C4-N9-C1'	-2.55	120.66	126.63
5	A	500	ATP	N3-C2-N1	-2.55	124.72	128.58
5	D	500	ATP	C5-N7-C8	2.53	107.42	103.45
5	D	500	ATP	C6-C5-N7	2.49	136.89	132.09
5	A	500	ATP	N9-C8-N7	-2.48	110.42	113.94
5	D	500	ATP	C2'-C3'-C4'	2.45	107.35	102.61
5	D	500	ATP	O4'-C1'-N9	-2.45	103.39	108.09
5	D	500	ATP	O2B-PB-O3B	2.45	113.88	107.27
5	C	500	ATP	O3G-PG-O2G	2.41	116.83	107.80
5	C	500	ATP	O3A-PA-O1A	-2.40	103.47	110.70
5	D	500	ATP	C2-N1-C6	2.36	122.61	118.73
5	B	500	ATP	C5-N7-C8	2.30	107.06	103.45
5	C	500	ATP	N3-C2-N1	-2.27	125.15	128.58
5	A	500	ATP	O2B-PB-O3B	2.26	113.37	107.27
5	A	500	ATP	C2-N1-C6	2.22	122.37	118.73
5	C	500	ATP	C6-C5-N7	2.20	136.33	132.09
5	B	500	ATP	C6-C5-N7	2.19	136.32	132.09
5	C	500	ATP	O2B-PB-O1B	2.16	122.48	112.44
5	C	500	ATP	C2'-C3'-C4'	2.15	106.76	102.61
5	B	500	ATP	O3'-C3'-C4'	-2.08	105.11	111.08
5	C	500	ATP	O2A-PA-O1A	2.07	122.09	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	500	ATP	O2B-PB-O3A	-2.05	101.73	107.27
5	D	500	ATP	N9-C8-N7	-2.05	111.03	113.94
5	A	500	ATP	O3A-PA-O1A	-2.05	104.55	110.70
5	C	500	ATP	O3'-C3'-C4'	-2.01	105.31	111.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

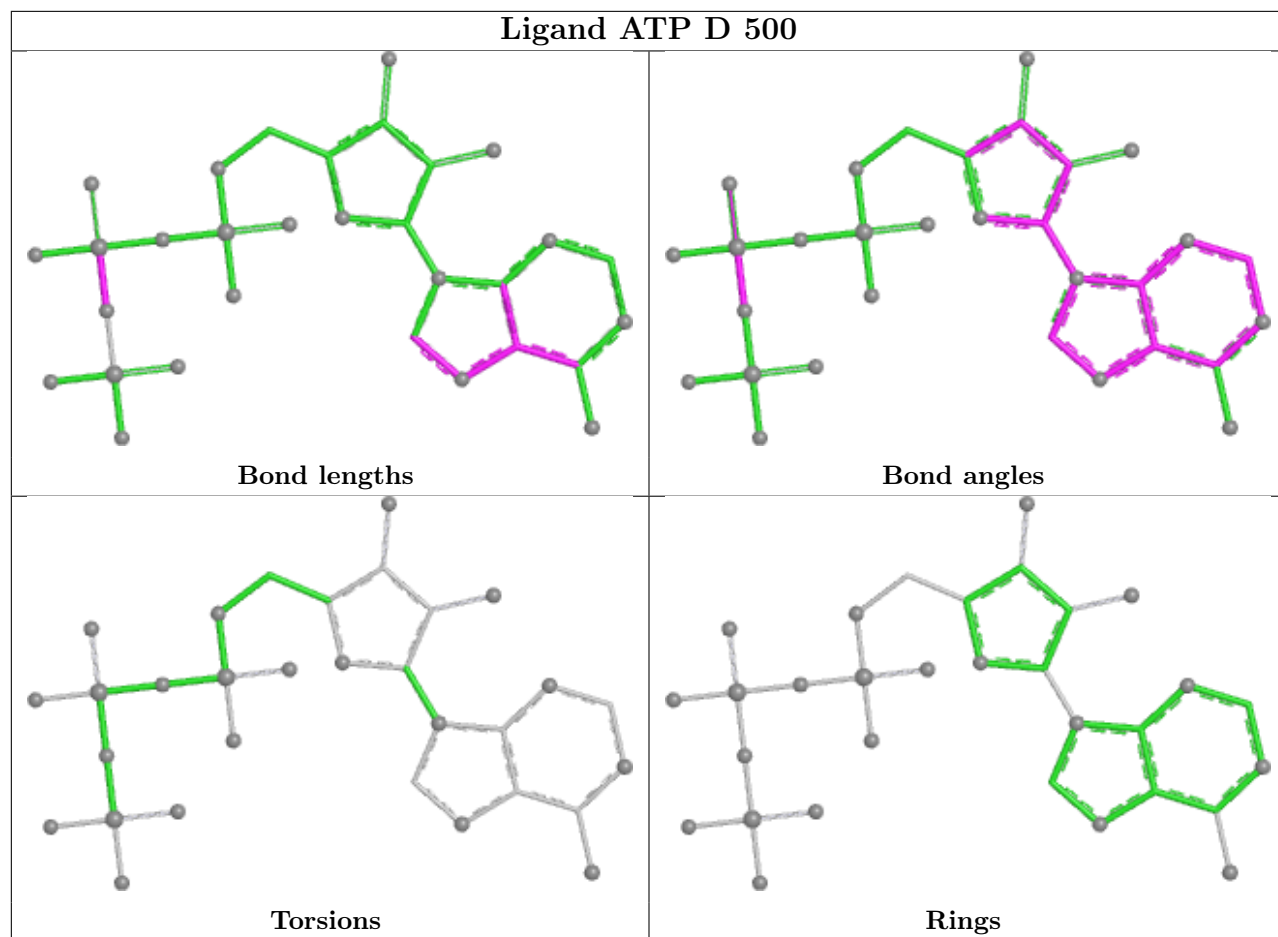
Mol	Chain	Res	Type	Atoms
5	C	500	ATP	PB-O3B-PG-O2G
5	B	500	ATP	PA-O3A-PB-O2B

