



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 12:05 AM JST

PDB ID : 7V3W
Title : Crystal Structure of VpsR display novel dimeric architecture and c-di-GMP binding: mechanistic implications in oligomerization, ATPase activity and DNA binding.
Authors : Chakraborty, T.; Sen, U.; Chowdhury, S.R.
Deposited on : 2021-08-11
Resolution : 3.21 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 : 2.27
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) : 2.27

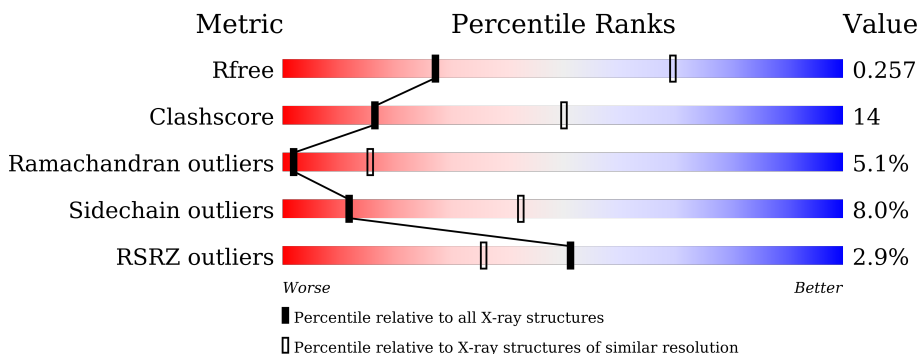
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	399	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>30%</div> <div>6% • 6%</div> </div> </div>
1	D	399	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>5% • 6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5944 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 VpsR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2936	1863	510	551	12			
1	D	376	Total	C	N	O	S	0	0	0
			2946	1869	512	553	12			

There are 34 discrepancies between the modelled and reference sequences:

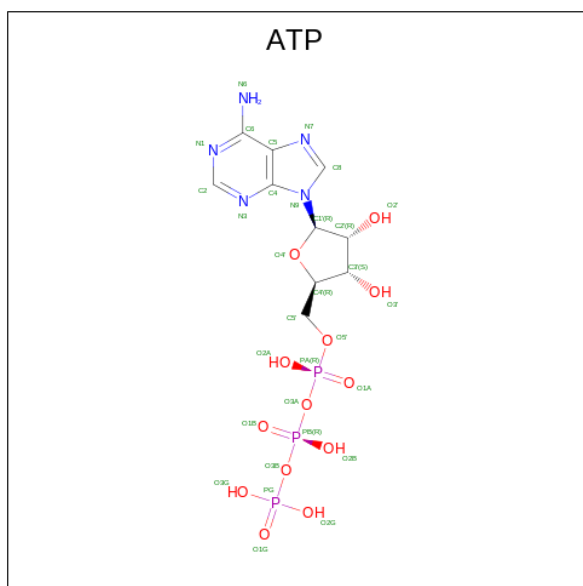
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q9AAQ41
A	-15	HIS	-	expression tag	UNP Q9AAQ41
A	-14	HIS	-	expression tag	UNP Q9AAQ41
A	-13	HIS	-	expression tag	UNP Q9AAQ41
A	-12	HIS	-	expression tag	UNP Q9AAQ41
A	-11	HIS	-	expression tag	UNP Q9AAQ41
A	-10	SER	-	expression tag	UNP Q9AAQ41
A	-9	SER	-	expression tag	UNP Q9AAQ41
A	-8	GLY	-	expression tag	UNP Q9AAQ41
A	-7	LEU	-	expression tag	UNP Q9AAQ41
A	-6	VAL	-	expression tag	UNP Q9AAQ41
A	-5	PRO	-	expression tag	UNP Q9AAQ41
A	-4	ARG	-	expression tag	UNP Q9AAQ41
A	-3	GLY	-	expression tag	UNP Q9AAQ41
A	-2	SER	-	expression tag	UNP Q9AAQ41
A	-1	HIS	-	expression tag	UNP Q9AAQ41
A	0	MET	-	expression tag	UNP Q9AAQ41
D	-16	HIS	-	expression tag	UNP Q9AAQ41
D	-15	HIS	-	expression tag	UNP Q9AAQ41
D	-14	HIS	-	expression tag	UNP Q9AAQ41
D	-13	HIS	-	expression tag	UNP Q9AAQ41
D	-12	HIS	-	expression tag	UNP Q9AAQ41
D	-11	HIS	-	expression tag	UNP Q9AAQ41
D	-10	SER	-	expression tag	UNP Q9AAQ41
D	-9	SER	-	expression tag	UNP Q9AAQ41

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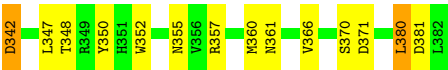
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP Q9AQ41
D	-7	LEU	-	expression tag	UNP Q9AQ41
D	-6	VAL	-	expression tag	UNP Q9AQ41
D	-5	PRO	-	expression tag	UNP Q9AQ41
D	-4	ARG	-	expression tag	UNP Q9AQ41
D	-3	GLY	-	expression tag	UNP Q9AQ41
D	-2	SER	-	expression tag	UNP Q9AQ41
D	-1	HIS	-	expression tag	UNP Q9AQ41
D	0	MET	-	expression tag	UNP Q9AQ41

