



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2026 – 10:02 AM EDT

PDB ID : 4DQW / pdb_00004dqw
Title : Crystal Structure Analysis of Pseudomonas aeruginosa IMPDH
Authors : Labesse, G.; Munier-Lehmann, H.
Deposited on : 2012-02-16
Resolution : 2.51 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

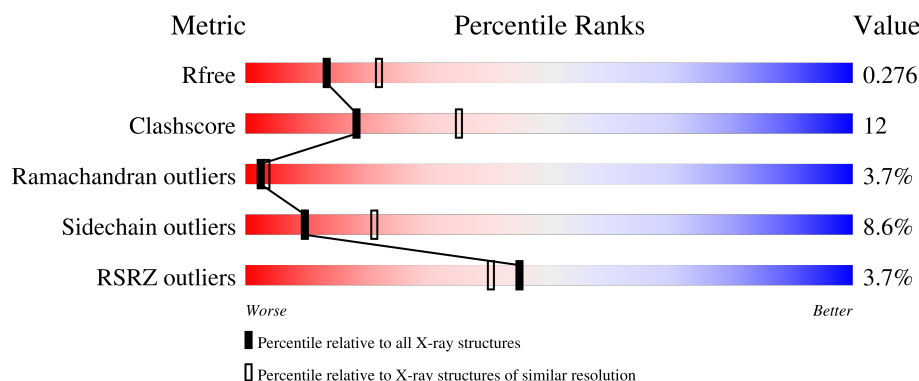
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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 ≥ 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	509	5% 59% 18% • • 18%
1	B	509	5% 59% 15% • • 21%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6384 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	2	0
			3073	1932	541	583	17			
1	B	404	Total	C	N	O	S	0	1	0
			2967	1868	519	563	17			

There are 40 discrepancies between the modelled and reference sequences:

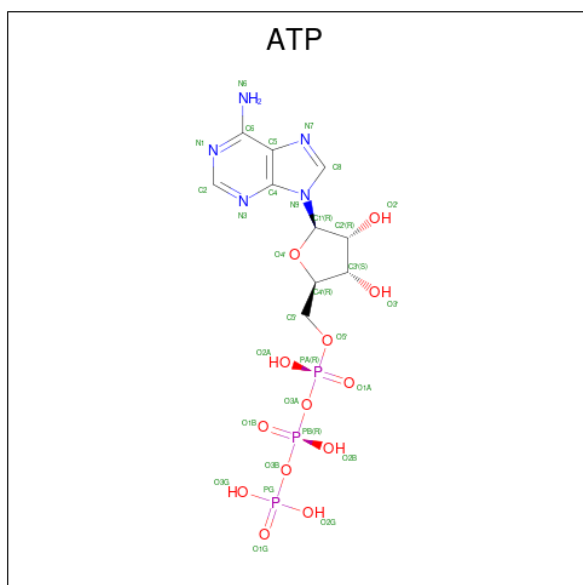
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q9HXM5
A	-18	GLY	-	expression tag	UNP Q9HXM5
A	-17	SER	-	expression tag	UNP Q9HXM5
A	-16	SER	-	expression tag	UNP Q9HXM5
A	-15	HIS	-	expression tag	UNP Q9HXM5
A	-14	HIS	-	expression tag	UNP Q9HXM5
A	-13	HIS	-	expression tag	UNP Q9HXM5
A	-12	HIS	-	expression tag	UNP Q9HXM5
A	-11	HIS	-	expression tag	UNP Q9HXM5
A	-10	HIS	-	expression tag	UNP Q9HXM5
A	-9	SER	-	expression tag	UNP Q9HXM5
A	-8	SER	-	expression tag	UNP Q9HXM5
A	-7	GLY	-	expression tag	UNP Q9HXM5
A	-6	LEU	-	expression tag	UNP Q9HXM5
A	-5	VAL	-	expression tag	UNP Q9HXM5
A	-4	PRO	-	expression tag	UNP Q9HXM5
A	-3	ARG	-	expression tag	UNP Q9HXM5
A	-2	GLY	-	expression tag	UNP Q9HXM5
A	-1	SER	-	expression tag	UNP Q9HXM5
A	0	HIS	-	expression tag	UNP Q9HXM5
B	-19	MET	-	expression tag	UNP Q9HXM5
B	-18	GLY	-	expression tag	UNP Q9HXM5
B	-17	SER	-	expression tag	UNP Q9HXM5
B	-16	SER	-	expression tag	UNP Q9HXM5
B	-15	HIS	-	expression tag	UNP Q9HXM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q9HXM5
B	-13	HIS	-	expression tag	UNP Q9HXM5
B	-12	HIS	-	expression tag	UNP Q9HXM5
B	-11	HIS	-	expression tag	UNP Q9HXM5
B	-10	HIS	-	expression tag	UNP Q9HXM5
B	-9	SER	-	expression tag	UNP Q9HXM5
B	-8	SER	-	expression tag	UNP Q9HXM5
B	-7	GLY	-	expression tag	UNP Q9HXM5
B	-6	LEU	-	expression tag	UNP Q9HXM5
B	-5	VAL	-	expression tag	UNP Q9HXM5
B	-4	PRO	-	expression tag	UNP Q9HXM5
B	-3	ARG	-	expression tag	UNP Q9HXM5
B	-2	GLY	-	expression tag	UNP Q9HXM5
B	-1	SER	-	expression tag	UNP Q9HXM5
B	0	HIS	-	expression tag	UNP Q9HXM5

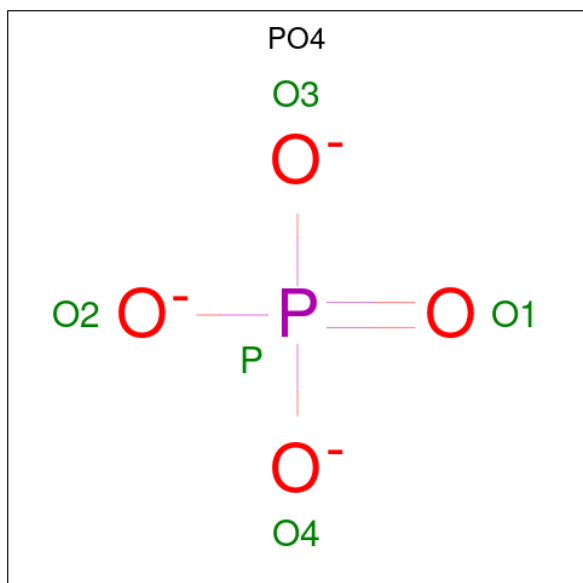
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