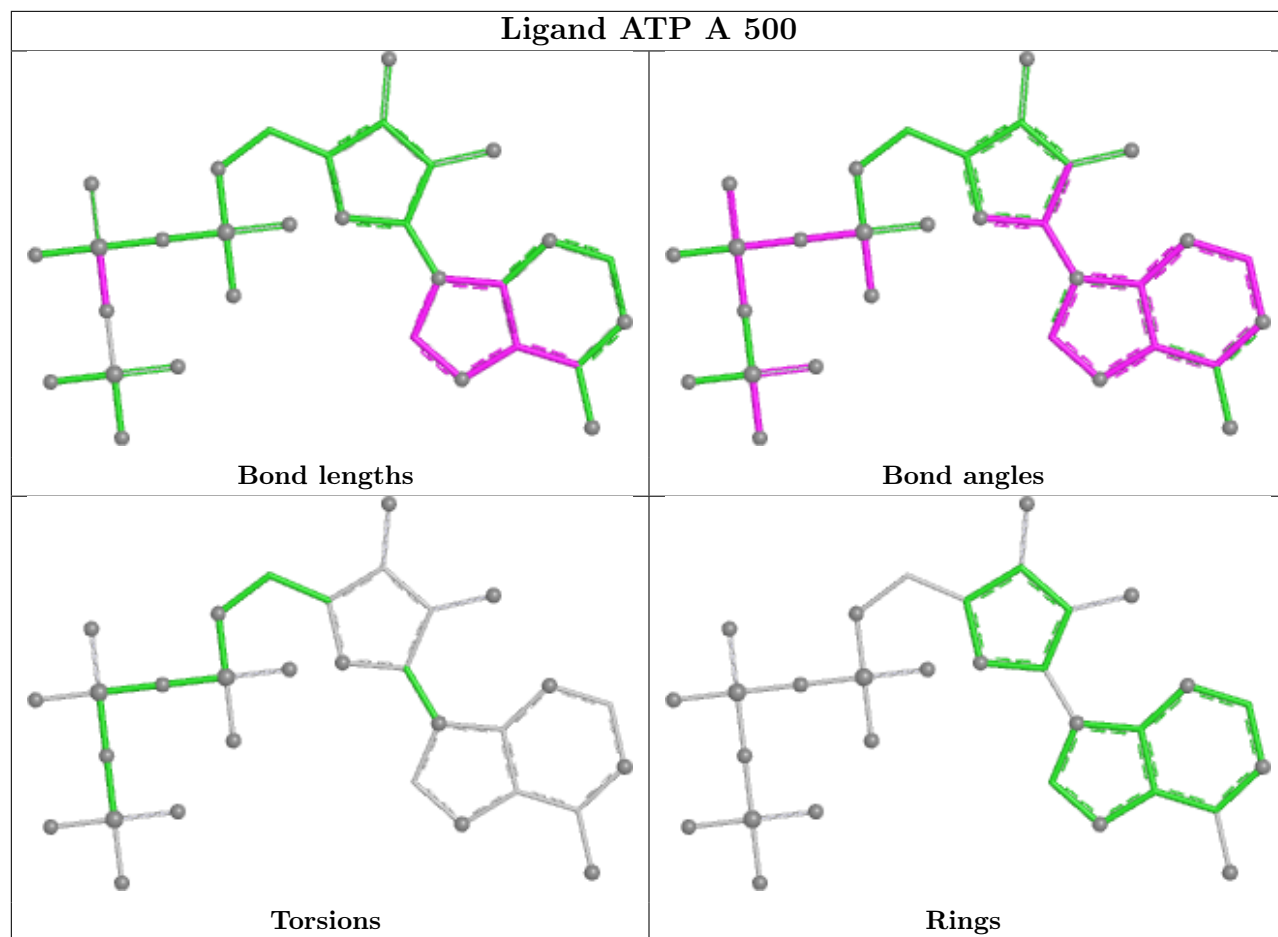
There are no ring outliers.