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	118.79Å 118.79Å 79.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.51 – 3.21 47.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.51-3.21) 97.6 (47.51-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.273 0.221 , 0.257	Depositor DCC
R_{free} test set	977 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	147.3	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 172.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.127 for -h,-k,l 0.499 for h,-h-k,-l 0.127 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5944	wwPDB-VP
Average B, all atoms (Å ²)	181.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: ATP

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	0.22	0/2990	0.46	2/4047 (0.0%)
1	D	0.24	0/3000	0.50	1/4061 (0.0%)
All	All	0.23	0/5990	0.48	3/8108 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	LEU	CA-CB-CG	7.08	131.57	115.30
1	A	14	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	91	LEU	CA-CB-CG	5.19	127.24	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	2936	0	2967	92	0
1	D	2946	0	2971	92	0
2	A	31	0	11	2	0
2	D	31	0	11	2	0
All	All	5944	0	5960	170	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 14.

All (170) 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:145:GLY:O	1:D:147:ILE:N	2.17	0.77
1:D:203:CYS:SG	1:D:204:ARG:N	2.60	0.75
1:D:160:ILE:HG23	1:D:187:ILE:HG22	1.70	0.74
1:A:288:ILE:HD12	1:D:306:ASN:HB3	1.71	0.71
1:A:42:ARG:HB3	1:D:258:GLN:HB3	1.71	0.70
1:D:87:ARG:NH1	1:D:109:THR:O	2.25	0.69
1:A:22:GLU:O	1:A:24:TRP:N	2.25	0.69
1:D:203:CYS:O	1:D:205:ALA:N	2.26	0.67
1:D:240:ASN:HD21	2:D:501:ATP:PG	2.16	0.67
1:D:87:ARG:HA	1:D:108:PHE:HB2	1.78	0.65
1:D:71:ALA:HB2	1:D:99:PHE:HE1	1.61	0.65
1:D:60:LEU:O	1:D:62:HIS:N	2.30	0.64
1:D:200:SER:HA	1:D:238:LEU:HB3	1.80	0.64
1:D:38:VAL:HG21	1:D:44:PRO:HB3	1.80	0.63
1:D:87:ARG:NH2	1:D:110:ALA:O	2.32	0.63
1:A:101:VAL:HA	1:D:80:VAL:HG21	1.80	0.62
1:D:22:GLU:O	1:D:24:TRP:N	2.32	0.62
1:A:61:SER:OG	1:A:63:ASP:OD1	2.17	0.61
1:D:287:LEU:HD23	1:D:292:PHE:HB3	1.83	0.61
1:A:341:ASP:OD1	1:A:341:ASP:N	2.24	0.61
1:D:222:GLU:OE2	1:D:266:GLN:NE2	2.28	0.61
1:A:199:ILE:HD12	1:A:232:ALA:HB2	1.84	0.59
1:A:89:ALA:O	1:A:91:LEU:N	2.35	0.59
1:D:212:GLU:HG2	1:D:216:PHE:HE1	1.68	0.59
1:D:175:GLU:O	1:D:180:LYS:NZ	2.35	0.59
1:D:310:LEU:HB3	1:D:317:ILE:HD11	1.85	0.59
1:A:101:VAL:HG23	1:D:80:VAL:HG11	1.84	0.58
1:D:93:SER:N	1:D:97:CYS:SG	2.77	0.57
1:D:105:ILE:HG13	1:D:106:ASP:N	2.18	0.57
1:A:138:PHE:O	1:A:157:ARG:NH1	2.37	0.57
1:A:104:CYS:O	1:A:106:ASP:N	2.37	0.57
1:A:44:PRO:O	1:A:48:PHE:N	2.34	0.57
1:A:240:ASN:HA	1:A:278:ALA:HB3	1.86	0.57
1:D:44:PRO:HA	1:D:47:LEU:HB3	1.85	0.56
1:A:22:GLU:O	1:A:25:LEU:N	2.22	0.56
1:A:137:HIS:O	1:A:139:GLY:N	2.37	0.56
1:D:283:ILE:HD12	1:D:283:ILE:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	2:A:501:ATP:O2A	2.38	0.56
