



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:00 AM UTC

PDB ID : 9I0S / pdb\_00009i0s  
Title : Structure of RecQL-ADP complex from Bos taurus  
Authors : Song, Z.Y.; Liu, N.N.; Ai, X.; Rety, S.; Xi, X.G.  
Deposited on : 2025-01-15  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 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

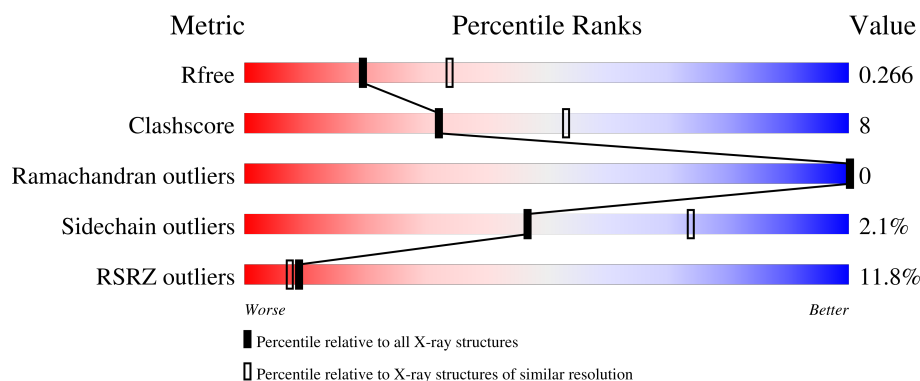
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	<div> <div>10%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	531	<div> <div>14%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8593 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 ATP-dependent DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	B	530	Total	C	N	O	S	0	1	0
			4231	2701	726	769	35			

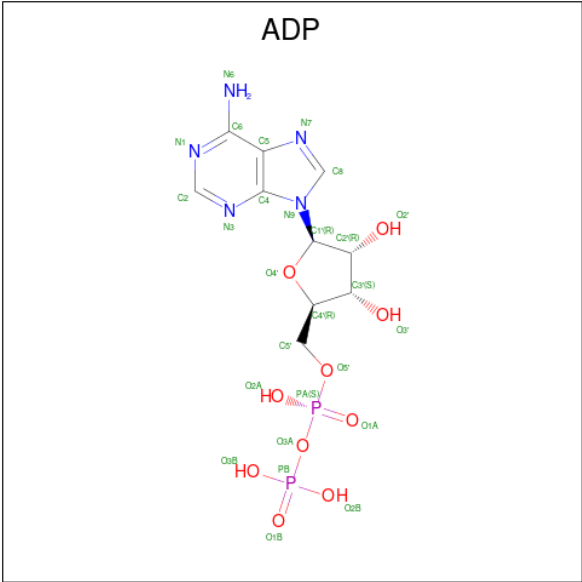
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	MET	-	initiating methionine	UNP A0JN36
B	62	MET	-	initiating methionine	UNP A0JN36

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

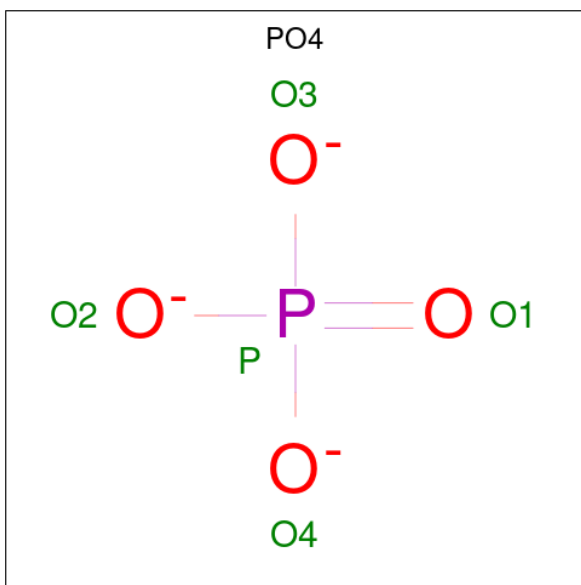


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

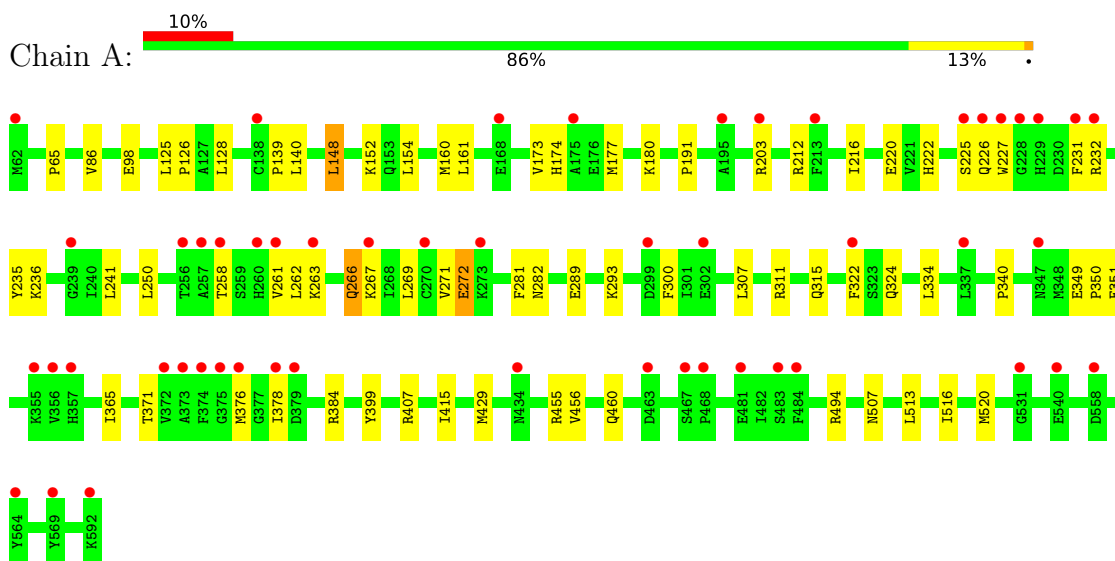
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	19	Total	O	0	0
			19	19		