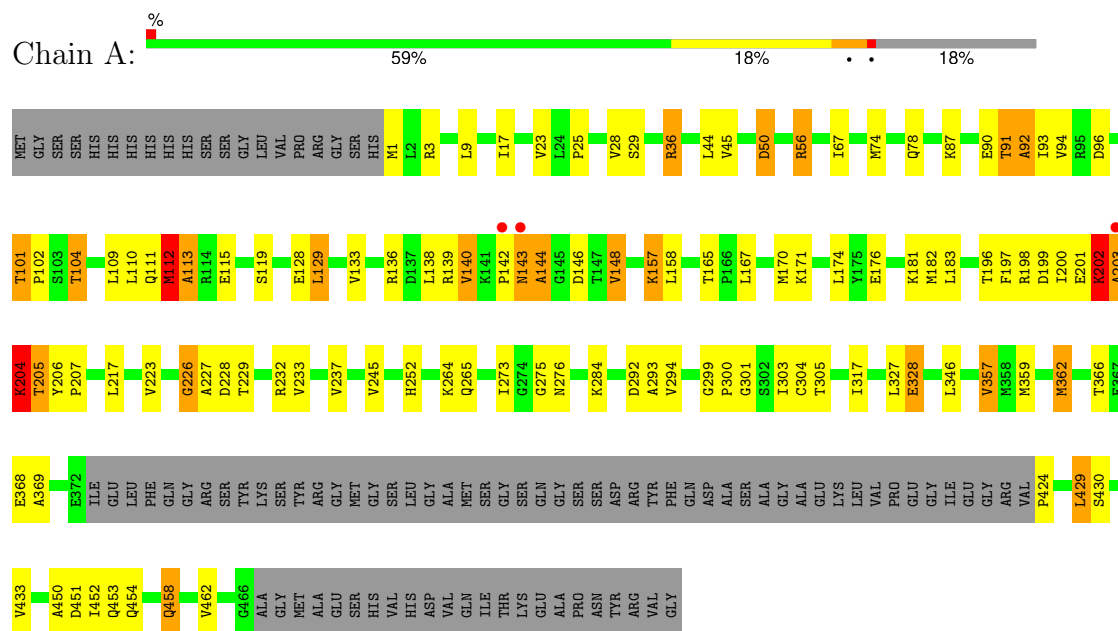
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	100	Total	O	0	0
			100	100		
6	B	105	Total	O	0	0
			105	105		

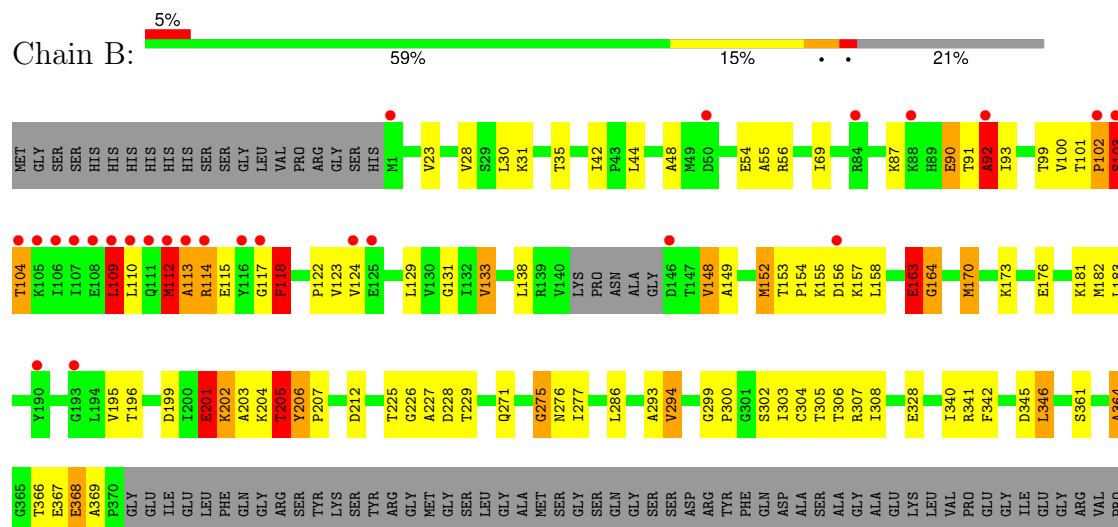
3 Residue-property plots [i](#)

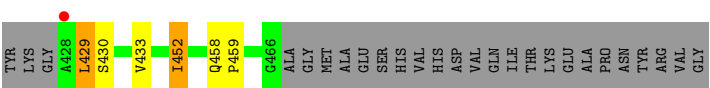
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	108.96Å 108.96Å 194.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.92 – 2.51 54.92 – 2.51	Depositor EDS
% Data completeness (in resolution range)	88.8 (54.92-2.51) 88.8 (54.92-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.284 0.210 , 0.276	Depositor DCC
R_{free} test set	1750 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6384	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ATP, MN, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	0/3123	0.91	2/4224 (0.0%)
1	B	0.66	1/3005 (0.0%)	0.97	7/4068 (0.2%)
All	All	0.67	1/6128 (0.0%)	0.94	9/8292 (0.1%)

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	9
1	B	0	12
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ALA	CA-CB	-5.35	1.48	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ALA	N-CA-C	7.46	121.30	111.75
1	B	153	THR	CA-C-N	7.13	127.30	120.31
1	B	153	THR	C-N-CA	7.13	127.30	120.31
1	B	276	ASN	N-CA-C	-6.70	96.83	108.69
1	B	91	THR	N-CA-C	-6.69	100.85	111.02
1	B	103	SER	N-CA-C	-6.15	97.70	110.80
1	A	276	ASN	N-CA-C	5.76	123.06	110.80
1	B	275	GLY	N-CA-C	5.47	118.01	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	227	ALA	N-CA-C	5.33	120.16	111.37

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	MET	Peptide
1	A	142	PRO	Peptide
1	A	144	ALA	Peptide
1	A	202	LYS	Peptide
1	A	204	LYS	Peptide
1	A	226	GLY	Peptide
1	A	275	GLY	Peptide,Mainchain
1	A	91	THR	Peptide
1	B	102	PRO	Peptide
1	B	109	LEU	Peptide
1	B	112	MET	Peptide
1	B	113	ALA	Peptide
1	B	117	GLY	Peptide
1	B	163	GLU	Peptide
1	B	201	GLU	Peptide
1	B	205	THR	Peptide
1	B	226	GLY	Peptide
1	B	275	GLY	Peptide
1	B	90	GLU	Peptide
1	B	92	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3073	0	3171	75	0
1	B	2967	0	3043	76	0
2	A	62	0	24	2	0
2	B	62	0	24	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
5	A	6	0	8	0	0
6	A	100	0	0	4	0
6	B	105	0	0	5	0
All	All	6384	0	6270	151	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 12.