1:A:44:PRO:HA	1:A:47:LEU:HB3	1.87	0.56
1:A:193:ARG:NH1	1:A:235:GLY:O	2.35	0.56
1:A:188:HIS:NE2	1:A:193:ARG:O	2.39	0.55
1:D:347:LEU:HD21	1:D:380:LEU:HG	1.88	0.55
1:D:22:GLU:N	1:D:23:PRO:HD2	2.21	0.55
1:A:145:GLY:O	1:A:147:ILE:N	2.32	0.55
1:A:264:THR:OG1	1:A:267:GLY:O	2.21	0.55
1:A:40:ASP:H	1:A:43:LYS:HD2	1.72	0.55
1:A:106:ASP:HA	1:D:127:MET:HE1	1.87	0.55
1:A:335:GLN:HE21	1:A:371:ASP:HA	1.72	0.54
1:D:212:GLU:HG2	1:D:216:PHE:CE1	2.42	0.54
1:A:100:ILE:HG23	1:A:104:CYS:HB2	1.89	0.54
1:D:191:SER:O	1:D:192:SER:OG	2.20	0.54
1:D:199:ILE:HD12	1:D:232:ALA:HB2	1.90	0.53
1:D:104:CYS:O	1:D:106:ASP:N	2.37	0.53
1:A:49:VAL:HB	1:A:78:LYS:HE3	1.90	0.53
1:A:22:GLU:N	1:A:23:PRO:HD2	2.24	0.52
1:D:11:PRO:HA	1:D:34:ARG:HB2	1.91	0.52
1:A:133:LYS:HZ2	1:D:98:GLN:HB2	1.74	0.52
1:D:188:HIS:CD2	1:D:198:PHE:HB2	2.44	0.52
1:D:240:ASN:ND2	2:D:501:ATP:O1G	2.43	0.52
1:A:120:THR:HA	1:D:123:HIS:CD2	2.45	0.52
1:D:308:PRO:HG2	1:D:313:ARG:HD2	1.92	0.51
1:D:360:MET:HG3	1:D:361:ASN:N	2.25	0.51
1:A:199:ILE:HG21	1:A:228:PHE:HD2	1.76	0.50
1:D:99:PHE:O	1:D:102:ASN:ND2	2.36	0.50
1:D:61:SER:O	1:D:63:ASP:N	2.44	0.50
1:A:135:TRP:O	1:A:137:HIS:N	2.44	0.50
1:D:230:LEU:HA	1:D:271:VAL:HG11	1.93	0.50
1:A:102:ASN:O	1:A:104:CYS:N	2.45	0.50
1:D:28:LEU:HA	1:D:31:VAL:HG12	1.93	0.49
1:D:342:ASP:N	1:D:342:ASP:OD1	2.45	0.49
1:A:127:MET:HE1	1:D:106:ASP:HA	1.95	0.49
1:A:213:SER:HA	1:A:217:GLY:HA2	1.94	0.49
1:A:87:ARG:HA	1:A:108:PHE:HB2	1.95	0.49
1:A:221:THR:HG21	1:A:225:GLN:HG2	1.95	0.49
1:D:243:LEU:H	1:D:243:LEU:HD23	1.78	0.48
1:D:308:PRO:O	1:D:313:ARG:NH2	2.39	0.48
1:A:90:GLN:O	1:A:92:SER:N	2.47	0.47
1:A:193:ARG:NH2	1:A:272:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:VAL:HG13	1:D:82:TRP:HZ3	1.79	0.47
1:A:326:GLN:HE21	1:A:330:LYS:HD3	1.79	0.47
1:A:53:PRO:HA	1:A:81:ARG:O	2.13	0.47
1:A:160:ILE:HG23	1:A:187:ILE:HG22	1.96	0.47
1:D:309:SER:HB2	1:D:355:ASN:ND2	2.29	0.47
1:D:113:PRO:HB2	1:D:116:GLN:HB3	1.96	0.47
1:D:58:VAL:O	1:D:87:ARG:N	2.42	0.47
1:D:113:PRO:O	1:D:117:LEU:N	2.42	0.47
1:D:142:GLY:O	1:D:144:MET:N	2.47	0.47
1:A:301:ASN:O	1:A:301:ASN:ND2	2.48	0.47
1:D:165:PRO:HD3	1:D:190:THR:HG22	1.96	0.47
1:D:105:ILE:HG13	1:D:106:ASP:H	1.80	0.46
1:A:40:ASP:O	1:A:42:ARG:N	2.43	0.46
1:D:86:ILE:HD12	1:D:100:ILE:HD12	1.96	0.46
1:A:257:LEU:HD13	1:A:299:TYR:HB3	1.96	0.46
1:A:174:GLY:O	1:A:280:SER:HA	2.16	0.46
1:D:156:LEU:HD12	1:D:305:ILE:HD11	1.98	0.46
1:D:173:TYR:CZ	1:D:306:ASN:HB2	2.50	0.46
1:D:380:LEU:HB3	1:D:381:ASP:H	1.50	0.46
1:A:225:GLN:OE1	1:A:226:GLN:N	2.49	0.46
1:A:227:PRO:HG3	1:A:264:THR:HG22	1.98	0.46
1:A:72:ASN:O	1:A:76:SER:N	2.49	0.46
1:A:133:LYS:NZ	1:D:94:ASP:O	2.49	0.46
1:D:48:PHE:HA	1:D:51:THR:HG22	1.97	0.46
1:A:146:LEU:HG	1:A:186:ALA:HB2	1.98	0.45
2:A:501:ATP:H8	2:A:501:ATP:H2'	1.63	0.45
1:D:329:SER:HA	1:D:334:ALA:HB3	1.98	0.45
1:A:173:TYR:HB3	1:A:304:ARG:HH12	1.81	0.45