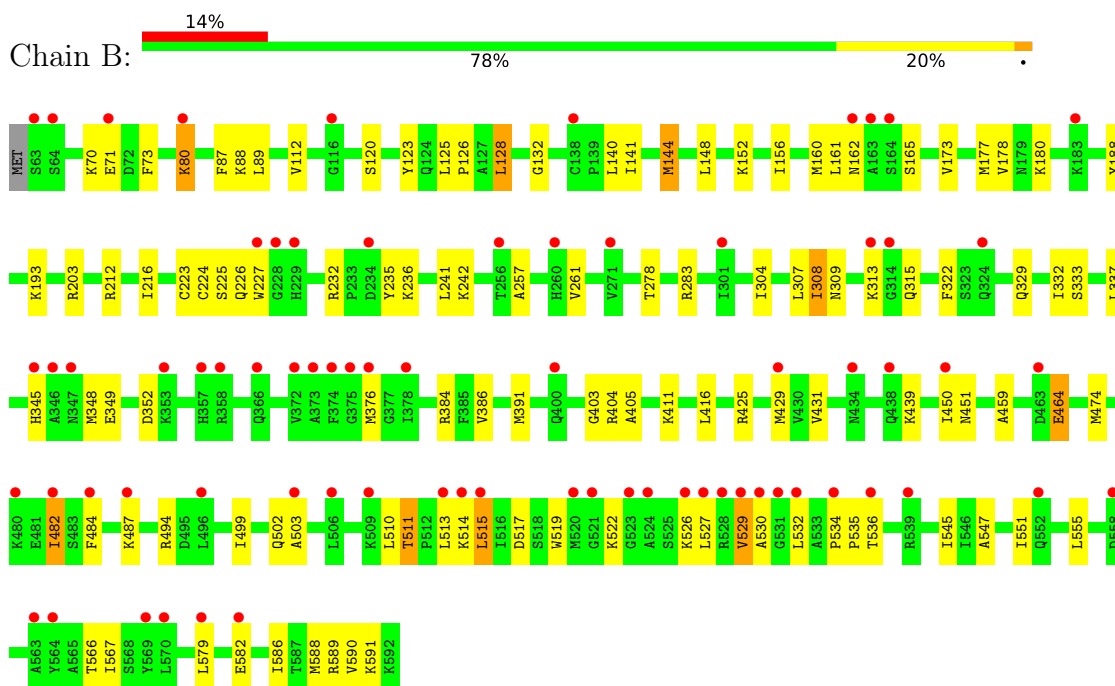
### 3 Residue-property plots [i](#)

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: ATP-dependent DNA helicase



#### • Molecule 1: ATP-dependent DNA helicase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.15Å 119.45Å 201.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.48 – 2.50 50.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.48-2.50) 100.0 (50.48-2.50)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.240 , 0.268 0.238 , 0.266	Depositor DCC
$R_{free}$ test set	2271 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ZN, ADP

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	0.14	0/4325	0.42	0/5830
1	B	0.17	0/4325	0.44	0/5830
All	All	0.15	0/8650	0.43	0/11660

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	GLU	Peptide
1	B	515	LEU	Peptide

