



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2021 – 06:08 PM JST

PDB ID : 7DWR
Title : Structure of Sulfolobus solfataricus SegA-ADP complex bound to DNA
Authors : Yen, C.Y.; Lin, M.G.; Hsiao, C.D.; Sun, Y.J.
Deposited on : 2021-01-17
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

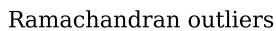
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.24
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

i

X-RAY DIFFRACTION

A.

Metric	Percentile Banks	Value
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 R_{free}

The numeric value for each fraction is indicated below the corresponding segment, with a dot

1

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Mol	Chain	Length	Quality of chain
3	F	24	 25% 79% 21%
3	H	24	 12% 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8947 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 SOJ protein (Soj).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1711	1104	283	321	3			
1	B	220	Total	C	N	O	S	0	0	0
			1711	1104	283	321	3			
1	C	220	Total	C	N	O	S	0	0	0
			1711	1104	283	321	3			
1	D	220	Total	C	N	O	S	0	0	0
			1711	1104	283	321	3			

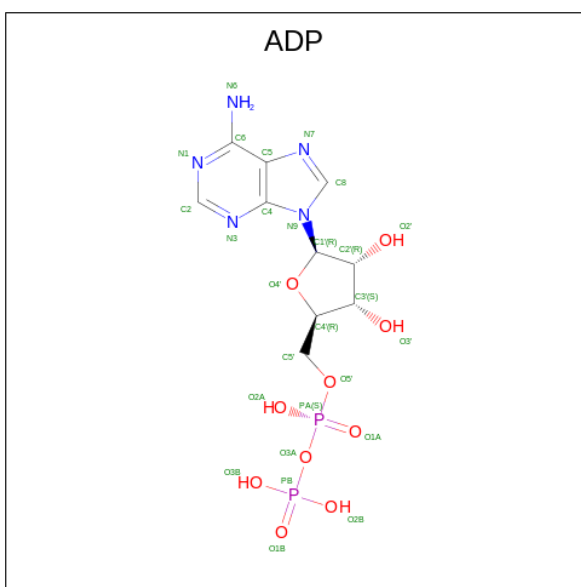
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*GP*GP*TP*GP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*CP*AP*GP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	24	Total	C	N	O	P	0	0	0
			501	236	100	141	24			
2	G	24	Total	C	N	O	P	0	0	0
			501	236	100	141	24			

- Molecule 3 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
3	F	24	Total	C	N	O	P	0	0	0
			483	231	81	147	24			
3	H	24	Total	C	N	O	P	0	0	0
			483	231	81	147	24			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

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

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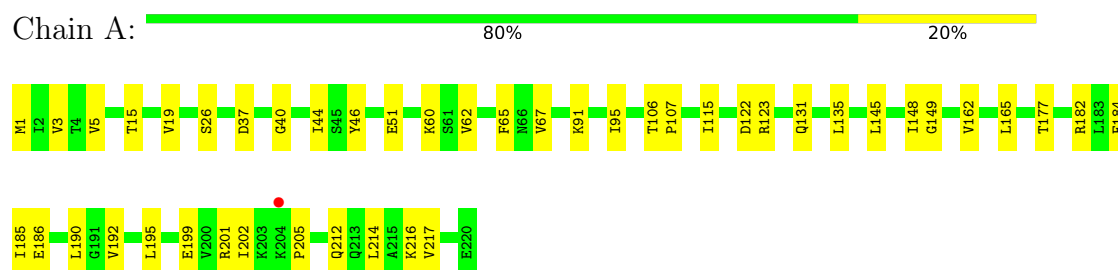
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	5	Total	O	0	0
			5	5		
6	C	6	Total	O	0	0
			6	6		
6	D	6	Total	O	0	0
			6	6		

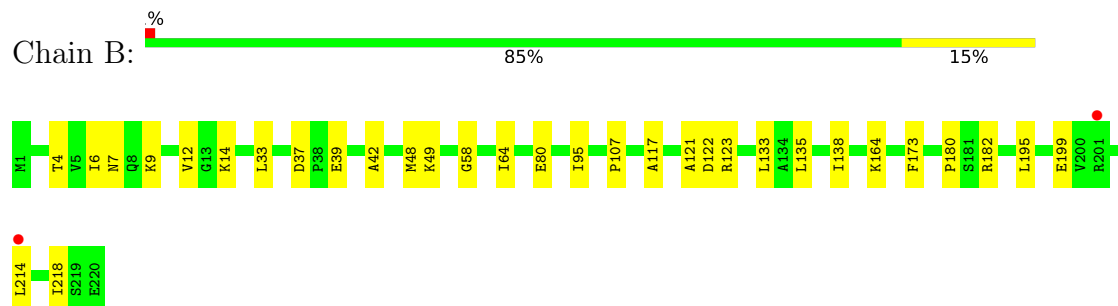
3 Residue-property plots

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.