1:A:212:GLU:HA	1:A:215:LEU:HD12	1.97	0.45
1:D:88:GLU:N	1:D:88:GLU:OE1	2.49	0.45
1:D:233:ASP:OD1	1:D:272:ASP:N	2.43	0.45
1:A:335:GLN:NE2	1:A:370:SER:O	2.50	0.45
1:D:301:ASN:O	1:D:301:ASN:ND2	2.50	0.45
1:A:49:VAL:HA	1:A:81:ARG:NH1	2.32	0.45
1:A:105:ILE:HD12	1:D:105:ILE:HG22	1.98	0.45
1:A:335:GLN:OE1	1:A:335:GLN:N	2.45	0.45
1:A:233:ASP:HA	1:A:273:VAL:HG22	1.98	0.45
1:D:293:ASN:HD21	1:D:295:GLU:HB3	1.82	0.45
1:A:239:LEU:O	1:A:278:ALA:N	2.39	0.45
1:A:150:SER:OG	1:A:151:MET:N	2.49	0.44
1:A:84:ALA:HB3	1:A:104:CYS:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD22	1:A:229:LEU:H	1.83	0.44
1:D:131:GLU:O	1:D:135:TRP:HB2	2.18	0.44
1:D:317:ILE:HG21	1:D:348:THR:HA	1.99	0.44
1:A:335:GLN:H	1:A:335:GLN:CD	2.18	0.44
1:D:112:ILE:O	1:D:114:ASP:N	2.51	0.44
1:A:284:GLU:OE1	1:D:159:GLN:NE2	2.50	0.44
1:A:30:LYS:HA	1:A:30:LYS:HD2	1.81	0.43
1:D:135:TRP:N	1:D:136:PRO:HD2	2.33	0.43
1:D:350:TYR:HB3	1:D:352:TRP:CE2	2.53	0.43
1:A:261:THR:HG22	1:A:270:ALA:HB2	2.00	0.43
1:A:215:LEU:HB2	1:A:216:PHE:H	1.62	0.43
1:A:158:ASP:HB3	1:A:162:ARG:HH12	1.83	0.43
1:D:151:MET:HB3	1:D:152:PRO:HD3	2.01	0.43
1:D:366:VAL:O	1:D:370:SER:N	2.49	0.43
1:A:88:GLU:N	1:A:88:GLU:OE2	2.51	0.43
1:A:120:THR:HG22	1:D:123:HIS:CG	2.53	0.43
1:A:128:LEU:HD22	1:A:128:LEU:HA	1.82	0.43
1:A:165:PRO:HB2	1:D:98:GLN:HG2	2.00	0.43
1:A:183:VAL:O	1:A:187:ILE:HG23	2.18	0.43
1:A:26:PRO:HA	1:A:29:GLU:HB2	1.99	0.43
1:A:20:THR:C	1:A:22:GLU:H	2.21	0.43
1:D:264:THR:OG1	1:D:267:GLY:O	2.31	0.43
1:D:143:ASN:O	1:D:145:GLY:N	2.52	0.42
1:A:123:HIS:HB3	1:D:106:ASP:OD2	2.19	0.42
1:D:83:LEU:HD13	1:D:124:GLN:HG3	2.02	0.42
1:D:245:LEU:O	1:D:250:GLN:NE2	2.52	0.42
1:A:166:THR:O	1:A:166:THR:OG1	2.38	0.42
1:D:40:ASP:O	1:D:42:ARG:N	2.42	0.42
1:D:103:PHE:C	1:D:105:ILE:H	2.23	0.42
1:A:188:HIS:O	1:A:191:SER:OG	2.28	0.42
1:A:223:GLU:HB2	1:A:224:GLY:H	1.68	0.42
1:A:140:SER:HA	1:A:157:ARG:NH2	2.35	0.41
1:D:219:GLY:O	1:D:221:THR:N	2.53	0.41
1:D:283:ILE:HD12	1:D:283:ILE:N	2.34	0.41
1:D:76:SER:O	1:D:77:HIS:HD2	2.04	0.41
1:A:82:TRP:CZ2	1:A:84:ALA:HA	2.55	0.41
1:A:124:GLN:NE2	1:D:105:ILE:O	2.53	0.41
1:A:113:PRO:HB2	1:A:116:GLN:HB3	2.02	0.41
1:A:263:GLU:HA	1:A:268:VAL:HG12	2.03	0.41
1:A:193:ARG:NH1	1:A:274:ARG:H	2.19	0.41
1:A:251:LEU:O	1:A:255:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:O	1:A:365:ARG:HG3	2.21	0.41
1:D:47:LEU:O	1:D:50:GLU:HG3	2.19	0.41
1:A:28:LEU:HB3	1:A:33:TRP:HE3	1.86	0.41
1:A:74:VAL:HG21	1:A:99:PHE:CZ	2.56	0.41
1:A:94:ASP:HB3	1:A:95:THR:H	1.76	0.41
1:A:213:SER:HA	1:A:218:LEU:N	2.35	0.40
1:A:350:TYR:HB3	1:A:352:TRP:CE2	2.56	0.40
1:D:99:PHE:C	1:D:101:VAL:H	2.24	0.40
1:D:74:VAL:HG13	1:D:82:TRP:CZ3	2.57	0.40
1:A:136:PRO:O	1:A:138:PHE:N	2.44	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	372/399 (93%)	300 (81%)	53 (14%)	19 (5%)	2	15
1	D	374/399 (94%)	302 (81%)	53 (14%)	19 (5%)	2	15
All	All	746/798 (94%)	602 (81%)	106 (14%)	38 (5%)	2	15