All (151) 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:163:GLU:HG3	1:B:164:GLY:H	1.28	0.98
1:A:357:VAL:HG23	1:A:359:MET:HE2	1.49	0.91
1:A:429:LEU:HD22	1:A:433:VAL:HG23	1.54	0.88
1:B:155:LYS:HA	1:B:158:LEU:HD13	1.57	0.86
1:B:163:GLU:HG3	1:B:164:GLY:N	1.88	0.85
1:B:101:THR:OG1	1:B:104:THR:HG23	1.77	0.83
1:A:92:ALA:HB1	1:A:199:ASP:HB3	1.64	0.78
1:B:23:VAL:CG2	6:B:604:HOH:O	2.32	0.77
1:B:303:ILE:O	1:B:303:ILE:HG22	1.84	0.77
1:A:245:VAL:HG22	1:A:273:ILE:HD12	1.68	0.76
1:B:429:LEU:HD22	1:B:433:VAL:HG23	1.68	0.75
1:A:357:VAL:CG2	1:A:359:MET:HE2	2.16	0.74
1:B:149:ALA:HA	1:B:152:MET:HE2	1.68	0.74
1:B:202:LYS:O	1:B:205:THR:O	2.06	0.73
1:A:101:THR:O	1:A:104:THR:HG23	1.87	0.73
1:B:109:LEU:O	1:B:113:ALA:HB2	1.87	0.73
1:B:92:ALA:CB	1:B:199:ASP:HB3	2.19	0.73
1:A:429:LEU:HD22	1:A:433:VAL:CG2	2.20	0.72
1:B:23:VAL:HG22	6:B:604:HOH:O	1.90	0.71
1:A:110:LEU:O	1:A:113:ALA:HB3	1.91	0.70
1:B:361:SER:O	1:B:364:ALA:HB2	1.91	0.69
1:A:429:LEU:CD2	1:A:433:VAL:HG23	2.22	0.68
1:B:201:GLU:HB2	1:B:202:LYS:HB2	1.75	0.67
1:A:109:LEU:O	1:A:113:ALA:HB2	1.96	0.65
1:A:424:PRO:N	6:A:644:HOH:O	2.30	0.64
1:B:109:LEU:HD23	1:B:138:LEU:HD21	1.79	0.64
1:B:154:PRO:O	1:B:158:LEU:HD12	1.97	0.64
1:B:170:MET:HE1	1:B:195:VAL:HG21	1.80	0.63
1:B:100:VAL:HG23	1:B:123:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ILE:HG23	1:B:308:ILE:HD11	1.80	0.63
1:B:129:LEU:HD21	1:B:158:LEU:CD2	2.28	0.62
1:A:1:MET:CG	1:A:1:MET:O	2.47	0.62
1:A:228:ASP:HA	6:A:658:HOH:O	2.00	0.61
1:B:199:ASP:O	1:B:203:ALA:CB	2.49	0.60
1:A:104:THR:O	1:A:148:VAL:HG12	2.01	0.60
1:B:101:THR:HG22	1:B:124:VAL:O	2.01	0.60
1:A:139:ARG:O	1:A:140:VAL:HB	2.00	0.59
1:A:36:ARG:HD3	1:A:292:ASP:HA	1.83	0.59
1:B:30:LEU:HA	1:B:452:ILE:HD12	1.85	0.59
1:A:17:ILE:HG12	1:A:462:VAL:HG13	1.85	0.58
1:B:154:PRO:O	1:B:158:LEU:CD1	2.51	0.58
1:A:92:ALA:CB	1:A:199:ASP:HB3	2.33	0.57
1:B:303:ILE:O	1:B:303:ILE:CG2	2.52	0.57
1:A:366:THR:HG23	1:A:369:ALA:H	1.69	0.57
1:B:102:PRO:HA	1:B:148:VAL:HG22	1.87	0.56
1:B:133:VAL:HG13	1:B:152:MET:HB2	1.86	0.56
1:A:112:MET:O	1:A:115:GLU:N	2.38	0.56
1:B:93:ILE:HA	1:B:195:VAL:HG22	1.86	0.56
1:A:301:GLY:O	1:A:304:CYS:SG	2.64	0.55
1:B:92:ALA:HB1	1:B:199:ASP:HB3	1.89	0.55
1:B:155:LYS:CA	1:B:158:LEU:HD13	2.35	0.54
1:A:165:THR:HB	1:A:170:MET:CE	2.39	0.53
1:B:206:TYR:N	1:B:207:PRO:CD	2.71	0.53
1:B:366:THR:O	1:B:369:ALA:N	2.39	0.53
1:B:170:MET:HG2	1:B:182:MET:HG2	1.90	0.53
1:B:199:ASP:O	1:B:203:ALA:HB2	2.09	0.53
1:A:362:MET:HA	1:A:362:MET:HE2	1.90	0.53
1:A:109:LEU:HD23	1:A:138:LEU:HD21	1.91	0.52
1:A:346:LEU:HD13	1:A:357:VAL:HG21	1.90	0.52
1:A:299:GLY:N	1:A:300:PRO:HD3	2.24	0.52
1:A:1:MET:O	1:A:1:MET:HG2	2.08	0.52
1:B:56:ARG:HG2	1:B:368:GLU:HA	1.92	0.51
1:A:226:GLY:HA2	6:A:632:HOH:O	2.10	0.51
1:B:271:GLN:NE2	6:B:620:HOH:O	2.23	0.51
1:A:17:ILE:CG1	1:A:462:VAL:HG13	2.40	0.51
1:B:429:LEU:CD2	1:B:433:VAL:HG23	2.40	0.51
1:A:200:ILE:C	1:A:202:LYS:H	2.18	0.50
1:B:87:LYS:NZ	1:B:212:ASP:OD2	2.39	0.50
1:B:103:SER:O	1:B:104:THR:C	2.55	0.50
1:B:196:THR:OG1	1:B:199:ASP:OD2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HG22	1:A:369:ALA:HB2	1.94	0.50
1:B:158:LEU:HD23	1:B:183:LEU:HD13	1.92	0.50
1:A:45:VAL:HG13	1:A:67:ILE:HG23	1.94	0.49
1:A:167:LEU:O	1:A:171:LYS:N	2.42	0.49
1:B:181:LYS:NZ	2:B:501:ATP:O1B	2.46	0.49
1:B:366:THR:O	1:B:367:GLU:C	2.56	0.49