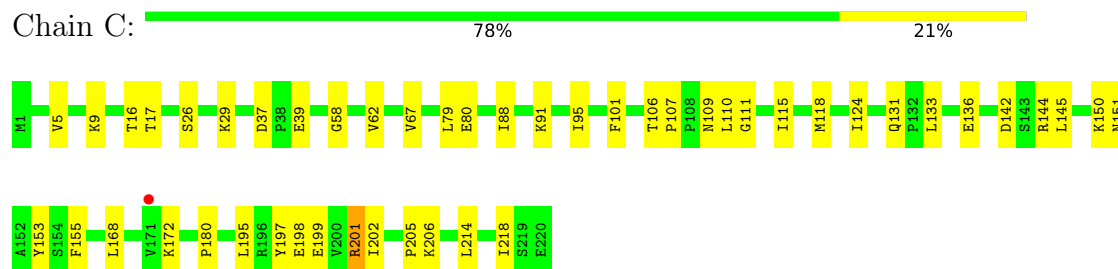
• Molecule 1: SOJ protein (Soj)



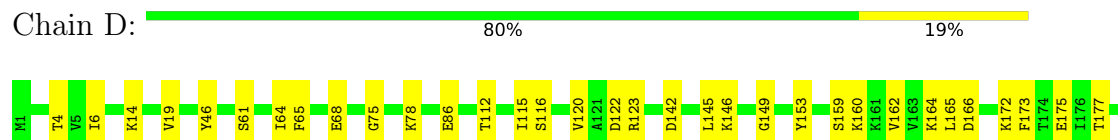
• Molecule 1: SOJ protein (Soj)

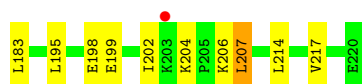


• Molecule 1: SOJ protein (Soj)

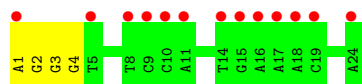
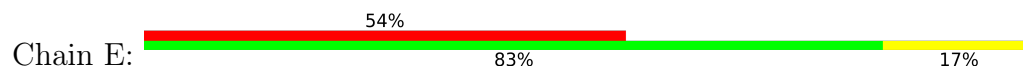


• Molecule 1: SOJ protein (Soj)

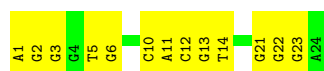




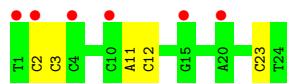
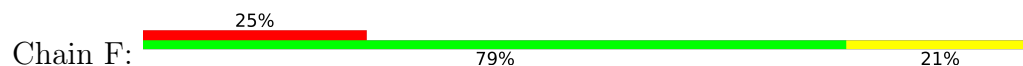
- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*CP*AP*GP*GP*GP*A)-3')



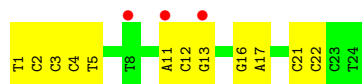
- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*TP*TP*CP*CP*AP*CP*GP*TP*GP*AP*AP*AP*CP*AP*GP*GP*GP*A)-3')



- Molecule 3: 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')



- Molecule 3: 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')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.00Å 60.54Å 132.14Å 90.00° 127.01° 90.00°	Depositor
Resolution (Å)	27.68 – 2.80 27.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (27.68-2.80) 86.5 (27.68-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.239 , 0.298 0.238 , 0.297	Depositor DCC
R_{free} test set	1987 reflections (6.61%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.447 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8947	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.38% 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	0.30	0/1738	0.52	1/2348 (0.0%)
1	B	0.28	0/1738	0.48	0/2348
1	C	0.34	0/1738	0.52	0/2348
1	D	0.32	0/1738	0.54	1/2348 (0.0%)
2	E	0.55	0/564	0.89	0/870
2	G	0.50	0/564	0.83	0/870
3	F	0.57	0/538	0.94	0/826
3	H	0.55	0/538	0.93	0/826
All	All	0.38	0/9156	0.64	2/12784 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLN	CA-CB-CG	6.71	128.16	113.40
1	D	207	LEU	CA-CB-CG	5.20	127.25	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1711	0	1813	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1711	0	1812	20	0
1	C	1711	0	1812	30	0
1	D	1711	0	1813	28	0
2	E	501	0	269	3	0
2	G	501	0	269	13	0
3	F	483	0	272	6	0
3	H	483	0	272	8	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	0	0	0
6	B	5	0	0	0	0
6	C	6	0	0	0	0
6	D	6	0	0	0	0
All	All	8947	0	8380	131	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 8.