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4237	0	4295	46	0
1	B	4231	0	4289	94	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
6	A	43	0	0	1	0
6	B	19	0	0	1	0
All	All	8593	0	8608	137	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (137) 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:B:322:PHE:HZ	1:B:429:MET:HG3	1.37	0.90
1:A:226:GLN:OE1	1:A:236:LYS:NZ	2.16	0.79
1:A:226:GLN:HB2	1:B:226:GLN:HB2	1.66	0.77
1:B:499:ILE:HG13	1:B:527:LEU:HD23	1.67	0.77
1:B:503:ALA:HB2	1:B:526:LYS:HZ1	1.49	0.76
1:B:141:ILE:HG23	1:B:160:MET:HE1	1.68	0.75
1:B:511:THR:HG22	1:B:514:LYS:HD3	1.68	0.74
1:B:144:MET:HE3	1:B:188:TYR:HB3	1.73	0.71
1:B:376:MET:HB2	1:B:404:ARG:HH12	1.53	0.71
1:B:160:MET:HE2	1:B:162:ASN:HD22	1.56	0.70
1:B:503:ALA:HB2	1:B:526:LYS:NZ	2.08	0.68
1:B:180:LYS:HA	1:B:212:ARG:HD2	1.77	0.66
1:B:144:MET:HE2	1:B:160:MET:HE3	1.79	0.64
1:B:510:LEU:HD11	1:B:526:LYS:NZ	2.13	0.64
1:B:482:ILE:HG13	1:B:484:PHE:HE2	1.63	0.63
1:B:225:SER:HB3	1:B:261:VAL:HG13	1.80	0.63
1:B:322:PHE:CZ	1:B:429:MET:HG3	2.27	0.63
1:B:309:ASN:O	1:B:313:LYS:HG2	2.00	0.62
1:B:511:THR:HG23	1:B:513:LEU:H	1.65	0.62
1:B:510:LEU:HD11	1:B:526:LYS:HZ1	1.65	0.61
1:B:484:PHE:CE1	1:B:591:LYS:HG2	2.34	0.61
1:A:227:TRP:HH2	1:B:227:TRP:CG	2.19	0.61
1:B:510:LEU:HD13	1:B:515:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:HB3	1:B:384:ARG:HG3	1.84	0.60
1:A:351:GLU:N	1:A:351:GLU:OE2	2.35	0.60
1:B:499:ILE:HD11	1:B:532:LEU:HD11	1.84	0.60
1:B:502:GLN:NE2	1:B:527:LEU:HD13	2.17	0.58
1:B:519:TRP:HA	1:B:532:LEU:HD21	1.87	0.57
1:A:340:PRO:HB2	1:A:365:ILE:HA	1.87	0.56
1:B:502:GLN:HE22	1:B:527:LEU:HD13	1.70	0.56
1:B:193:LYS:NZ	6:B:1102:HOH:O	2.33	0.56
1:B:144:MET:HE2	1:B:160:MET:HB2	1.86	0.55
1:A:216:ILE:HD13	1:A:241:LEU:HB3	1.88	0.55
1:A:307:LEU:HD11	1:A:311:ARG:HH11	1.71	0.55
1:B:283:ARG:NH1	1:B:403:GLY:O	2.29	0.55
1:A:65:PRO:HB2	1:A:98:GLU:HG2	1.87	0.55
1:B:386:VAL:HG23	1:B:405:ALA:HB2	1.89	0.55
1:A:173:VAL:O	1:A:177:MET:HG3	2.07	0.55
1:B:482:ILE:CG1	1:B:484:PHE:HE2	2.20	0.54
1:B:89:LEU:HD13	3:B:1002:ADP:C6	2.44	0.53
1:B:431:VAL:HG11	1:B:566:THR:HG21	1.91	0.52
1:B:216:ILE:HD13	1:B:241:LEU:HB3	1.92	0.52
1:A:250:LEU:HD22	1:A:271:VAL:HG11	1.91	0.51
1:A:140:LEU:HD12	1:A:232:ARG:HH21	1.76	0.51
1:B:148:LEU:HD11	1:B:160:MET:HB3	1.93	0.51
1:B:226:GLN:HE22	1:B:236:LYS:NZ	2.08	0.50
1:B:527:LEU:HD12	1:B:529:VAL:H	1.76	0.50
1:B:345:HIS:HB2	1:B:348:MET:HG3	1.93	0.50
1:A:293:LYS:HE3	1:A:300:PHE:CE2	2.47	0.50
1:B:322:PHE:HD2	1:B:425:ARG:NH2	2.10	0.49
1:B:450:ILE:HD12	1:B:451:ASN:N	2.27	0.49
1:A:263:LYS:O	1:A:267:LYS:HG3	2.11	0.49
1:B:87:PHE:O	1:B:88:LYS:HG2	2.12	0.49
1:B:140:LEU:O	1:B:144:MET:HG2	2.12	0.49
1:B:529:VAL:HG12	1:B:530:ALA:H	1.78	0.49
1:B:71:GLU:OE2	1:B:80:LYS:HE3	2.13	0.49
1:B:178:VAL:HG11	1:B:203:ARG:HH21	1.78	0.49
1:A:258:THR:O	1:A:261:VAL:N	2.47	0.48
1:A:269:LEU:HB2	1:A:271:VAL:HG22	1.93	0.48
1:B:173:VAL:O	1:B:177:MET:HG3	2.14	0.48
1:B:547:ALA:O	1:B:551:ILE:HG12	2.13	0.48
1:A:281:PHE:O	1:A:399:TYR:OH	2.25	0.48
1:B:519:TRP:HD1	1:B:532:LEU:HD21	1.79	0.48
1:A:174:HIS:O	1:A:203:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HB	1:B:278:THR:HG23	1.97	0.47
1:B:348:MET:HE3	1:B:352:ASP:HB3	1.96	0.47
1:A:322:PHE:CZ	1:A:429:MET:HG3	2.50	0.47
1:A:494:ARG:HD3	6:A:1122:HOH:O	2.14	0.47
1:B:494:ARG:HH22	1:B:582:GLU:HA	1.80	0.47
1:B:511:THR:HG23	1:B:513:LEU:N	2.28	0.47
1:A:227:TRP:CH2	1:B:227:TRP:CD2	3.03	0.47
1:A:267:LYS:HG2	1:A:272:GLU:CD	2.39	0.47
1:B:391:MET:HB3	1:B:416:LEU:HD21	1.96	0.47
1:B:112:VAL:HG11	1:B:257:ALA:HA	1.96	0.46
1:B:376:MET:HE3	1:B:376:MET:HB3	1.60	0.46
1:A:456:VAL:O	1:A:460:GLN:HG2	2.16	0.46
1:A:315:GLN:HB3	1:A:384:ARG:HG3	1.97	0.46
1:B:514:LYS:O	1:B:515:LEU:HB3	2.15	0.46
1:B:545:ILE:HG12	1:B:588:MET:HE1	1.98	0.46
1:A:148:LEU:O	1:A:152:LYS:HB2	2.16	0.46
1:A:267:LYS:HA	1:A:272:GLU:HG2	1.98	0.46
1:A:148:LEU:HD21	1:A:160:MET:HB3	1.97	0.46
1:B:333:SER:O	1:B:337:LEU:HD23	2.16	0.46
1:B:484:PHE:HE1	1:B:591:LYS:HG2	1.77	0.46
1:A:226:GLN:HA	1:A:231:PHE:CD1	2.52	0.45
1:B:450:ILE:HD13	1:B:484:PHE:CD1	2.52	0.45
1:B:223:CYS:HB3	1:B:232:ARG:HG3	1.99	0.45
1:B:534:PRO:HA	1:B:535:PRO:HD3	1.83	0.45
1:B:376:MET:CB	1:B:404:ARG:HH12	2.27	0.45
1:A:139:PRO:HB2	1:A:232:ARG:HE	1.82	0.45
1:B:517:ASP:O	1:B:522:LYS:N	2.42	0.45
1:A:289:GLU:OE1	1:A:415:ILE:HD12	2.16	0.45
1:B:494:ARG:HG3	1:B:579:LEU:HD13	1.99	0.44
1:B:459:ALA:HB1	1:B:464:GLU:HB3	1.98	0.44
1:B:499:ILE:HG22	1:B:526:LYS:NZ	2.32	0.44
1:B:120:SER:HA	1:B:123:TYR:CE2	2.53	0.44
1:B:80:LYS:N	1:B:80:LYS:HD3	2.33	0.44
1:B:132:GLY:HA3	1:B:212:ARG:O	2.17	0.44
1:B:304:ILE:O	1:B:308:ILE:HD12	2.17	0.44
1:B:535:PRO:O	1:B:536:THR:OG1	2.30	0.44
1:B:128:LEU:HD11	1:B:156:ILE:HG12	2.00	0.44
1:B:160:MET:HE2	1:B:162:ASN:ND2	2.29	0.43
1:A:191:PRO:HG3	1:A:235:TYR:CE1	2.53	0.43
1:A:516:ILE:O	1:A:520:MET:HG3	2.18	0.43
1:A:322:PHE:HZ	1:A:429:MET:HG3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD23	1:B:161:LEU:HA	1.84	0.43
1:A:282:ASN:OD1	1:A:455:ARG:HD3	2.18	0.43
1:B:224:CYS:HA	1:B:235:TYR:HB3	2.00	0.43
1:B:484:PHE:CD1	1:B:590:VAL:C	2.96	0.43
1:A:376:MET:HB2	1:A:376:MET:HE2	1.65	0.43
1:B:144:MET:HG2	1:B:144:MET:H	1.56	0.43
1:A:180:LYS:HA	1:A:212:ARG:HD2	2.00	0.43
1:A:86:VAL:HG11	1:A:128:LEU:HD23	2.01	0.43
1:A:349:GLU:OE1	1:A:350:PRO:HD2	2.18	0.43
1:B:450:ILE:HD12	1:B:451:ASN:HB3	2.01	0.43
1:B:579:LEU:HD21	1:B:586:ILE:HD11	2.01	0.43
1:B:499:ILE:HG22	1:B:526:LYS:HZ2	1.84	0.42
1:A:125:LEU:HB3	1:A:126:PRO:HD3	2.02	0.42
1:B:242:LYS:HD2	1:B:242:LYS:HA	1.82	0.42
1:B:70:LYS:HE3	1:B:73:PHE:CZ	2.55	0.42
1:A:86:VAL:O	1:A:154:LEU:HD22	2.20	0.42
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.89	0.42
1:A:407:ARG:HA	1:A:407:ARG:HD3	1.86	0.42
1:A:220:GLU:OE1	1:A:222:HIS:HE1	2.03	0.41
1:A:262:LEU:O	1:A:266:GLN:HG2	2.19	0.41
1:B:180:LYS:HB3	1:B:180:LYS:HE3	1.91	0.41
1:B:411:LYS:HG3	1:B:474:MET:HE1	2.02	0.41
1:B:527:LEU:CD1	1:B:529:VAL:H	2.33	0.41
1:B:439:LYS:HD2	1:B:439:LYS:HA	1.90	0.41
1:B:566:THR:C	1:B:567:ILE:HD12	2.45	0.41
1:A:371:THR:O	1:A:376:MET:HE1	2.21	0.40
1:B:125:LEU:HB3	1:B:126:PRO:HD3	2.02	0.40
1:A:376:MET:HG3	1:A:378:ILE:HG12	2.03	0.40
1:B:519:TRP:HA	1:B:532:LEU:CD2	2.50	0.40
1:A:225:SER:HB3	1:A:261:VAL:HG13	2.03	0.40
1:B:487:LYS:HG3	1:B:590:VAL:CG2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLU:OE2	1:B:589:ARG:NH2[1_655]	2.19	0.01