1:A:56[A]:ARG:HG3	1:A:56[A]:ARG:HH11	1.78	0.48
1:B:277:ILE:HD11	1:B:294:VAL:CG1	2.43	0.48
1:A:196:THR:HG22	1:A:198:ARG:H	1.79	0.47
1:A:204:LYS:O	1:A:206:TYR:CD1	2.67	0.47
1:A:50:ASP:OD1	1:A:50:ASP:N	2.44	0.47
1:A:223:VAL:HG12	1:A:232:ARG:HD3	1.97	0.47
1:A:23:VAL:HG21	1:A:450:ALA:HA	1.96	0.47
1:A:25:PRO:O	1:A:28:VAL:HG22	2.15	0.47
1:B:341:ARG:NH2	6:B:613:HOH:O	2.46	0.47
1:B:361:SER:O	1:B:364:ALA:CB	2.60	0.47
1:A:203:ALA:O	1:A:204:LYS:HB2	2.14	0.47
1:B:23:VAL:HG23	6:B:604:HOH:O	2.08	0.46
1:B:155:LYS:C	1:B:157:LYS:H	2.23	0.46
1:A:346:LEU:HD13	1:A:357:VAL:CG2	2.44	0.46
1:B:23:VAL:HG21	1:B:28:VAL:HG12	1.98	0.46
1:B:299:GLY:N	1:B:300:PRO:HD3	2.30	0.46
1:B:154:PRO:C	1:B:158:LEU:CD1	2.88	0.46
1:B:346:LEU:HD12	1:B:346:LEU:O	2.16	0.46
1:A:273:ILE:HG12	1:A:293:ALA:HB3	1.98	0.46
1:B:35:THR:HA	1:B:293:ALA:HB2	1.98	0.46
1:B:340:ILE:HG23	1:B:345:ASP:HB2	1.98	0.46
1:A:327:LEU:O	1:A:328:GLU:C	2.59	0.45
1:B:303:ILE:HG23	1:B:308:ILE:CD1	2.46	0.45
1:B:277:ILE:HD11	1:B:294:VAL:HG11	1.98	0.45
1:A:157:LYS:O	1:A:158:LEU:HB2	2.15	0.45
1:A:368:GLU:N	1:A:368:GLU:OE2	2.50	0.45
1:A:454:GLN:NE2	1:A:458:GLN:OE1	2.48	0.45
1:B:102:PRO:HB3	1:B:152:MET:HE1	1.99	0.45
1:B:131:GLY:HA2	1:B:158:LEU:HD11	1.97	0.45
1:A:174:LEU:HD21	1:A:181:LYS:C	2.41	0.45
1:A:101:THR:O	1:A:102:PRO:C	2.59	0.45
1:A:74:MET:HE2	1:A:78:GLN:HB3	1.98	0.44
1:B:99:THR:HG22	1:B:122:PRO:HG2	1.98	0.44
1:A:90:GLU:HB2	1:A:93:ILE:HD12	1.99	0.44
1:A:366:THR:CG2	1:A:369:ALA:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:O	1:B:112:MET:N	2.46	0.44
1:B:346:LEU:HD12	1:B:346:LEU:C	2.43	0.43
1:B:429:LEU:HD22	1:B:429:LEU:O	2.18	0.43
1:A:44:LEU:CD2	1:A:359:MET:HE1	2.48	0.43
1:A:252:HIS:ND1	6:A:612:HOH:O	2.29	0.43
1:A:196:THR:HG22	1:A:197:PHE:N	2.34	0.43
1:A:233:VAL:O	1:A:237:VAL:HG23	2.19	0.43
1:A:129:LEU:HD11	1:A:183:LEU:HD13	1.99	0.43
1:A:451:ASP:OD2	1:A:451:ASP:C	2.61	0.43
1:B:42:ILE:HD12	1:B:44:LEU:HD12	2.01	0.43
1:A:87:LYS:NZ	1:A:217:LEU:O	2.45	0.42
1:A:303:ILE:HG22	1:A:303:ILE:O	2.19	0.42
1:B:100:VAL:HG21	1:B:133:VAL:HG21	2.01	0.42
1:B:458:GLN:HB2	1:B:459:PRO:HD3	2.02	0.42
1:A:136:ARG:HD2	2:A:501:ATP:H5'2	2.01	0.42
1:B:205:THR:HG22	1:B:207:PRO:HD3	2.02	0.42
1:A:90:GLU:CB	1:A:93:ILE:HD12	2.50	0.42
1:A:170:MET:CG	1:A:182:MET:HG2	2.50	0.42
1:A:202:LYS:O	1:A:203:ALA:CB	2.65	0.42
1:A:109:LEU:O	1:A:113:ALA:CB	2.64	0.41
1:B:129:LEU:CD2	1:B:158:LEU:CD2	2.96	0.41
1:B:304:CYS:SG	1:B:307:ARG:HG3	2.60	0.41
1:A:205:THR:O	1:A:207:PRO:HD3	2.20	0.41
1:B:118:PHE:CD2	1:B:118:PHE:C	2.98	0.41
1:A:204:LYS:O	1:A:206:TYR:CE1	2.73	0.41
1:A:94:VAL:HG11	2:A:503:ATP:C2	2.55	0.41
1:B:286:LEU:HD12	1:B:294:VAL:HG22	2.02	0.41
1:A:167:LEU:HD22	1:A:200:ILE:HG12	2.03	0.41
1:A:205:THR:O	1:A:205:THR:OG1	2.32	0.41
1:B:48:ALA:HB2	1:B:69:ILE:CG2	2.51	0.41
1:B:92:ALA:HB3	1:B:199:ASP:HB3	2.00	0.41
1:B:129:LEU:C	1:B:129:LEU:HD23	2.45	0.41
1:A:36:ARG:CD	1:A:292:ASP:HA	2.48	0.40
1:B:206:TYR:H	1:B:207:PRO:CD	2.33	0.40
1:A:9:LEU:O	1:A:317:ILE:HB	2.21	0.40
1:A:74:MET:O	1:A:232:ARG:NH1	2.54	0.40
1:A:452:ILE:O	1:A:453:GLN:C	2.64	0.40
1:B:228:ASP:O	1:B:229:THR:C	2.64	0.40
1:B:305:THR:O	1:B:306:THR:C	2.64	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	413/509 (81%)	383 (93%)	17 (4%)	13 (3%)	3	5
1	B	399/509 (78%)	348 (87%)	34 (8%)	17 (4%)	2	2
All	All	812/1018 (80%)	731 (90%)	51 (6%)	30 (4%)	2	3