All (131) 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:198:GLU:OE2	1:D:207:LEU:N	2.17	0.76
1:A:135:LEU:HD22	1:A:165:LEU:HD11	1.75	0.69
1:D:164:LYS:NZ	1:D:175:GLU:OE2	2.30	0.63
1:D:162:VAL:HG11	1:D:164:LYS:HE3	1.80	0.63
1:C:142:ASP:OD2	1:C:168:LEU:HB3	1.99	0.63
1:B:80:GLU:OE2	1:B:107:PRO:HG2	2.00	0.62
1:C:109:ASN:OD1	1:C:111:GLY:N	2.30	0.61
2:G:14:DT:H3	3:H:11:DA:H61	1.46	0.61
2:G:12:DC:H2''	2:G:13:DG:C8	2.36	0.60
3:F:3:DC:OP2	3:F:3:DC:H6	1.86	0.58
1:A:51:GLU:OE2	1:A:60:LYS:HE2	2.05	0.57
1:A:162:VAL:HG22	1:A:177:THR:HB	1.86	0.57
1:A:1:MET:HE2	1:A:3:VAL:HG22	1.86	0.56
1:A:202:ILE:HD11	1:A:205:PRO:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:DA:H1'	3:H:12:DC:H5'	1.88	0.56
1:D:162:VAL:CG1	1:D:164:LYS:HE3	2.35	0.56
1:A:1:MET:HE1	1:A:123:ARG:HD3	1.86	0.56
1:A:216:LYS:HA	1:A:216:LYS:HE2	1.88	0.55
1:D:142:ASP:O	1:D:146:LYS:HG3	2.07	0.55
1:A:131:GLN:NE2	3:F:23:DC:H2'	2.22	0.55
1:B:37:ASP:OD2	1:B:39:GLU:HB3	2.08	0.54
1:B:195:LEU:O	1:B:199:GLU:HG3	2.08	0.54
2:E:1:DA:H2''	2:E:2:DG:N7	2.24	0.53
1:C:17:THR:HG1	1:C:155:PHE:HZ	1.53	0.53
2:E:1:DA:H2''	2:E:2:DG:C5	2.44	0.53
1:B:48:MET:CE	1:B:64:ILE:HG13	2.39	0.52
2:G:1:DA:H2''	2:G:2:DG:C8	2.45	0.52
1:C:153:TYR:CZ	1:C:172:LYS:HD2	2.45	0.52
1:A:122:ASP:O	1:A:123:ARG:NH1	2.42	0.52
1:A:184:PHE:HD2	4:A:301:ADP:C6	2.28	0.52
1:D:198:GLU:HG3	1:D:202:ILE:HD11	1.91	0.52
2:G:13:DG:H2''	2:G:14:DT:OP2	2.10	0.52
1:B:48:MET:HE1	1:B:64:ILE:HG13	1.90	0.52
2:G:2:DG:H2''	2:G:3:DG:C8	2.45	0.52
1:A:37:ASP:HA	1:A:107:PRO:HG3	1.92	0.52
1:A:201:ARG:O	1:A:201:ARG:NH2	2.43	0.52
1:C:9:LYS:NZ	1:C:131:GLN:HE21	2.08	0.51
1:C:37:ASP:OD2	1:C:39:GLU:HB2	2.11	0.51
1:D:195:LEU:O	1:D:199:GLU:HG3	2.11	0.51
1:C:80:GLU:O	1:C:80:GLU:HG3	2.11	0.50
1:D:86:GLU:OE2	1:D:86:GLU:HA	2.11	0.50
1:B:48:MET:O	1:B:49:LYS:HE2	2.12	0.50
1:B:135:LEU:O	1:B:138:ILE:HG22	2.13	0.49
1:C:153:TYR:CE2	1:C:172:LYS:HD2	2.46	0.49
1:D:112:THR:O	1:D:115:ILE:HG22	2.12	0.49
1:C:58:GLY:HA3	1:C:95:ILE:HD11	1.93	0.49
1:C:16:THR:OG1	4:C:301:ADP:O1A	2.26	0.49
1:A:214:LEU:HA	1:A:217:VAL:HG12	1.95	0.49
1:C:133:LEU:O	1:C:136:GLU:HG3	2.13	0.48
1:A:5:VAL:O	1:A:106:THR:OG1	2.26	0.48
1:B:9:LYS:HE3	1:B:133:LEU:HD22	1.96	0.48
1:A:40:GLY:O	1:A:44:ILE:HG12	2.12	0.48
2:G:11:DA:OP2	2:G:11:DA:H8	1.96	0.48
1:A:19:VAL:HG13	1:A:46:TYR:CE1	2.48	0.48
1:A:65:PHE:CZ	1:A:192:VAL:HG12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:22:DG:H2''	2:G:23:DG:H5''	1.94	0.48
1:B:4:THR:HG22	1:B:6:ILE:HG12	1.96	0.47
1:C:180:PRO:HA	4:C:301:ADP:N1	2.29	0.47
1:D:159:SER:OG	1:D:160:LYS:N	2.44	0.47
1:B:122:ASP:O	1:B:123:ARG:HG2	2.14	0.47
1:B:164:LYS:HG2	1:B:173:PHE:HB3	1.96	0.47
1:D:198:GLU:OE2	1:D:206:LYS:N	2.42	0.47
3:H:21:DC:H1'	3:H:22:DC:H5'	1.96	0.47
2:G:10:DC:H2''	2:G:11:DA:OP2	2.14	0.46
1:D:19:VAL:HG13	1:D:46:TYR:CE1	2.50	0.46
1:D:64:ILE:HG22	1:D:65:PHE:CD1	2.51	0.46
3:F:11:DA:H2''	3:F:12:DC:O4'	2.16	0.46
1:A:1:MET:CE	1:A:123:ARG:HD3	2.46	0.46
1:A:62:VAL:HG11	1:C:62:VAL:HG11	1.98	0.46
1:C:29:LYS:HG3	1:C:101:PHE:HE1	1.79	0.46
1:C:110:LEU:HD13	1:C:144:ARG:HG2	1.97	0.46
1:C:202:ILE:HD11	1:C:205:PRO:HA	1.97	0.46
1:A:195:LEU:O	1:A:199:GLU:HG3	2.16	0.46
1:B:7:ASN:N	1:B:14:LYS:HD3	2.31	0.46
1:B:58:GLY:HA3	1:B:95:ILE:HD11	1.98	0.46
1:C:198:GLU:OE2	1:C:206:LYS:N	2.46	0.45
1:D:164:LYS:HG2	1:D:173:PHE:HB3	1.98	0.45
1:D:214:LEU:HA	1:D:217:VAL:HG12	1.99	0.45
1:D:61:SER:OG	1:D:68:GLU:HG3	2.16	0.45
1:C:79:LEU:HD22	1:C:88:ILE:HD11	1.99	0.45
1:D:198:GLU:OE2	1:D:207:LEU:HD22	2.17	0.45
1:C:197:TYR:CZ	1:C:201:ARG:HG3	2.51	0.45
1:C:109:ASN:O	1:C:110:LEU:HD23	2.17	0.45
1:D:153:TYR:CE2	1:D:172:LYS:HD2	2.52	0.45
1:D:198:GLU:CD	1:D:206:LYS:H	2.20	0.45
1:C:118:MET:HG2	1:C:124:ILE:HD13	1.99	0.45
1:B:182:ARG:NH1	2:G:1:DA:O3'	2.49	0.44
1:A:91:LYS:O	1:A:95:ILE:HG13	2.17	0.44
1:A:131:GLN:HE21	3:F:23:DC:H2'	1.82	0.44
1:C:115:ILE:HD11	1:C:144:ARG:NE	2.33	0.44
1:D:145:LEU:O	1:D:149:GLY:N	2.51	0.44
1:D:122:ASP:O	1:D:123:ARG:HD3	2.18	0.43
1:C:145:LEU:HB3	1:C:150:LYS:O	2.17	0.43
1:C:91:LYS:O	1:C:95:ILE:HG13	2.18	0.43
1:B:182:ARG:NH1	2:G:2:DG:O4'	2.51	0.43
1:C:26:SER:HB3	1:C:67:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:GLY:O	1:D:78:LYS:HB3	2.18	0.43
2:E:3:DG:H2''	2:E:4:DG:C8	2.54	0.43
1:C:214:LEU:O	1:C:218:ILE:HG12	2.19	0.43
1:D:4:THR:HG22	1:D:6:ILE:HG12	2.00	0.43
2:G:21:DG:H2''	2:G:22:DG:H5'	2.01	0.43
1:A:185:ILE:HG13	1:A:186:GLU:N	2.33	0.42
3:H:3:DC:H2'	3:H:4:DC:C6	2.53	0.42
3:H:12:DC:H2''	3:H:13:DG:N7	2.33	0.42
1:A:26:SER:OG	1:A:67:VAL:HG22	2.19	0.42
1:D:14:LYS:HB3	1:D:14:LYS:HE2	1.90	0.42
1:D:165:LEU:O	1:D:166:ASP:OD1	2.37	0.42
3:F:3:DC:OP2	3:F:3:DC:H2'	2.19	0.42
3:H:16:DG:H2'	3:H:17:DA:C8	2.54	0.42
1:B:7:ASN:ND2	1:B:12:VAL:HG21	2.34	0.42
1:D:162:VAL:HG22	1:D:177:THR:HB	2.02	0.42
2:G:10:DC:H2''	2:G:11:DA:C8	2.55	0.42
1:B:180:PRO:HA	4:B:301:ADP:N1	2.35	0.41
1:A:201:ARG:HA	1:A:201:ARG:HD2	1.87	0.41
1:C:151:ASN:HB3	1:C:172:LYS:NZ	2.35	0.41
1:B:117:ALA:O	1:B:121:ALA:HB2	2.19	0.41
2:G:5:DT:H2''	2:G:6:DG:C8	2.54	0.41
1:D:183:LEU:HD13	1:D:207:LEU:HD21	2.02	0.41
3:F:2:DC:C2'	3:F:3:DC:H5'	2.50	0.41
1:A:15:THR:O	1:A:19:VAL:HG23	2.19	0.41
1:A:115:ILE:HD11	1:A:148:ILE:HG21	2.01	0.41
3:H:4:DC:H3'	3:H:5:DT:H72	2.03	0.41
1:C:107:PRO:O	1:C:109:ASN:N	2.52	0.41
1:C:195:LEU:O	1:C:199:GLU:HG3	2.20	0.41
3:H:1:DT:H2''	3:H:2:DC:O5'	2.21	0.41
1:A:145:LEU:O	1:A:149:GLY:N	2.53	0.41
1:B:33:LEU:HD21	1:B:42:ALA:HB1	2.03	0.41
1:C:5:VAL:O	1:C:106:THR:OG1	2.32	0.41
1:A:190:LEU:HD22	1:A:192:VAL:HG22	2.04	0.40
1:B:214:LEU:O	1:B:218:ILE:HG23	2.21	0.40
1:D:116:SER:O	1:D:120:VAL:HG22	2.21	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	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
1	B	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
1	C	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
1	D	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
All	All	872/880 (99%)	843 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	194/194 (100%)	193 (100%)	1 (0%)	88	96
1	B	194/194 (100%)	194 (100%)	0	100	100
1	C	194/194 (100%)	193 (100%)	1 (0%)	88	96
1	D	194/194 (100%)	193 (100%)	1 (0%)	88	96
All	All	776/776 (100%)	773 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ARG
1	C	201	ARG
1	D	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	131	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 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	$\# Z > 2$
4	ADP	D	301	5	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
4	ADP	C	301	5	24,29,29	0.94	1 (4%)	29,45,45	1.35	3 (10%)
4	ADP	B	301	5	24,29,29	0.93	1 (4%)	29,45,45	1.40	4 (13%)
4	ADP	A	301	5	24,29,29	0.96	1 (4%)	29,45,45	1.36	3 (10%)