## 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	529/531 (100%)	529 (100%)	0	0	100	100
1	B	529/531 (100%)	529 (100%)	0	0	100	100
All	All	1058/1062 (100%)	1058 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 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	469/469 (100%)	463 (99%)	6 (1%)	61	82
1	B	469/469 (100%)	455 (97%)	14 (3%)	36	64
All	All	938/938 (100%)	918 (98%)	20 (2%)	47	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	266	GLN
1	A	324	GLN
1	A	334	LEU
1	A	507	ASN
1	A	513	LEU
1	B	80	LYS
1	B	128	LEU

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Mol	Chain	Res	Type
1	B	144	MET
1	B	152	LYS
1	B	165	SER
1	B	307	LEU
1	B	308	ILE
1	B	329	GLN
1	B	332	ILE
1	B	464	GLU
1	B	482	ILE
1	B	511	THR
1	B	529	VAL
1	B	555	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	324	GLN
1	A	345	HIS
1	A	389	HIS
1	B	226	GLN
1	B	502	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADP	A	1002	4	28,29,29	1.41	4 (14%)	43,45,45	1.80	10 (23%)
3	ADP	B	1002	4	28,29,29	1.42	4 (14%)	43,45,45	1.81	9 (20%)
5	PO4	A	1004	-	4,4,4	1.57	1 (25%)	6,6,6	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1002	4	-	3/16/32/32	0/3/3/3
3	ADP	B	1002	4	-	3/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	ADP	C5-C4	4.73	1.47	1.39
3	B	1002	ADP	C5-C4	4.71	1.47	1.39
3	B	1002	ADP	C5-C6	2.79	1.48	1.41
3	A	1002	ADP	C5-C6	2.76	1.48	1.41
5	A	1004	PO4	P-O1	2.73	1.57	1.50
3	B	1002	ADP	C8-N7	2.45	1.36	1.31
3	A	1002	ADP	C8-N7	2.44	1.36	1.31
3	B	1002	ADP	C5-N7	-2.14	1.35	1.39
3	A	1002	ADP	C5-N7	-2.08	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	ADP	C5-C4-N3	-5.77	118.77	126.72
3	A	1002	ADP	C5-C4-N3	-5.50	119.15	126.72
3	B	1002	ADP	N3-C4-N9	4.50	134.81	127.17
3	A	1002	ADP	N3-C4-N9	4.33	134.53	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	ADP	C2-N3-C4	3.74	120.96	111.83
3	A	1002	ADP	C2-N3-C4	3.68	120.83	111.83
3	B	1002	ADP	C4-C5-N7	-3.58	106.49	110.58
3	A	1002	ADP	C4-C5-N7	-3.49	106.59	110.58
3	A	1002	ADP	N3-C2-N1	-3.48	123.32	128.58
3	B	1002	ADP	N3-C2-N1	-3.33	123.54	128.58
3	A	1002	ADP	C4-N9-C8	2.80	108.68	105.74
3	B	1002	ADP	C4-N9-C8	2.68	108.55	105.74
3	B	1002	ADP	C5-N7-C8	2.61	107.55	103.45
3	A	1002	ADP	C5-N7-C8	2.53	107.42	103.45
3	A	1002	ADP	C6-C5-N7	2.29	136.50	132.09
3	B	1002	ADP	C6-C5-N7	2.21	136.35	132.09
3	A	1002	ADP	C2-N1-C6	2.09	122.16	118.73
3	B	1002	ADP	N9-C8-N7	-2.08	110.99	113.94
3	A	1002	ADP	N9-C8-N7	-2.08	110.99	113.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	ADP	C5'-O5'-PA-O2A
3	A	1002	ADP	C5'-O5'-PA-O3A
3	B	1002	ADP	C5'-O5'-PA-O2A
3	B	1002	ADP	C5'-O5'-PA-O3A
3	A	1002	ADP	C5'-O5'-PA-O1A
3	B	1002	ADP	C5'-O5'-PA-O1A