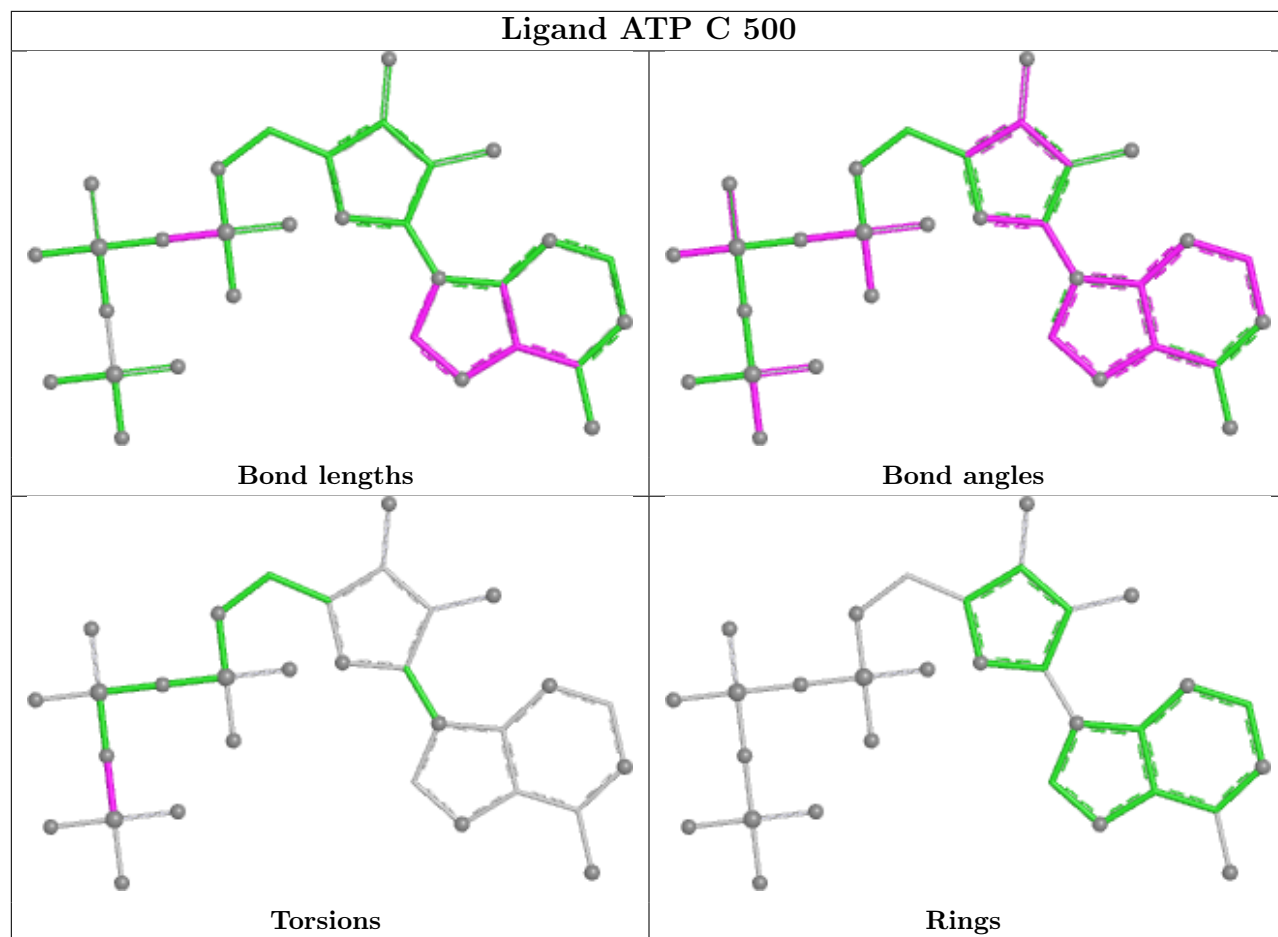
1 monomer is involved in 1 short contact:

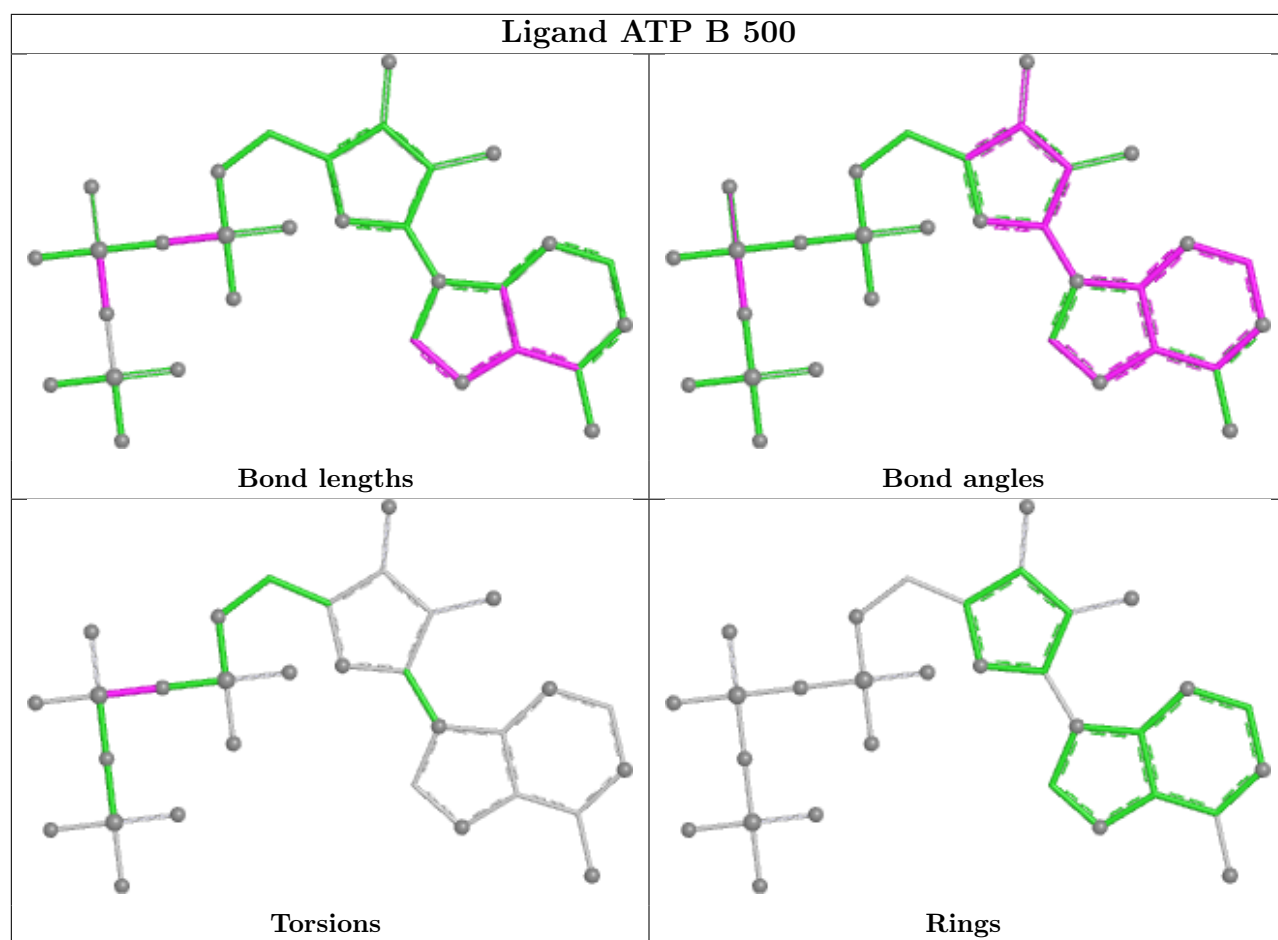
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	500	ATP	1	0