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
4	ADP	D	301	5	-	4/12/32/32	0/3/3/3
4	ADP	C	301	5	-	6/12/32/32	0/3/3/3
4	ADP	B	301	5	-	4/12/32/32	0/3/3/3
4	ADP	A	301	5	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	ADP	C5-C4	2.47	1.47	1.40
4	D	301	ADP	C5-C4	2.43	1.47	1.40
4	B	301	ADP	C5-C4	2.40	1.47	1.40
4	C	301	ADP	C5-C4	2.35	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	ADP	PA-O3A-PB	-3.41	121.11	132.83
4	B	301	ADP	N3-C2-N1	-3.31	123.50	128.68
4	D	301	ADP	N3-C2-N1	-3.31	123.50	128.68
4	A	301	ADP	N3-C2-N1	-3.28	123.56	128.68
4	C	301	ADP	N3-C2-N1	-3.20	123.68	128.68
4	C	301	ADP	PA-O3A-PB	-3.09	122.21	132.83
4	D	301	ADP	PA-O3A-PB	-3.07	122.28	132.83
4	A	301	ADP	C4-C5-N7	-2.75	106.53	109.40
4	C	301	ADP	C4-C5-N7	-2.72	106.57	109.40
4	A	301	ADP	PA-O3A-PB	-2.67	123.68	132.83
4	D	301	ADP	C4-C5-N7	-2.60	106.69	109.40
4	B	301	ADP	C4-C5-N7	-2.56	106.73	109.40
4	D	301	ADP	C3'-C2'-C1'	2.36	104.53	100.98
4	B	301	ADP	C3'-C2'-C1'	2.10	104.14	100.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	ADP	C5'-O5'-PA-O1A
4	C	301	ADP	C5'-O5'-PA-O2A
4	D	301	ADP	C5'-O5'-PA-O1A
4	C	301	ADP	PA-O3A-PB-O1B
4	B	301	ADP	C5'-O5'-PA-O3A
4	C	301	ADP	C5'-O5'-PA-O3A