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	23	PRO
1	A	61	SER
1	A	136	PRO
1	A	146	LEU
1	D	23	PRO
1	D	61	SER
1	D	140	SER

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Mol	Chain	Res	Type
1	D	144	MET
1	D	146	LEU
1	D	147	ILE
1	D	204	ARG
1	D	220	GLU
1	A	76	SER
1	A	91	LEU
1	A	92	SER
1	A	93	SER
1	A	103	PHE
1	A	220	GLU
1	D	62	HIS
1	D	137	HIS
1	D	145	GLY
1	A	94	ASP
1	A	138	PHE
1	D	76	SER
1	D	93	SER
1	D	103	PHE
1	A	40	ASP
1	D	40	ASP
1	D	203	CYS
1	D	111	PRO
1	A	90	GLN
1	A	114	ASP
1	D	167	ASP
1	A	135	TRP
1	A	18	GLY
1	A	147	ILE
1	D	105	ILE

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	325/348 (93%)	303 (93%)	22 (7%)	16 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	325/348 (93%)	295 (91%)	30 (9%)	9	33
All	All	650/696 (93%)	598 (92%)	52 (8%)	12	42

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	22	GLU
1	A	38	VAL
1	A	43	LYS
1	A	77	HIS
1	A	86	ILE
1	A	91	LEU
1	A	128	LEU
1	A	130	LEU
1	A	135	TRP
1	A	149	GLU
1	A	215	LEU
1	A	218	LEU
1	A	220	GLU
1	A	222	GLU
1	A	223	GLU
1	A	225	GLN
1	A	226	GLN
1	A	243	LEU
1	A	262	VAL
1	A	318	VAL
1	A	341	ASP
1	D	24	TRP
1	D	35	CYS
1	D	38	VAL
1	D	40	ASP
1	D	41	LEU
1	D	62	HIS
1	D	79	GLN
1	D	86	ILE
1	D	90	GLN
1	D	95	THR
1	D	105	ILE
1	D	117	LEU
1	D	118	LEU
1	D	128	LEU

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Mol	Chain	Res	Type
1	D	135	TRP
1	D	147	ILE
1	D	204	ARG
1	D	223	GLU
1	D	240	ASN
1	D	243	LEU
1	D	245	LEU
1	D	247	LYS
1	D	253	LEU
1	D	283	ILE
1	D	318	VAL
1	D	333	ASN
1	D	342	ASP
1	D	357	ARG
1	D	371	ASP
1	D	380	LEU

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	77	HIS
1	A	90	GLN
1	A	226	GLN
1	A	249	GLN
1	A	266	GLN
1	A	326	GLN
1	A	361	ASN
1	A	362	GLN
1	A	379	GLN
1	D	77	HIS
1	D	79	GLN
1	D	98	GLN
1	D	226	GLN
1	D	240	ASN
1	D	293	ASN
1	D	355	ASN
1	D	362	GLN
1	D	379	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ATP	D	501	-	26,33,33	4.77	9 (34%)	31,52,52	2.80	7 (22%)
2	ATP	A	501	-	26,33,33	4.75	9 (34%)	31,52,52	2.83	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	501	-	-	8/18/38/38	0/3/3/3
2	ATP	A	501	-	-	2/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ATP	C2'-C1'	-15.64	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ATP	O4'-C1'	15.52	1.62	1.41
2	A	501	ATP	O4'-C1'	15.50	1.62	1.41
2	A	501	ATP	C2'-C1'	-15.47	1.30	1.53
2	A	501	ATP	O4'-C4'	-6.55	1.30	1.45
2	D	501	ATP	O4'-C4'	-6.53	1.30	1.45
2	A	501	ATP	C2-N1	3.58	1.40	1.33
2	D	501	ATP	C2-N1	3.52	1.40	1.33
2	A	501	ATP	C6-N6	3.39	1.46	1.34
2	D	501	ATP	C6-N6	3.38	1.46	1.34
2	A	501	ATP	O2'-C2'	3.14	1.50	1.43
2	D	501	ATP	O2'-C2'	3.08	1.50	1.43
2	D	501	ATP	O3'-C3'	-2.79	1.36	1.43
2	A	501	ATP	O3'-C3'	-2.74	1.36	1.43
2	D	501	ATP	C5'-C4'	2.49	1.59	1.51
2	A	501	ATP	C5'-C4'	2.42	1.59	1.51
2	A	501	ATP	C5-C4	-2.17	1.35	1.40
2	D	501	ATP	C5-C4	-2.15	1.35	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	ATP	C5-C6-N6	10.61	136.47	120.35
2	A	501	ATP	C5-C6-N6	10.53	136.35	120.35
2	D	501	ATP	N6-C6-N1	-7.20	103.62	118.57
2	A	501	ATP	N6-C6-N1	-7.11	103.82	118.57
2	A	501	ATP	N3-C2-N1	-5.59	119.95	128.68
2	D	501	ATP	N3-C2-N1	-5.53	120.04	128.68
2	A	501	ATP	C3'-C2'-C1'	4.32	107.48	100.98
2	D	501	ATP	PA-O3A-PB	-3.68	120.19	132.83
2	A	501	ATP	PA-O3A-PB	-3.23	121.75	132.83
2	D	501	ATP	C3'-C2'-C1'	3.06	105.58	100.98
2	A	501	ATP	PB-O3B-PG	-2.39	124.62	132.83
2	D	501	ATP	PB-O3B-PG	-2.38	124.65	132.83
2	D	501	ATP	O3G-PG-O3B	2.29	112.31	104.64
2	A	501	ATP	C2'-C3'-C4'	2.03	106.59	102.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	ATP	PB-O3B-PG-O3G
2	D	501	ATP	C3'-C4'-C5'-O5'