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	264/264 (100%)	-1.05	0 100 100	22, 44, 86, 114	0
1	B	264/264 (100%)	-1.09	0 100 100	22, 43, 86, 136	0
1	C	264/264 (100%)	-1.07	0 100 100	21, 44, 87, 123	0
1	D	264/264 (100%)	-1.10	0 100 100	22, 43, 80, 134	0
2	E	24/24 (100%)	-0.86	0 100 100	30, 55, 134, 152	0
3	F	24/24 (100%)	-0.81	0 100 100	32, 49, 135, 149	0
4	K	10/10 (100%)	-0.35	0 100 100	67, 94, 109, 119	0
4	L	10/10 (100%)	-0.34	0 100 100	68, 95, 127, 134	0
4	M	10/10 (100%)	-0.31	0 100 100	76, 91, 101, 112	0
4	N	8/10 (80%)	-0.71	0 100 100	68, 83, 97, 102	0
All	All	1142/1144 (99%)	-1.04	0 100 100	21, 45, 96, 152	0

There are no RSRZ outliers to report.

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 oligosaccharides 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,

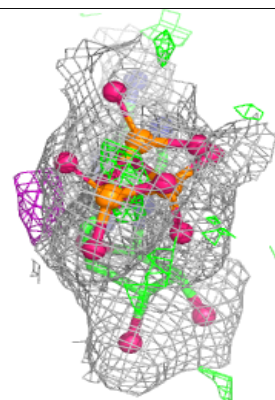
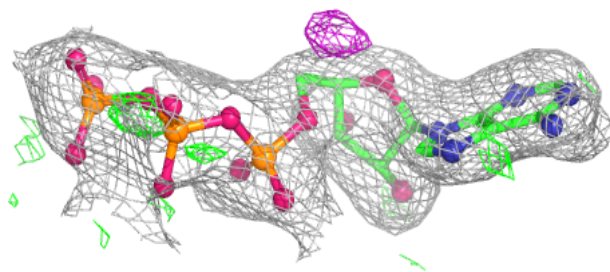
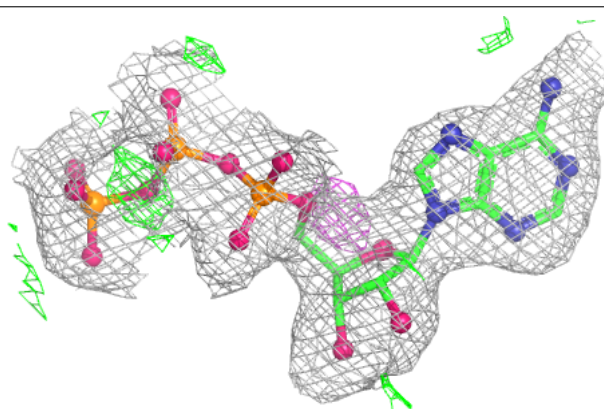
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ATP	B	500	31/31	0.99	0.04	19,21,39,45	0
5	ATP	C	500	31/31	0.99	0.04	17,21,39,51	0
5	ATP	D	500	31/31	0.99	0.04	19,22,34,38	0
6	MG	A	501	1/1	0.99	0.06	42,42,42,42	0
6	MG	B	501	1/1	0.99	0.06	49,49,49,49	0
6	MG	C	501	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	501	1/1	0.99	0.06	40,40,40,40	0
5	ATP	A	500	31/31	1.00	0.03	17,21,33,45	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.