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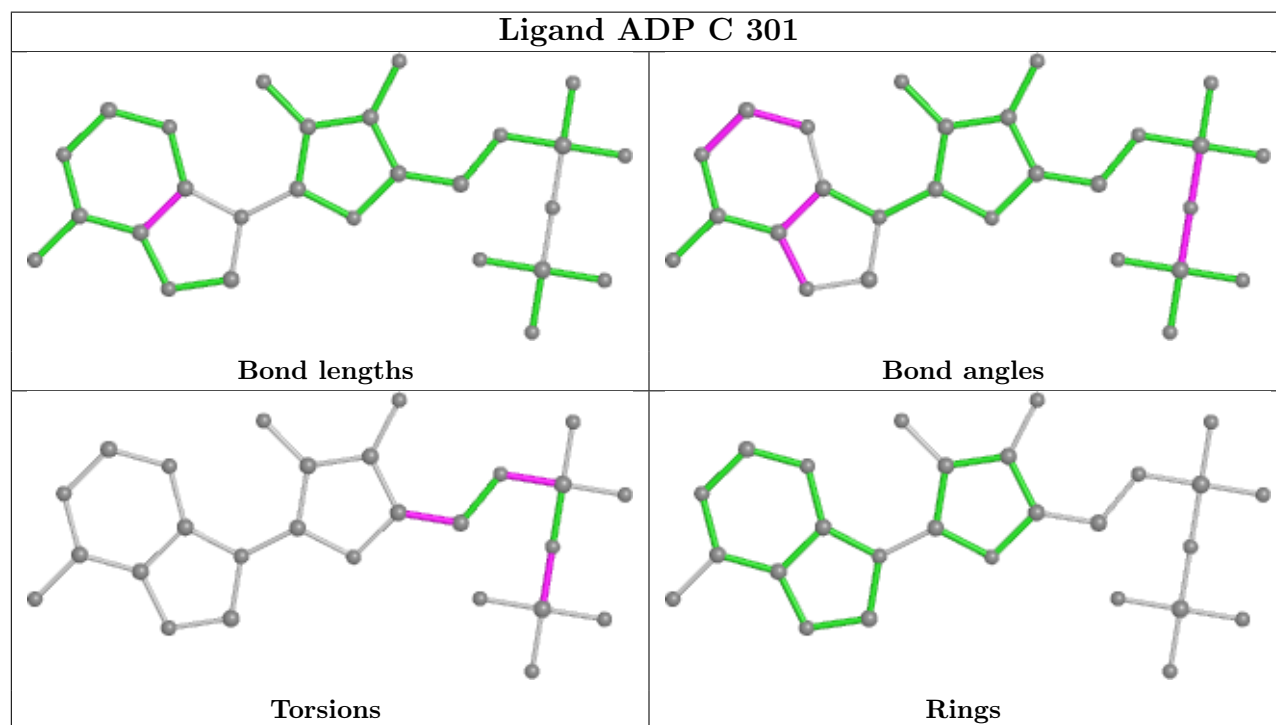
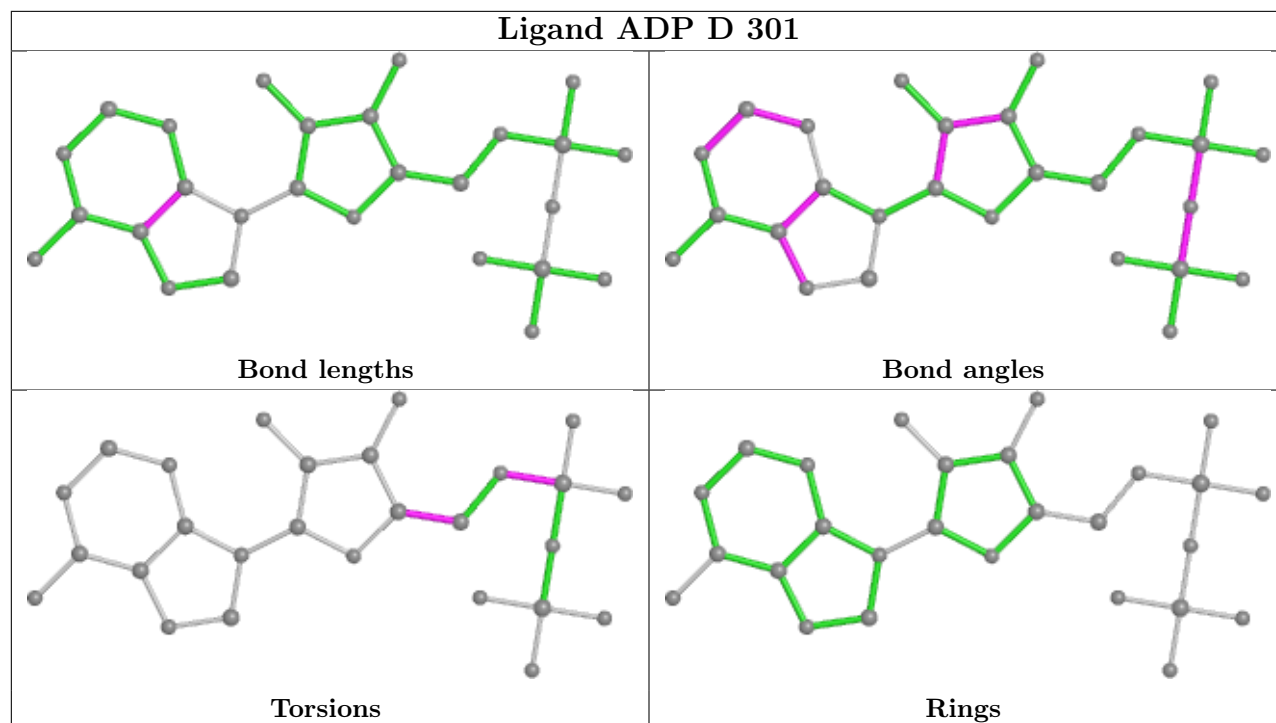
Mol	Chain	Res	Type	Atoms
4	D	301	ADP	C5'-O5'-PA-O3A
4	B	301	ADP	C5'-O5'-PA-O2A
4	C	301	ADP	C5'-O5'-PA-O1A
4	D	301	ADP	C5'-O5'-PA-O2A
4	C	301	ADP	O4'-C4'-C5'-O5'
4	D	301	ADP	O4'-C4'-C5'-O5'
4	B	301	ADP	PA-O3A-PB-O1B
4	A	301	ADP	PA-O3A-PB-O3B
4	C	301	ADP	C3'-C4'-C5'-O5'