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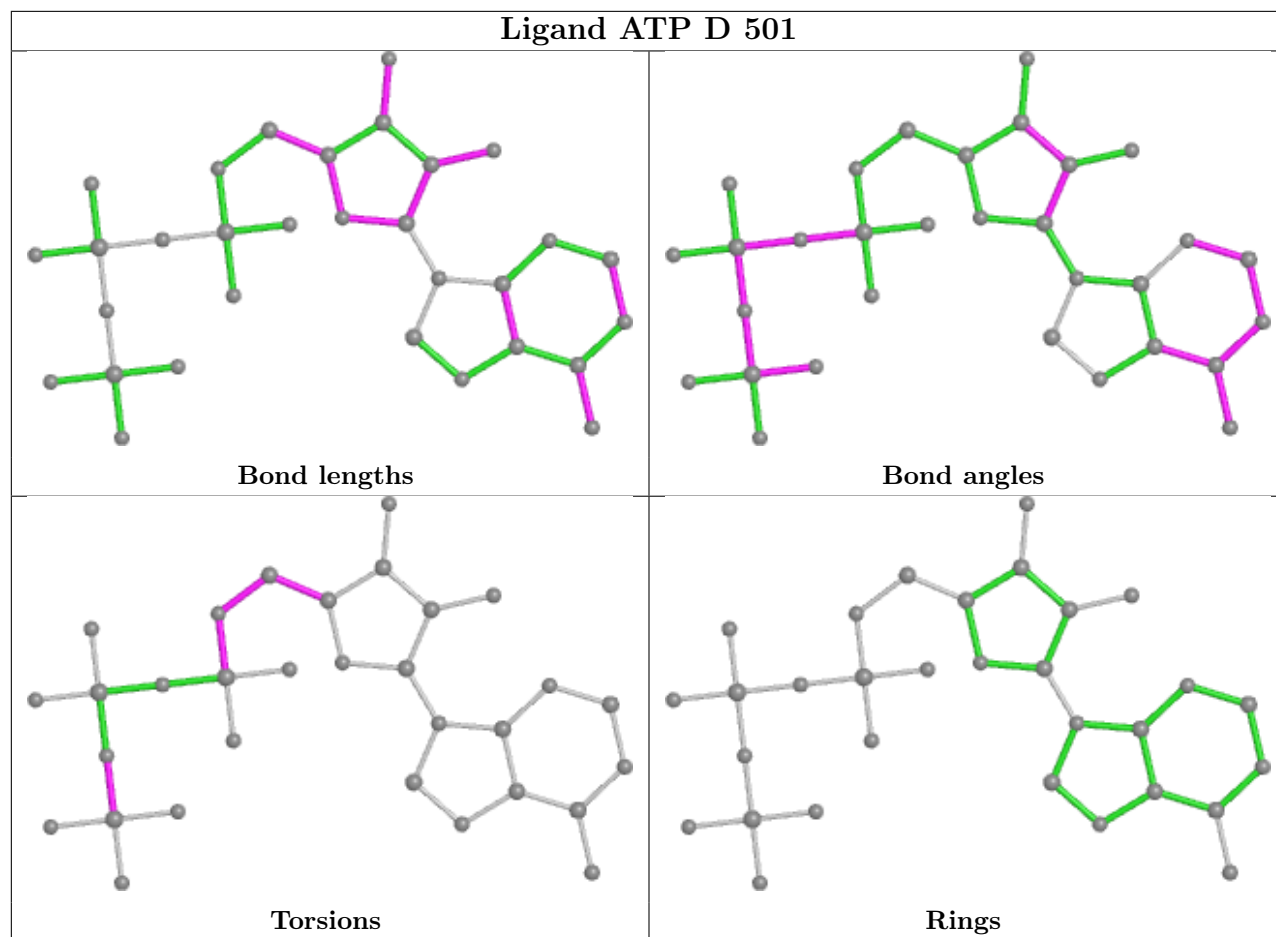
Mol	Chain	Res	Type	Atoms
2	D	501	ATP	O4'-C4'-C5'-O5'
2	D	501	ATP	C5'-O5'-PA-O3A
2	D	501	ATP	C5'-O5'-PA-O1A
2	A	501	ATP	O4'-C4'-C5'-O5'
2	D	501	ATP	C4'-C5'-O5'-PA
2	A	501	ATP	PA-O3A-PB-O3B
2	D	501	ATP	PB-O3B-PG-O2G
2	D	501	ATP	PB-O3B-PG-O1G