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ALA
1	A	140	VAL
1	A	143	ASN
1	A	203	ALA
1	A	328	GLU
1	B	55	ALA
1	B	103	SER
1	B	110	LEU
1	B	112	MET
1	B	114	ARG
1	B	118	PHE
1	B	164	GLY
1	B	201	GLU
1	B	302	SER
1	B	328	GLU
1	B	364	ALA
1	A	112	MET
1	A	157	LYS
1	A	205	THR
1	B	90	GLU
1	B	204	LYS
1	A	113	ALA
1	A	201	GLU
1	B	104	THR
1	B	109	LEU

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Mol	Chain	Res	Type
1	B	156	ASP
1	B	206	TYR
1	A	144	ALA
1	A	204	LYS
1	A	458	GLN

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	318/390 (82%)	287 (90%)	31 (10%)	8	17
1	B	303/390 (78%)	280 (92%)	23 (8%)	12	26
All	All	621/780 (80%)	567 (91%)	54 (9%)	10	21

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	29	SER
1	A	36	ARG
1	A	50	ASP
1	A	56[A]	ARG
1	A	56[B]	ARG
1	A	91	THR
1	A	96	ASP
1	A	101	THR
1	A	104	THR
1	A	111	GLN
1	A	119	SER
1	A	128	GLU
1	A	129	LEU
1	A	133	VAL
1	A	143	ASN
1	A	146	ASP
1	A	148	VAL

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Mol	Chain	Res	Type
1	A	176	GLU
1	A	202	LYS
1	A	204	LYS
1	A	229	THR
1	A	264	LYS
1	A	265	GLN
1	A	284	LYS
1	A	294	VAL
1	A	305	THR
1	A	357	VAL
1	A	362	MET
1	A	429	LEU
1	A	430	SER
1	B	31	LYS
1	B	54	GLU
1	B	114	ARG
1	B	115	GLU
1	B	118	PHE
1	B	133	VAL
1	B	148	VAL
1	B	152	MET
1	B	163	GLU
1	B	170	MET
1	B	173	LYS
1	B	176	GLU
1	B	201	GLU
1	B	202	LYS
1	B	205	THR
1	B	225	THR
1	B	294	VAL
1	B	342	PHE
1	B	346	LEU
1	B	368	GLU
1	B	429	LEU
1	B	430	SER
1	B	452	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	143	ASN

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Mol	Chain	Res	Type
1	A	322	ASN
1	A	454	GLN
1	A	458	GLN
1	B	111	GLN
1	B	435	GLN
1	B	453	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	A	506	-	5,5,5	0.49	0	5,5,5	0.51	0
2	ATP	A	501	3	32,33,33	1.35	6 (18%)	48,52,52	1.75	10 (20%)
4	PO4	A	505	-	4,4,4	0.71	0	6,6,6	0.56	0
2	ATP	B	501	3	32,33,33	1.51	7 (21%)	48,52,52	1.77	11 (22%)
2	ATP	A	503	3	32,33,33	1.51	5 (15%)	48,52,52	1.78	7 (14%)
2	ATP	B	503	3	32,33,33	1.39	6 (18%)	48,52,52	1.72	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	506	-	-	2/4/4/4	-
2	ATP	A	501	3	-	1/22/38/38	0/3/3/3
2	ATP	B	501	3	-	6/22/38/38	0/3/3/3
2	ATP	A	503	3	-	0/22/38/38	0/3/3/3
2	ATP	B	503	3	-	3/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	ATP	C5-C4	4.86	1.47	1.39
2	B	503	ATP	C5-C4	4.74	1.47	1.39
2	B	501	ATP	C5-C4	4.59	1.47	1.39
2	A	501	ATP	C5-C4	4.21	1.46	1.39
2	A	503	ATP	C5-N7	-3.20	1.33	1.39
2	A	501	ATP	PB-O3B	2.95	1.62	1.59
2	B	501	ATP	C5-C6	2.83	1.48	1.41
2	A	503	ATP	C5-C6	2.80	1.48	1.41
2	A	501	ATP	C4-N9	-2.61	1.32	1.37
2	B	503	ATP	C5-C6	2.51	1.48	1.41
2	A	501	ATP	C8-N7	2.51	1.36	1.31
2	B	501	ATP	C8-N7	2.51	1.36	1.31
2	B	503	ATP	C5-N7	-2.48	1.34	1.39
2	B	501	ATP	PB-O3A	2.44	1.62	1.59
2	B	501	ATP	PB-O3B	2.41	1.62	1.59
2	A	503	ATP	PB-O3B	2.37	1.62	1.59
2	B	501	ATP	C4-N9	-2.31	1.32	1.37
2	A	501	ATP	C5-N7	-2.31	1.34	1.39
2	A	503	ATP	C8-N7	2.29	1.36	1.31
2	A	501	ATP	C5-C6	2.19	1.47	1.41
2	B	503	ATP	PB-O3B	2.18	1.61	1.59
2	B	503	ATP	C8-N7	2.15	1.35	1.31
2	B	501	ATP	PA-O3A	2.12	1.61	1.59
2	B	503	ATP	C4-N9	-2.11	1.33	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	ATP	C5-C4-N3	-6.25	118.12	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	ATP	C5-C4-N3	-5.76	118.78	126.72
2	A	501	ATP	C5-C4-N3	-5.07	119.73	126.72
2	B	501	ATP	C5-C4-N3	-4.75	120.17	126.72
2	A	503	ATP	N3-C4-N9	4.70	135.16	127.17
2	B	503	ATP	N3-C4-N9	4.53	134.86	127.17
2	B	501	ATP	N3-C2-N1	-3.93	122.64	128.58
2	A	501	ATP	N3-C4-N9	3.90	133.79	127.17
2	A	503	ATP	C4-C5-N7	-3.89	106.13	110.58
2	A	501	ATP	N3-C2-N1	-3.77	122.88	128.58
2	B	501	ATP	N3-C4-N9	3.73	133.51	127.17
2	B	503	ATP	C2-N3-C4	3.72	120.91	111.83
2	A	501	ATP	C2-N3-C4	3.70	120.87	111.83
2	B	501	ATP	C2-N3-C4	3.64	120.71	111.83
2	B	503	ATP	N3-C2-N1	-3.61	123.11	128.58
2	A	503	ATP	C2-N3-C4	3.61	120.65	111.83
2	B	501	ATP	C4-C5-N7	-3.49	106.59	110.58
2	B	501	ATP	C4-N9-C8	3.32	109.22	105.74
2	B	503	ATP	C4-C5-N7	-3.14	107.00	110.58
2	A	503	ATP	N3-C2-N1	-3.05	123.97	128.58
2	A	501	ATP	C4-N9-C8	3.00	108.89	105.74
2	A	501	ATP	C4-C5-N7	-2.99	107.17	110.58
2	A	503	ATP	C5-N7-C8	2.91	108.02	103.45
2	B	501	ATP	C6-C5-N7	2.64	137.19	132.09
2	B	501	ATP	C5-N7-C8	2.57	107.49	103.45
2	B	501	ATP	C2-N1-C6	2.52	122.86	118.73
2	A	501	ATP	N9-C8-N7	-2.51	110.37	113.94
2	B	501	ATP	N9-C8-N7	-2.51	110.38	113.94
2	A	501	ATP	C6-C5-N7	2.46	136.83	132.09
2	A	501	ATP	C5-N7-C8	2.31	107.09	103.45
2	B	503	ATP	C2-N1-C6	2.26	122.44	118.73
2	B	503	ATP	C4-N9-C8	2.22	108.06	105.74
2	B	503	ATP	C5-N7-C8	2.21	106.92	103.45
2	A	501	ATP	C2-N1-C6	2.15	122.27	118.73
2	A	503	ATP	C2-N1-C6	2.08	122.15	118.73
2	B	501	ATP	C4-N9-C1'	-2.07	121.79	126.63