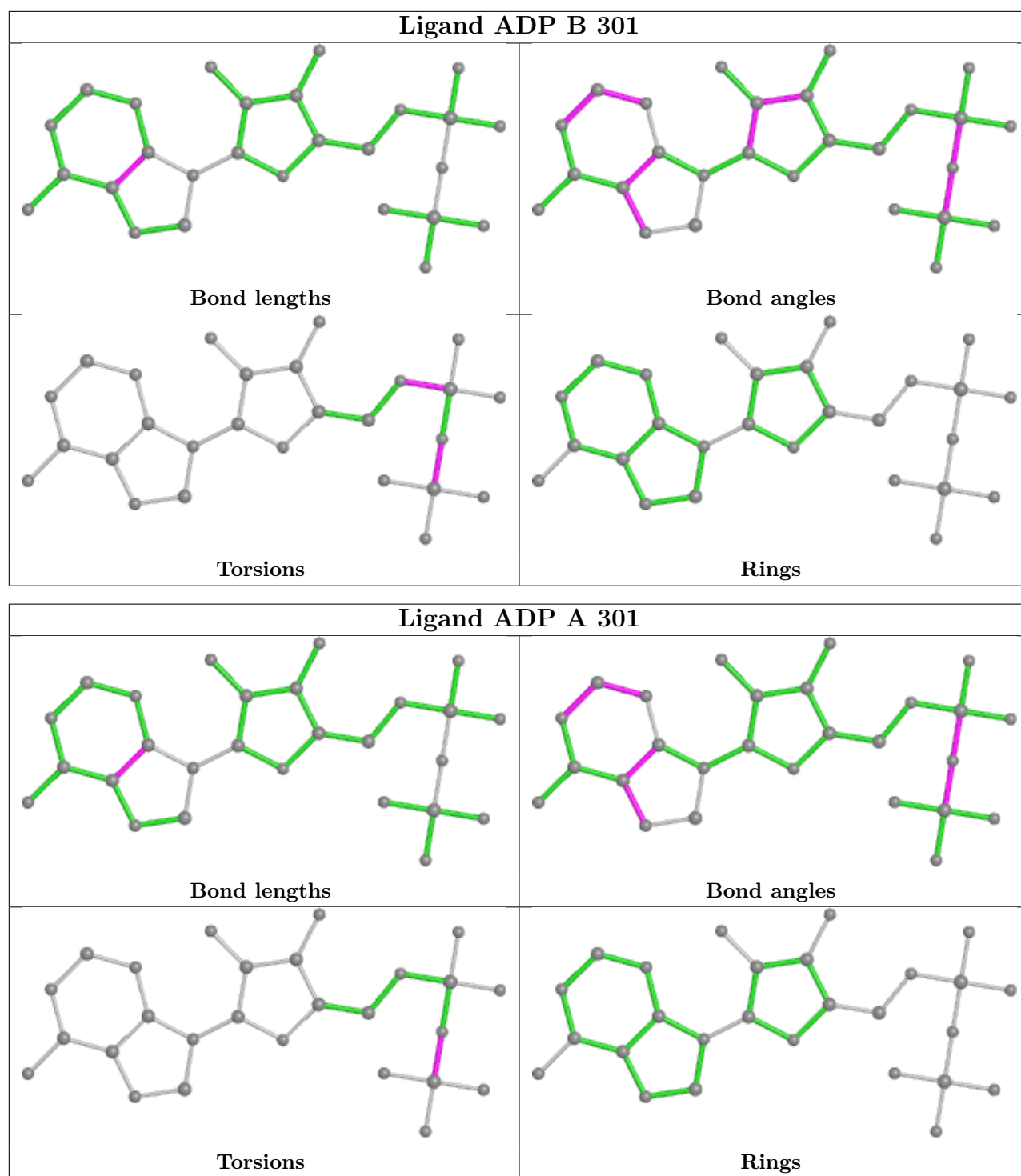
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	ADP	2	0
4	B	301	ADP	1	0
4	A	301	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	220/220 (100%)	-0.12	1 (0%) 91 88	25, 37, 63, 81	0
1	B	220/220 (100%)	-0.06	2 (0%) 84 80	25, 40, 67, 80	0
1	C	220/220 (100%)	-0.12	1 (0%) 91 88	24, 40, 63, 76	0
1	D	220/220 (100%)	-0.08	1 (0%) 91 88	24, 37, 62, 86	0
2	E	24/24 (100%)	2.14	13 (54%) 0 0	106, 128, 139, 140	0
2	G	24/24 (100%)	0.29	0 100 100	90, 116, 119, 121	0
3	F	24/24 (100%)	1.42	6 (25%) 0 0	79, 128, 134, 135	0
3	H	24/24 (100%)	0.78	3 (12%) 3 2	72, 118, 128, 130	0
All	All	976/976 (100%)	0.03	27 (2%) 53 43	24, 40, 120, 140	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	10	DC	4.8
2	E	10	DC	4.1
3	F	15	DG	4.0
2	E	15	DG	3.9
2	E	19	DC	3.7
2	E	16	DA	3.7
2	E	18	DA	3.6
2	E	17	DA	3.5
3	H	8	DT	3.5
2	E	5	DT	3.1
2	E	14	DT	2.7
2	E	9	DC	2.6
2	E	11	DA	2.6
1	C	171	VAL	2.5
1	A	204	LYS	2.5
2	E	1	DA	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	2	DC	2.3
3	F	20	DA	2.3
3	F	4	DC	2.3
3	H	13	DG	2.2
1	B	201	ARG	2.1
2	E	8	DT	2.1
2	E	24	DA	2.1
1	D	203	LYS	2.1
1	B	214	LEU	2.0
3	H	11	DA	2.0
3	F	1	DT	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](#)