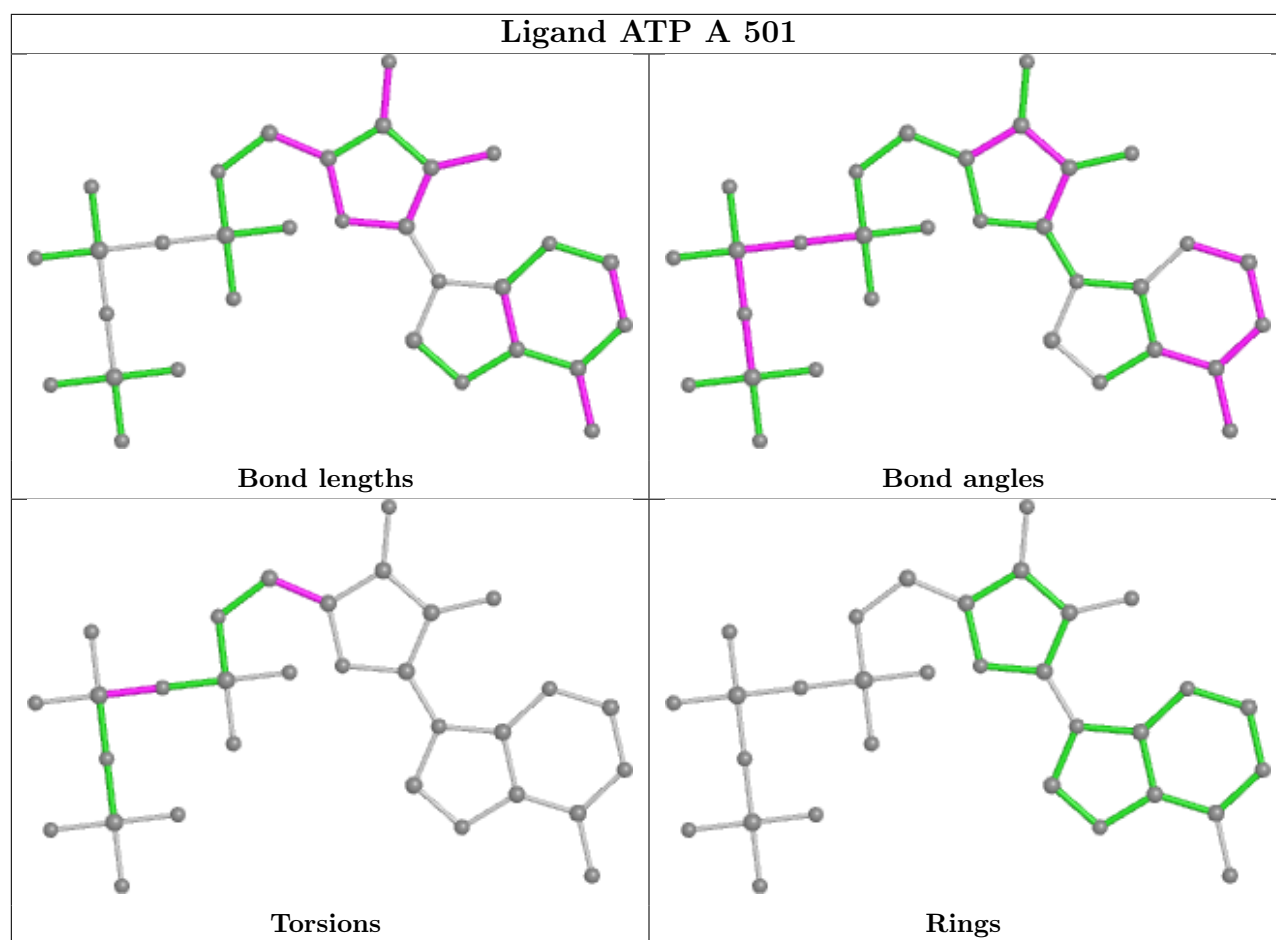
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	ATP	2	0
2	A	501	ATP	2	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, 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	374/399 (93%)	0.02	8 (2%) 63 49	121, 176, 220, 277	0
1	D	376/399 (94%)	0.05	14 (3%) 41 26	120, 180, 223, 287	0
All	All	750/798 (93%)	0.03	22 (2%) 51 36	120, 178, 223, 287	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	85	PHE	9.3
1	D	16	VAL	4.5
1	A	134	VAL	4.4
1	D	292	PHE	3.4
1	A	86	ILE	3.3
1	D	13	SER	2.9
1	D	242	ILE	2.8
1	D	103	PHE	2.7
1	D	14	LEU	2.6
1	D	86	ILE	2.5
1	A	324	PHE	2.5
1	D	276	LEU	2.5
1	A	309	SER	2.4
1	D	209	LYS	2.4
1	D	232	ALA	2.4
1	D	339	PHE	2.4
1	A	339	PHE	2.3
1	A	80	VAL	2.3
1	A	336	ALA	2.2
1	A	310	LEU	2.2
1	D	128	LEU	2.2
1	D	10	VAL	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](#)