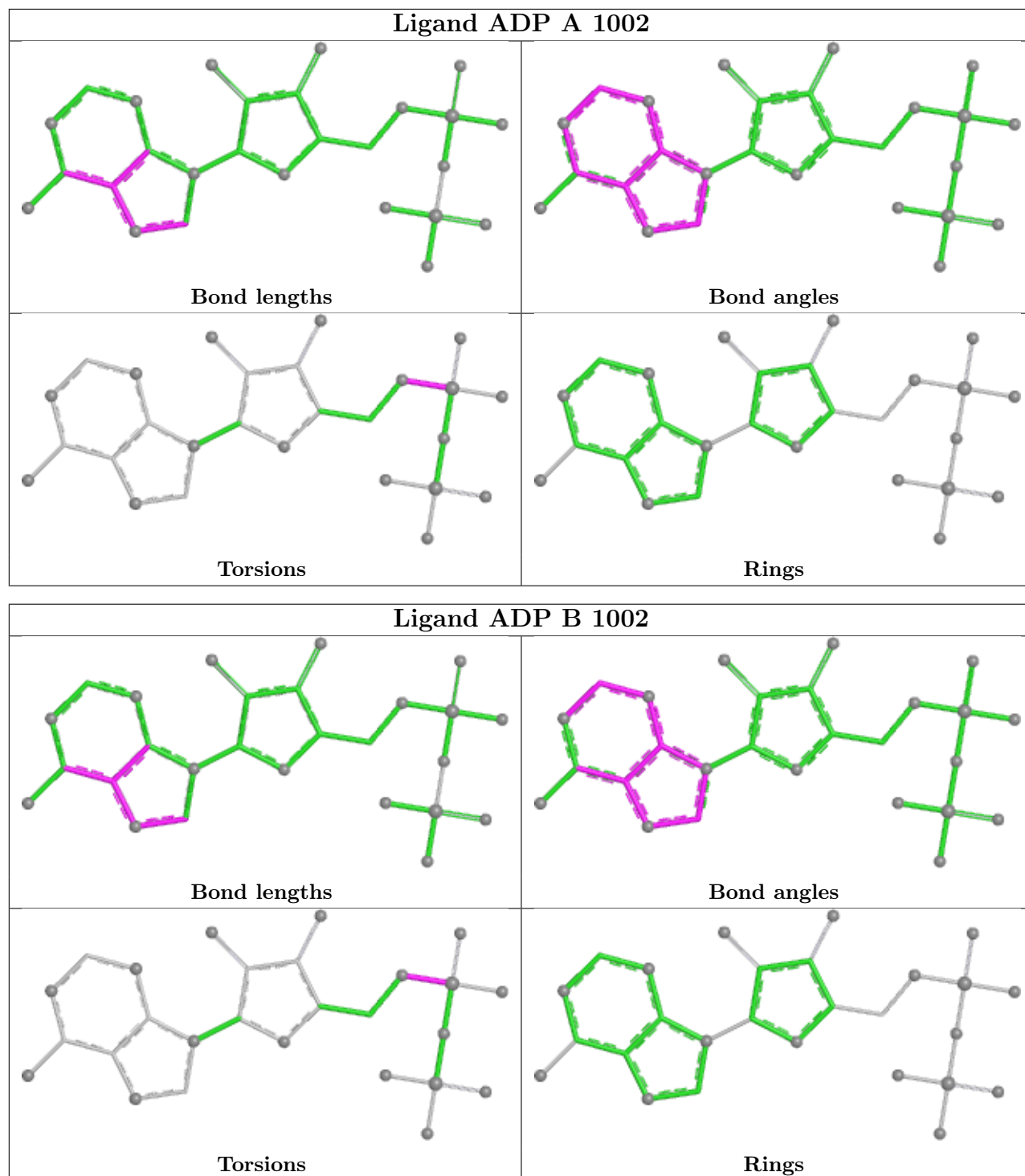
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	531/531 (100%)	0.79	52 (9%) 13 11	37, 68, 110, 152	0
1	B	530/531 (99%)	0.99	73 (13%) 6 5	40, 72, 133, 218	1 (0%)
All	All	1061/1062 (99%)	0.89	125 (11%) 9 7	37, 70, 126, 218	1 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	375	GLY	6.4
1	B	373	ALA	5.3
1	A	569	TYR	5.2
1	B	526	LYS	5.1
1	A	375	GLY	5.1
1	A	227	TRP	5.1
1	A	257	ALA	4.8
1	B	374	PHE	4.8
1	B	484	PHE	4.7
1	A	378	ILE	4.6
1	A	229	HIS	4.5
1	B	515	LEU	4.3
1	B	260	HIS	4.3
1	B	482	ILE	4.2
1	B	80	LYS	4.2
1	A	376	MET	4.1
1	B	563	ALA	4.1
1	A	463	ASP	4.1
1	B	521	GLY	4.1
1	A	540	GLU	4.0
1	B	376	MET	4.0
1	A	467	SER	4.0
1	A	232	ARG	4.0
1	A	256	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	313	LYS	3.8
1	A	372	VAL	3.8
1	B	63	SER	3.8
1	B	372	VAL	3.8
1	B	530	ALA	3.7
1	A	374	PHE	3.7
1	B	529	VAL	3.5
1	B	64	SER	3.5
1	B	506	LEU	3.5
1	A	260	HIS	3.4
1	B	513	LEU	3.4
1	B	345	HIS	3.4
1	A	564	TYR	3.4
1	B	346	ALA	3.4
1	B	539	ARG	3.4
1	B	229	HIS	3.3
1	B	378	ILE	3.3
1	A	225	SER	3.3
1	B	523	GLY	3.2
1	A	231	PHE	3.1
1	A	228	GLY	3.1
1	B	536	THR	3.1
1	A	379	ASP	3.1
1	B	532	LEU	3.1
1	A	273	LYS	3.0
1	B	438	GLN	3.0
1	A	468	PRO	3.0
1	A	483	SER	2.8
1	B	570	LEU	2.8
1	B	434	ASN	2.8
1	B	527	LEU	2.8
1	B	520	MET	2.8
1	A	226	GLN	2.8
1	A	347	ASN	2.7
1	A	357	HIS	2.7
1	A	322	PHE	2.7
1	B	314	GLY	2.7
1	B	582	GLU	2.7
1	B	324	GLN	2.7
1	B	301	ILE	2.6
1	B	347	ASN	2.6
1	B	534	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	558	ASP	2.6
1	B	228	GLY	2.5
1	B	162	ASN	2.5
1	A	138	CYS	2.5
1	B	256	THR	2.5
1	B	227	TRP	2.5
1	B	138	CYS	2.5
1	B	514	LYS	2.5
1	A	175	ALA	2.5
1	B	524	ALA	2.5
1	B	564	TYR	2.4
1	B	357	HIS	2.4
1	A	434	ASN	2.4
1	A	481	GLU	2.4
1	B	234	ASP	2.4
1	A	270	CYS	2.4
1	B	163	ALA	2.4
1	A	62	MET	2.3
1	B	429	MET	2.3
1	A	373	ALA	2.3
1	B	358	ARG	2.3
1	A	203	ARG	2.3
1	A	531	GLY	2.3
1	B	552	GLN	2.3
1	A	263	LYS	2.3
1	B	509	LYS	2.3
1	B	503	ALA	2.3
1	A	558	ASP	2.3
1	B	71	GLU	2.3
1	A	337	LEU	2.2
1	A	356	VAL	2.2
1	A	195	ALA	2.2
1	A	355	LYS	2.2
1	B	531	GLY	2.2
1	B	450	ILE	2.2
1	A	592	LYS	2.2
1	B	183	LYS	2.2
1	B	569	TYR	2.2
1	B	366	GLN	2.1
1	B	116	GLY	2.1
1	A	302	GLU	2.1
1	A	213	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	484	PHE	2.1
1	A	261	VAL	2.1
1	B	528	ARG	2.1
1	B	463	ASP	2.1
1	B	400	GLN	2.1
1	B	579	LEU	2.1
1	B	271	VAL	2.0
1	A	168	GLU	2.0
1	A	239	GLY	2.0
1	A	258	THR	2.0
1	A	267	LYS	2.0
1	B	353	LYS	2.0
1	B	480	LYS	2.0
1	B	487	LYS	2.0
1	A	299	ASP	2.0
1	B	164	SER	2.0
1	B	496	LEU	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 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	1003	1/1	0.60	0.26	71,71,71,71	0
5	PO4	A	1004	5/5	0.81	0.25	67,76,87,106	0
4	MG	A	1003	1/1	0.93	0.20	58,58,58,58	0
3	ADP	B	1002	27/27	0.94	0.09	49,64,74,77	0
3	ADP	A	1002	27/27	0.96	0.07	44,51,60,61	0
2	ZN	A	1001	1/1	0.99	0.02	48,48,48,48	0