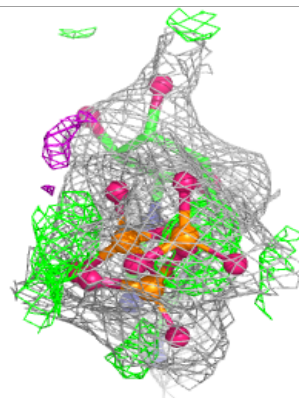
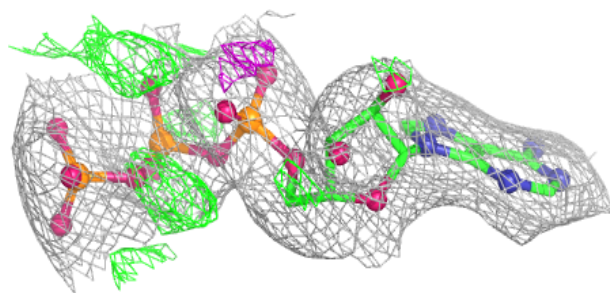
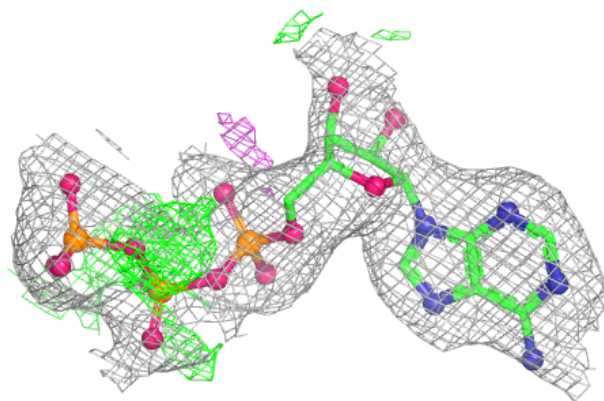
Electron density around ATP B 500:

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

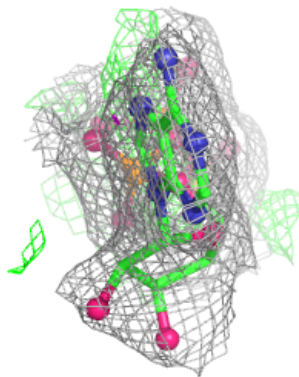
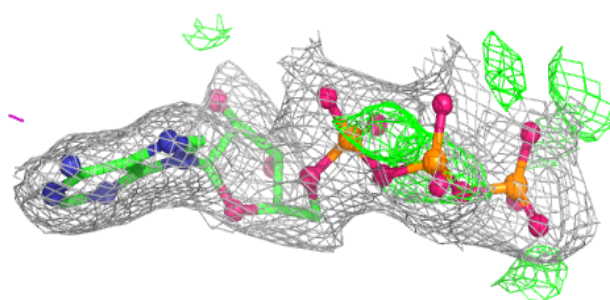
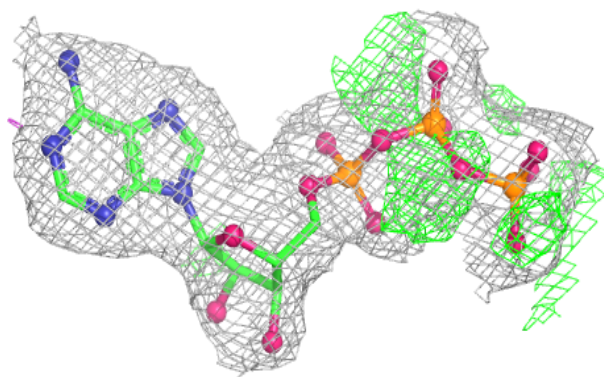