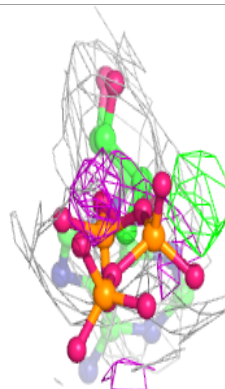
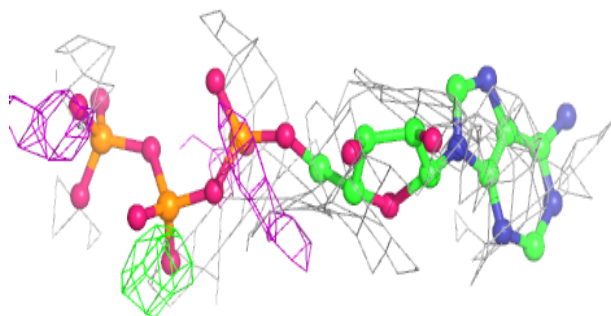
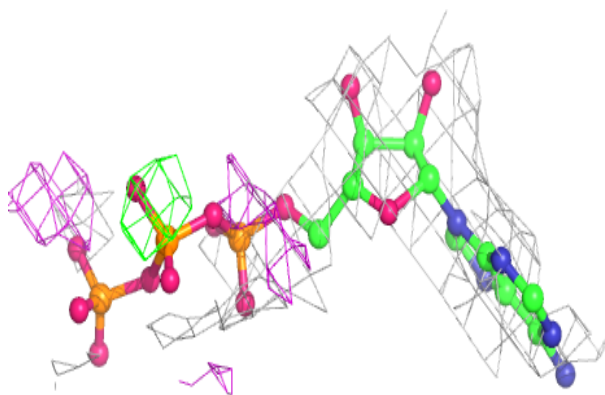
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	A	501	31/31	0.84	0.17	228,288,293,296	0
2	ATP	D	501	31/31	0.88	0.23	215,308,320,324	0

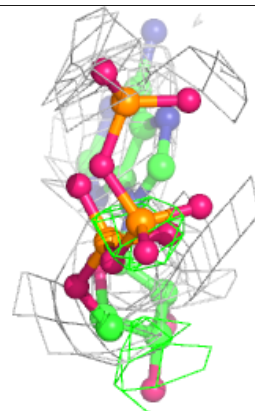
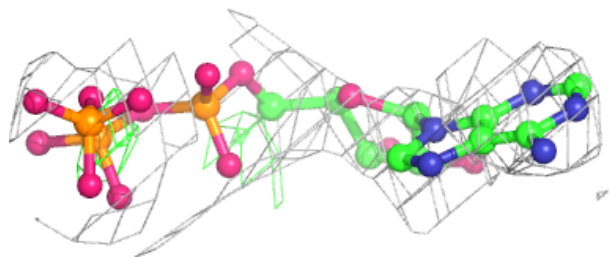
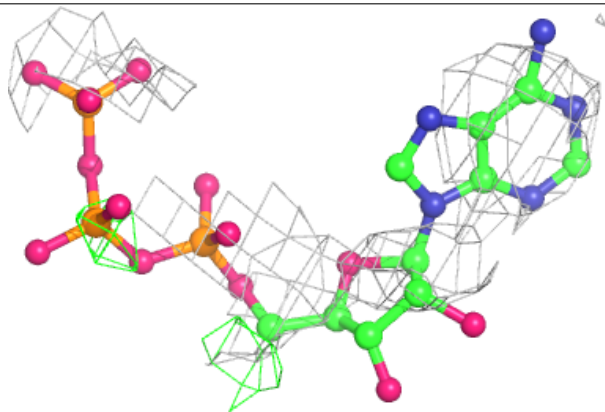
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 501:

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

**Electron density around ATP D 501:**

$2mF_o-DF_c$ (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.