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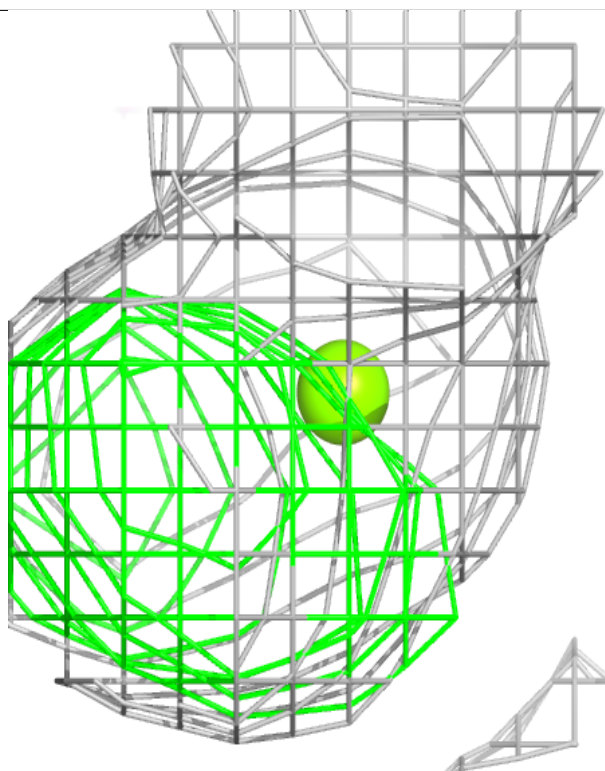
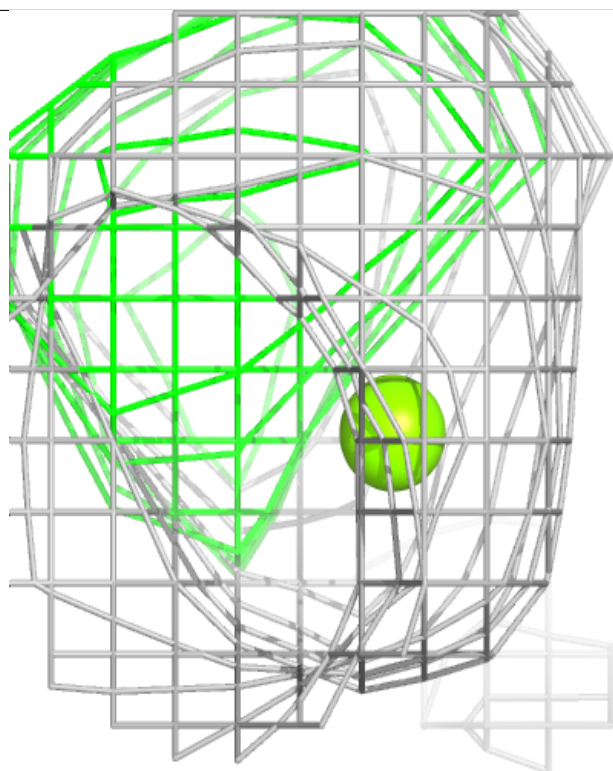
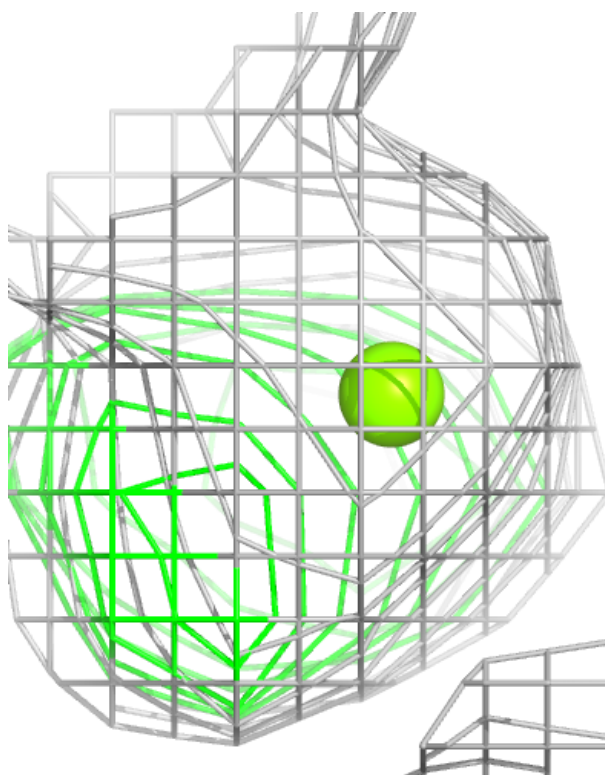
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	1001	1/1	1.00	0.01	45,45,45,45	0

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.