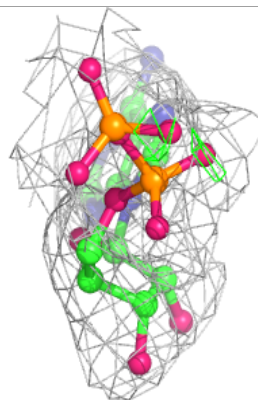
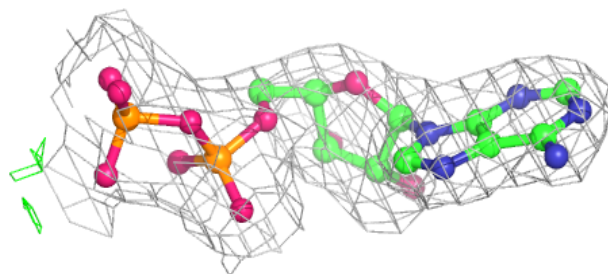
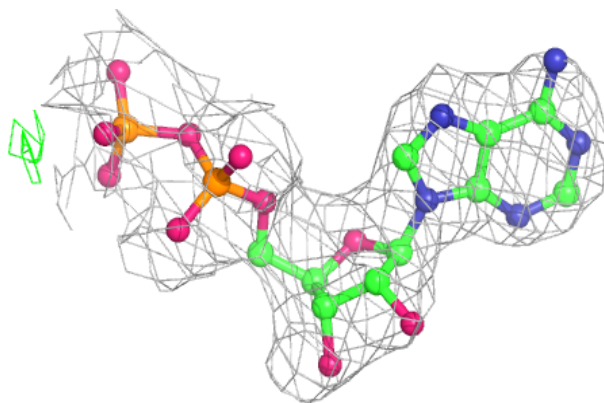
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	302	1/1	0.91	0.18	40,40,40,40	0
4	ADP	D	301	27/27	0.96	0.17	34,47,52,54	0
4	ADP	C	301	27/27	0.96	0.17	37,46,52,54	0
4	ADP	B	301	27/27	0.97	0.16	32,41,49,53	0
4	ADP	A	301	27/27	0.97	0.18	35,47,52,54	0
5	MG	B	302	1/1	0.97	0.16	28,28,28,28	0
5	MG	C	302	1/1	0.99	0.20	26,26,26,26	0
5	MG	D	302	1/1	0.99	0.21	32,32,32,32	0