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	503	ATP	C5'-O5'-PA-O2A
2	B	503	ATP	C5'-O5'-PA-O3A

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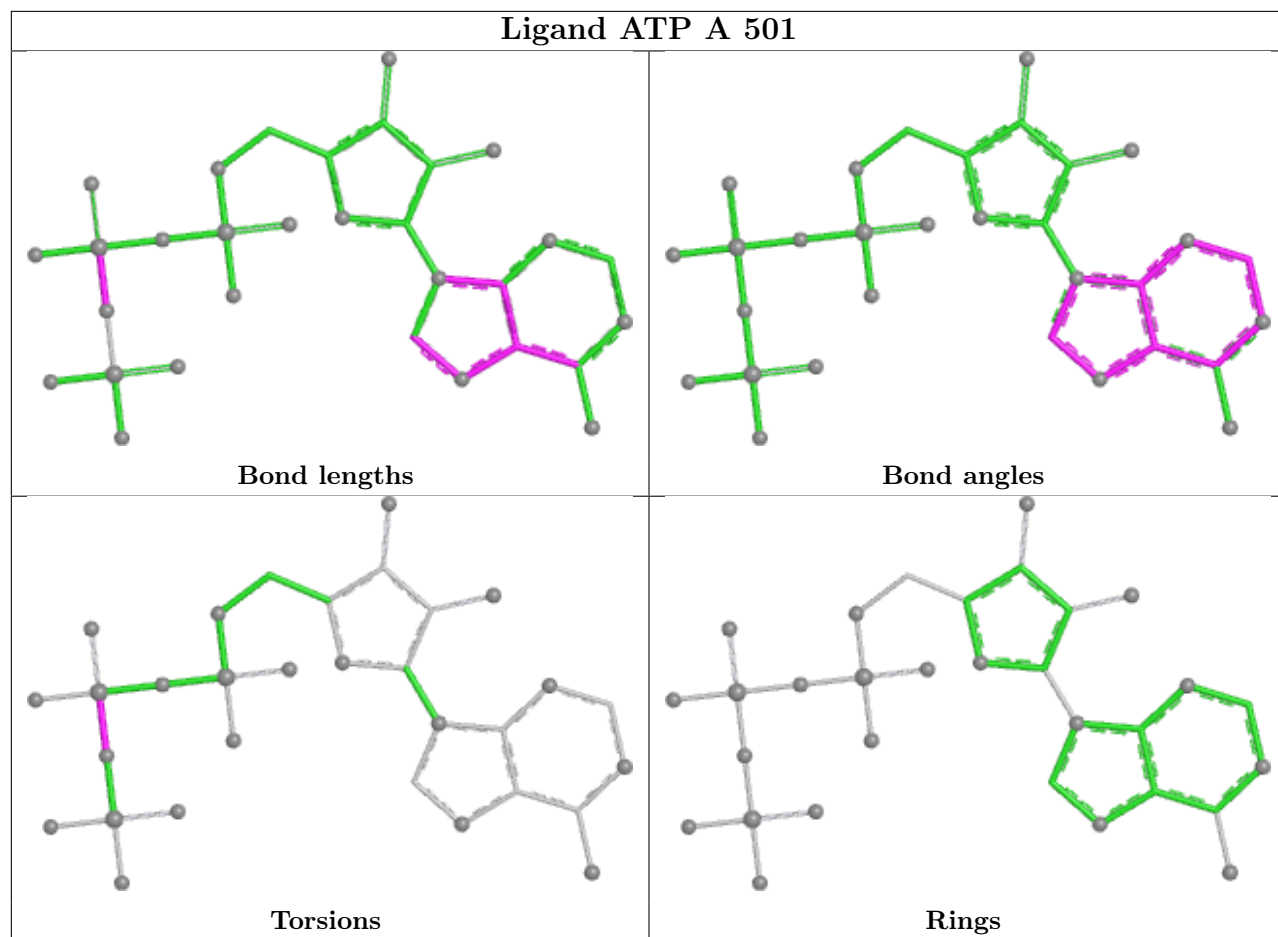
Mol	Chain	Res	Type	Atoms
5	A	506	GOL	O1-C1-C2-O2
5	A	506	GOL	O1-C1-C2-C3
2	B	501	ATP	PB-O3A-PA-O1A
2	B	501	ATP	C5'-O5'-PA-O3A
2	B	503	ATP	O4'-C4'-C5'-O5'
2	B	501	ATP	PG-O3B-PB-O2B
2	B	501	ATP	O4'-C4'-C5'-O5'
2	B	501	ATP	PG-O3B-PB-O1B
2	B	501	ATP	PB-O3A-PA-O2A
2	A	501	ATP	PG-O3B-PB-O2B