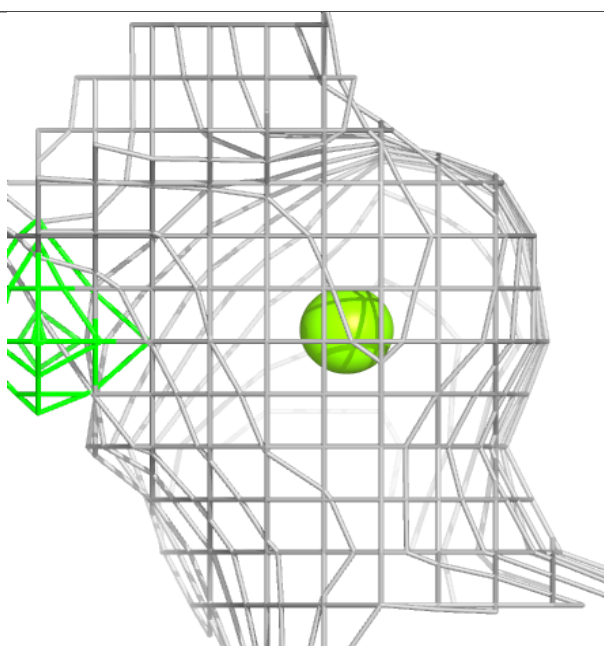
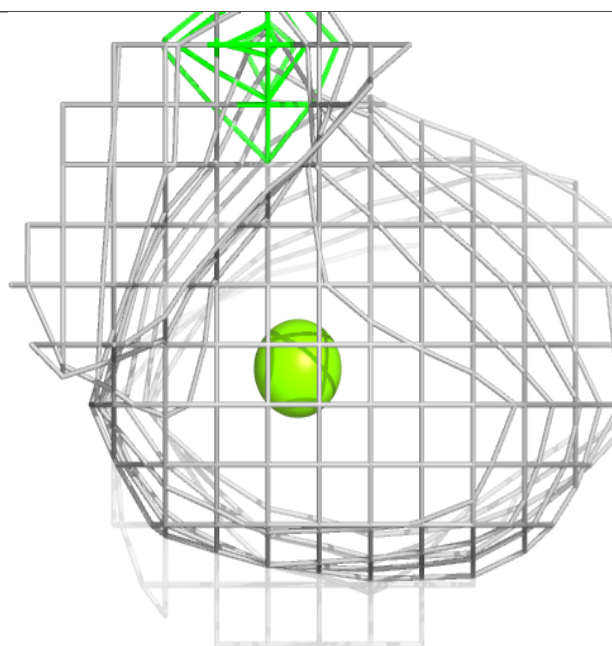
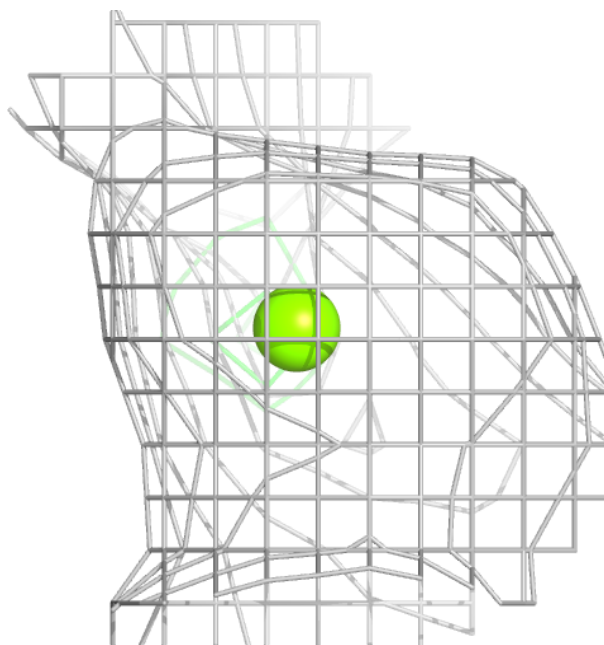
**Electron density around MG B 1003:**

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



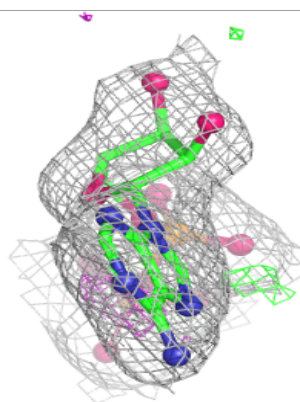
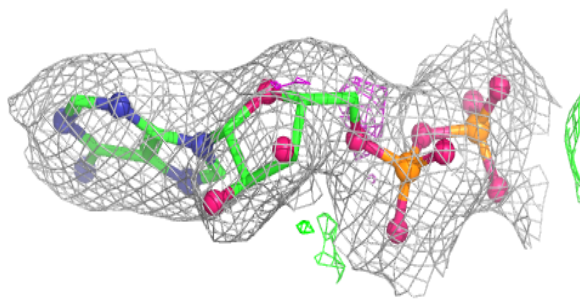
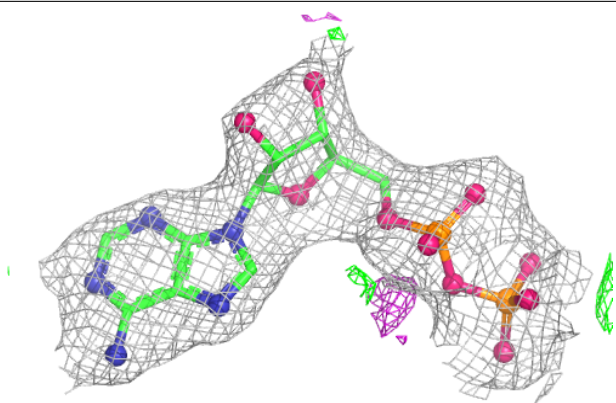
**Electron density around MG A 1003:**

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

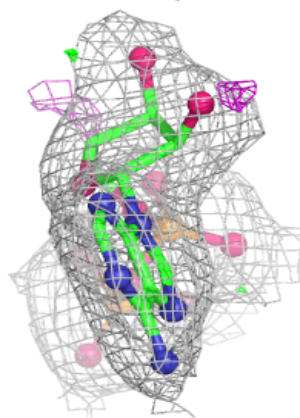
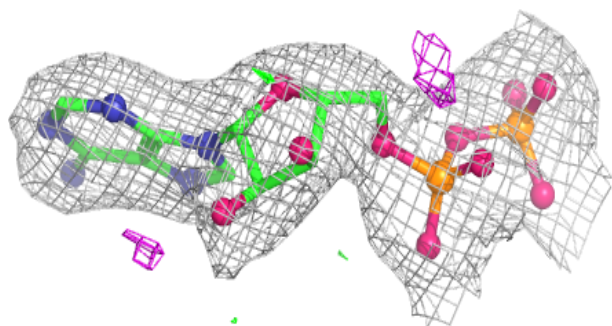
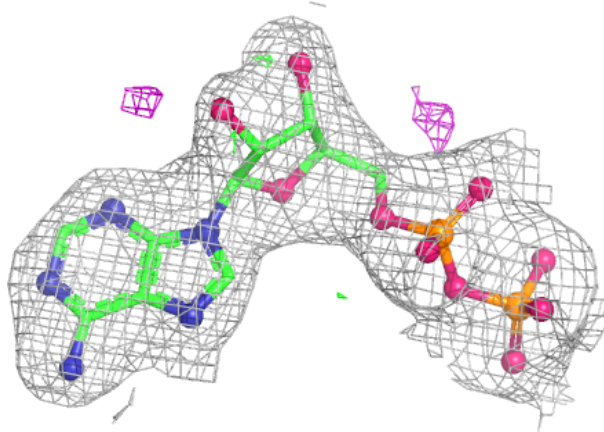