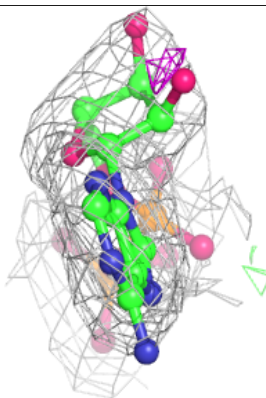
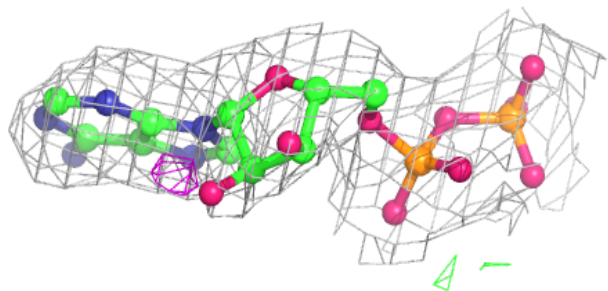
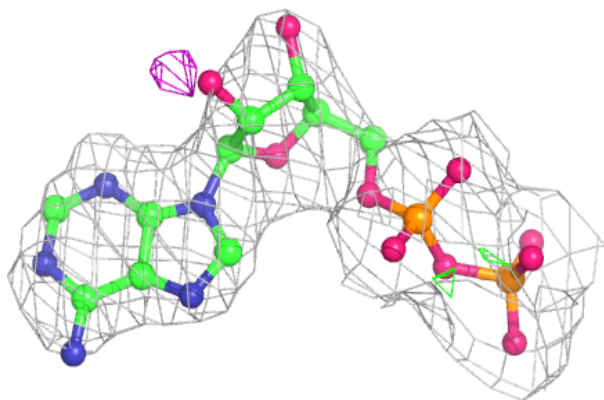
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP D 301:

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

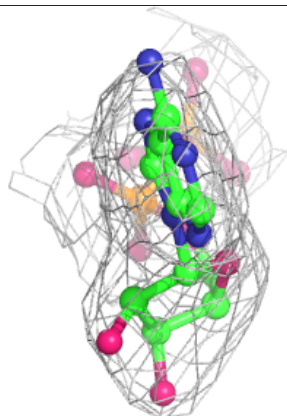
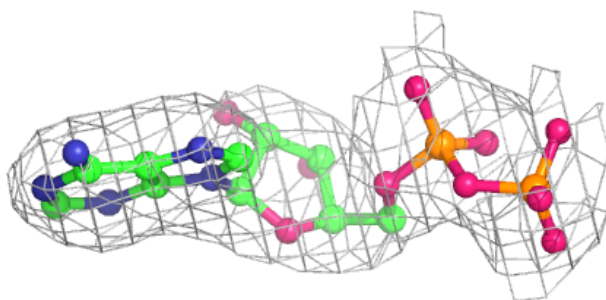
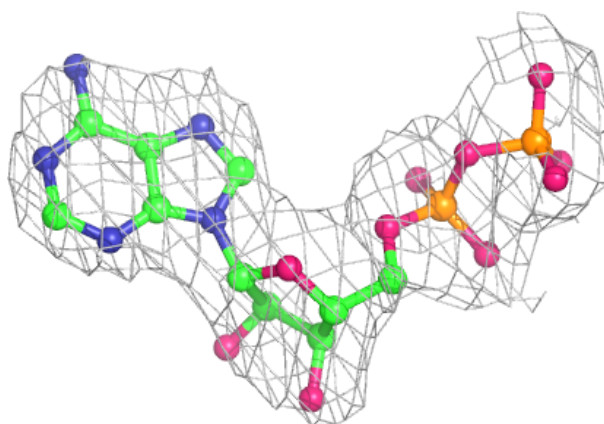
**Electron density around ADP C 301:**

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

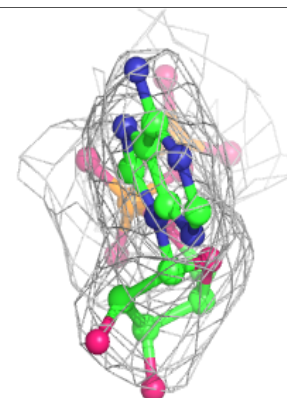
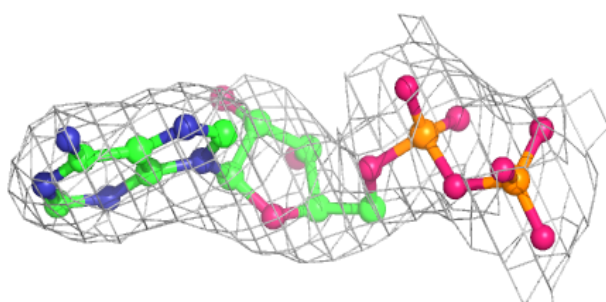
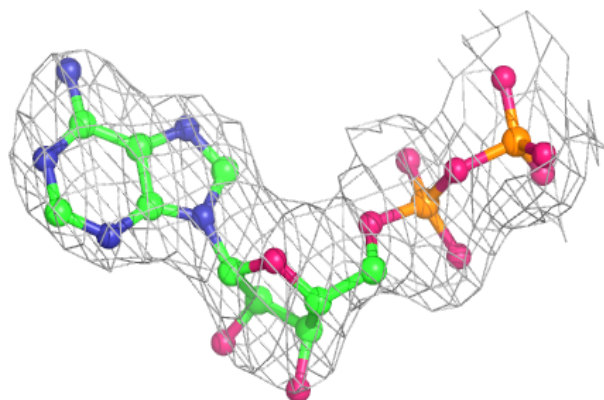


Electron density around ADP B 301:

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

**Electron density around ADP A 301:**

$2mF_o-DF_c$ (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.