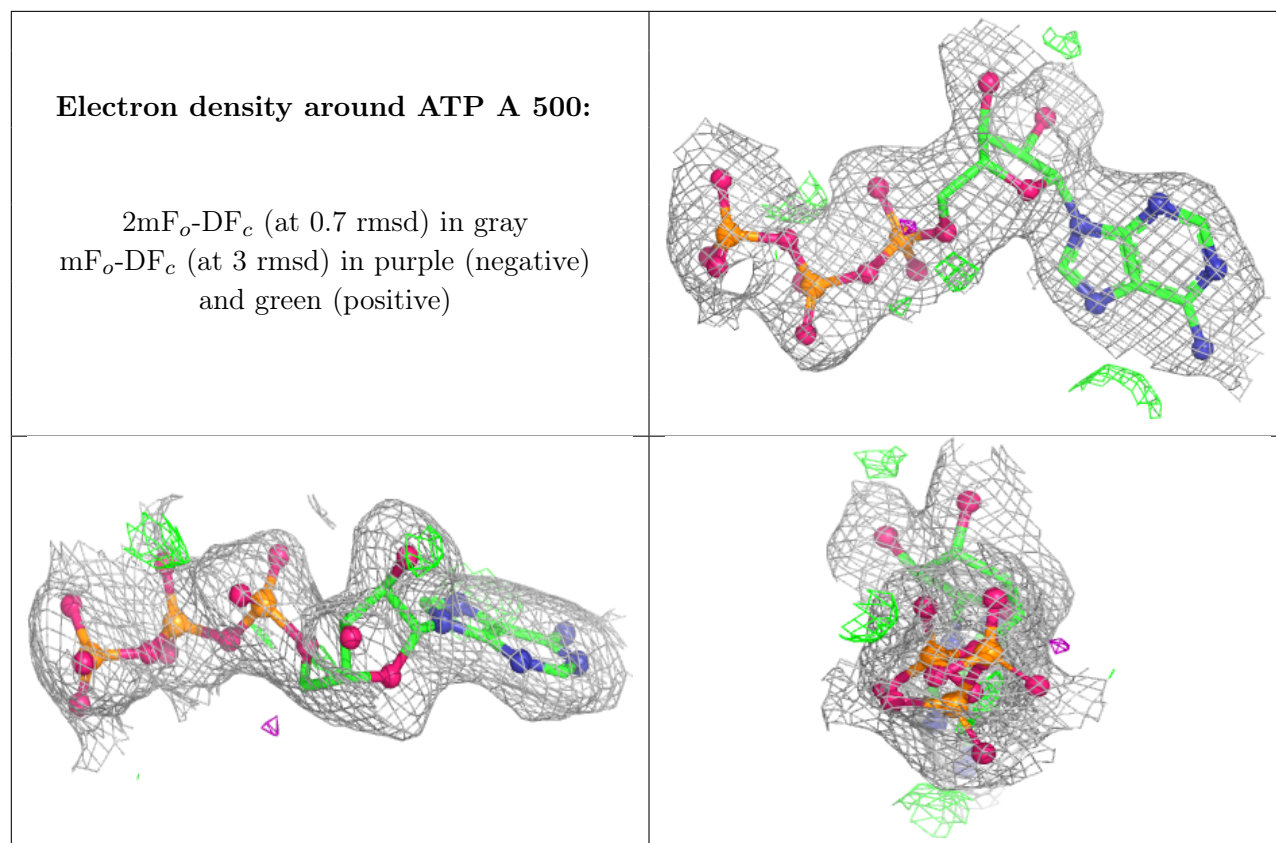
Electron density around ATP C 500:

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

**Electron density around ATP D 500:**

$2mF_o-DF_c$ (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.