**Electron density around ADP B 1002:**

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

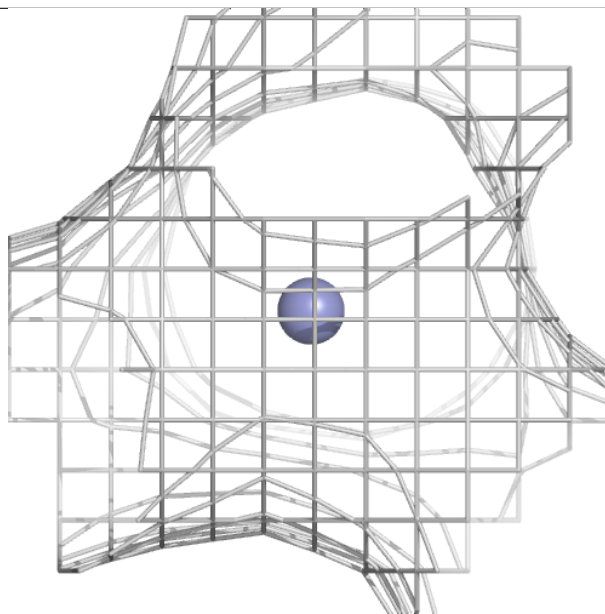
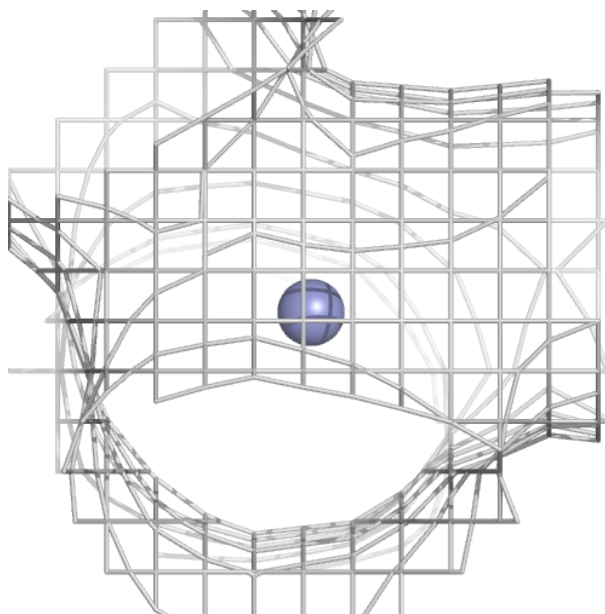
**Electron density around ADP A 1002:**

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



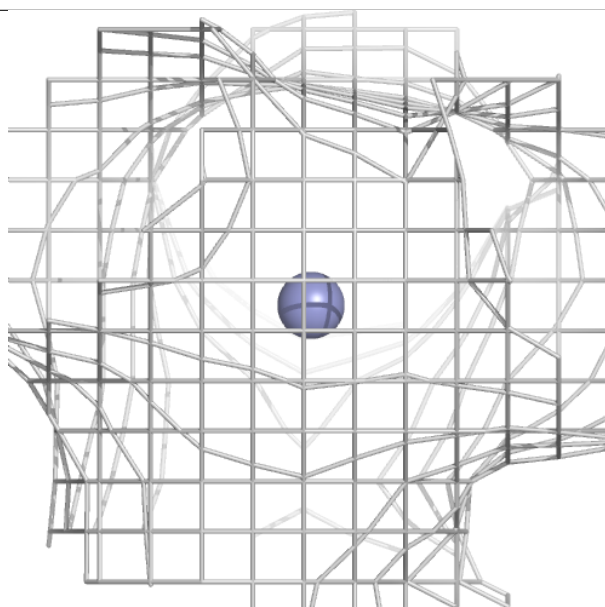
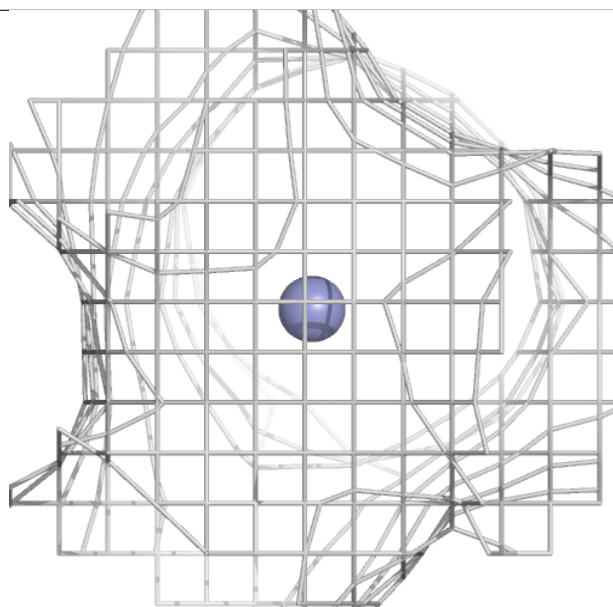
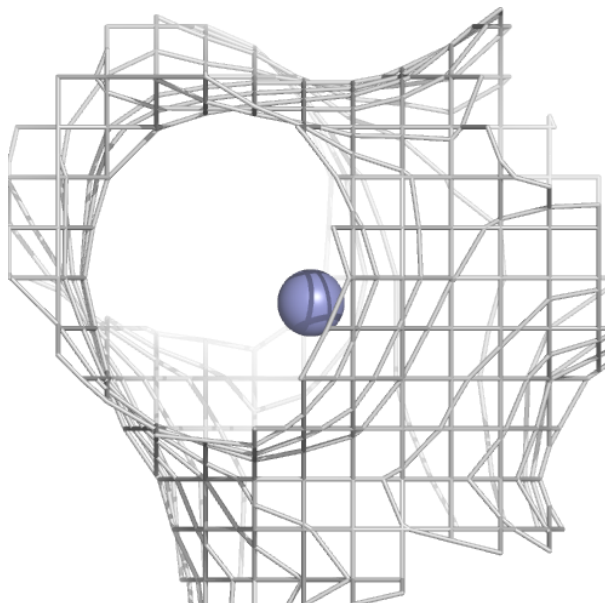
**Electron density around ZN A 1001:**

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



**Electron density around ZN B 1001:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.