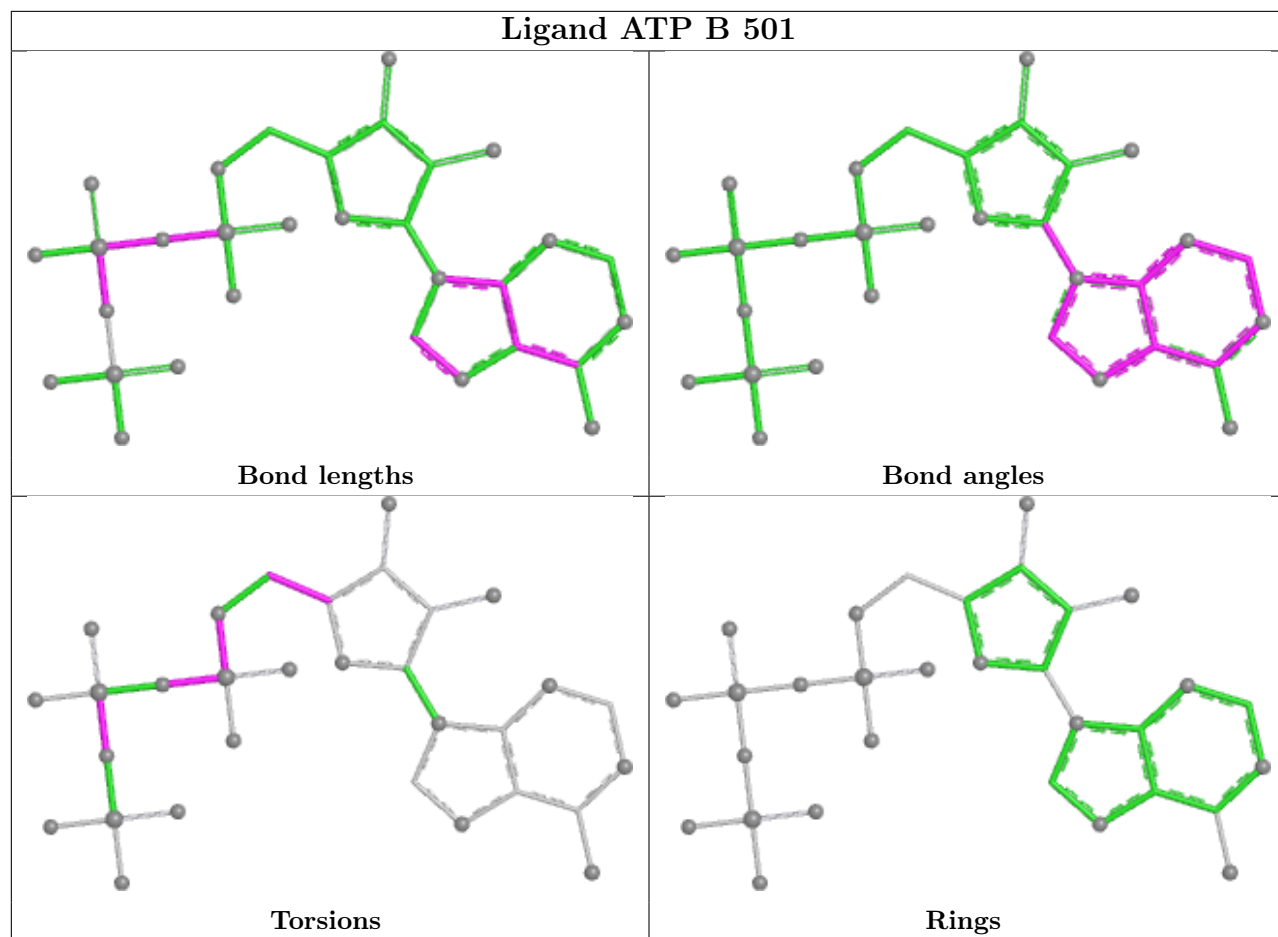
There are no ring outliers.

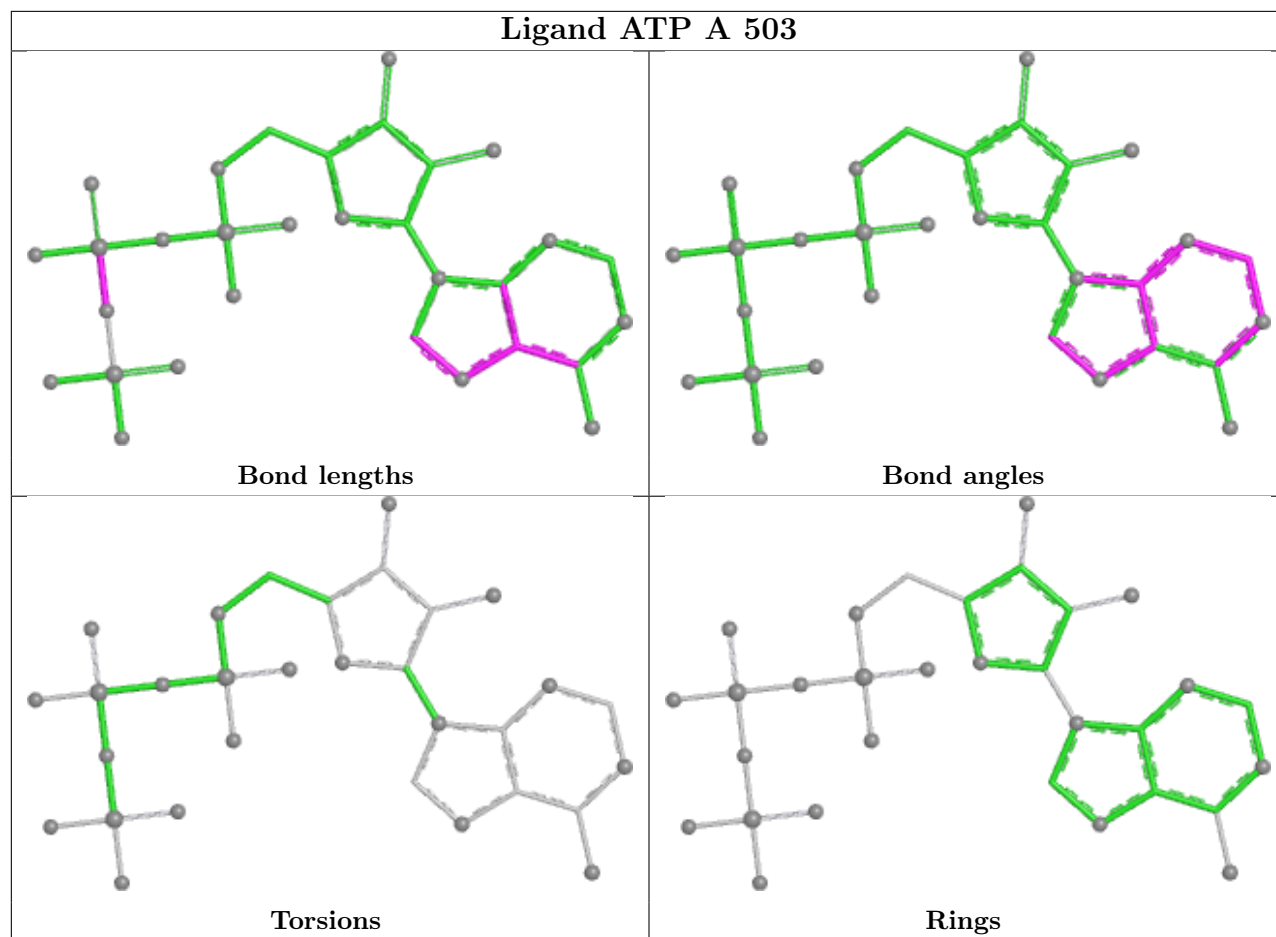
3 monomers are involved in 3 short contacts:

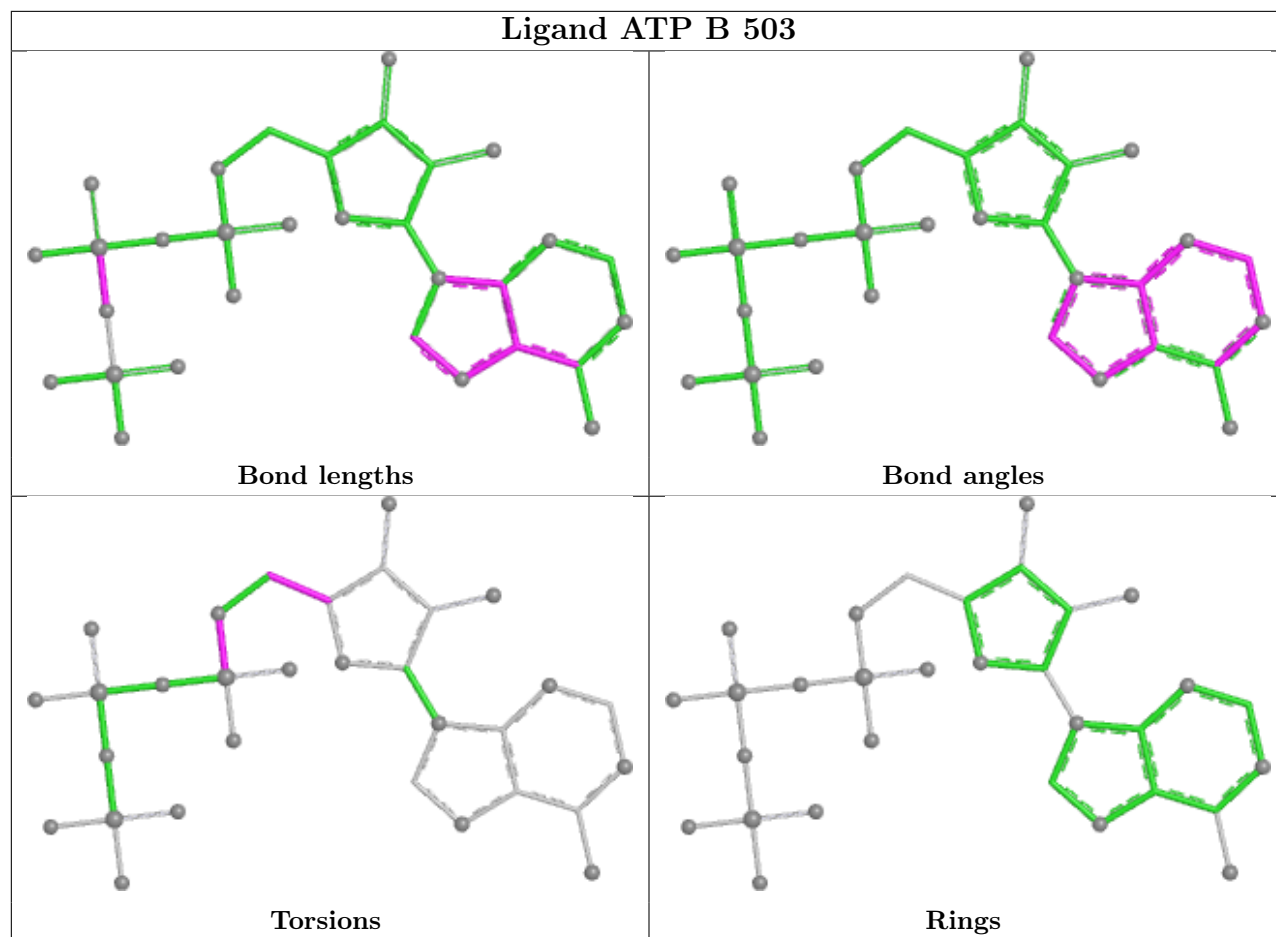
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ATP	1	0
2	B	501	ATP	1	0
2	A	503	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	415/509 (81%)	-0.30	3 (0%) 84 81	21, 37, 65, 83	20 (4%)
1	B	404/509 (79%)	0.24	27 (6%) 24 21	23, 56, 97, 122	34 (8%)
All	All	819/1018 (80%)	-0.03	30 (3%) 45 40	21, 44, 90, 122	54 (6%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	ILE	7.7
1	B	106	ILE	6.2
1	B	156	ASP	5.5
1	B	110	LEU	5.0
1	A	142	PRO	4.8
1	B	109	LEU	4.6
1	B	105	LYS	4.6
1	B	113	ALA	3.6
1	B	146	ASP	3.6
1	B	104	THR	3.6
1	B	125	GLU	3.6
1	A	203	ALA	3.5
1	B	111	GLN	3.2
1	B	108	GLU	3.0
1	B	103	SER	2.9
1	B	117	GLY	2.7
1	B	114	ARG	2.7
1	B	102	PRO	2.6
1	B	190	TYR	2.6
1	B	193	GLY	2.5
1	B	92	ALA	2.5
1	B	1	MET	2.4
1	B	124	VAL	2.3
1	B	88	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	143	ASN	2.1
1	B	116	TYR	2.1
1	B	50	ASP	2.1
1	B	112	MET	2.1
1	B	84	ARG	2.0
1	B	428	ALA	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](#)

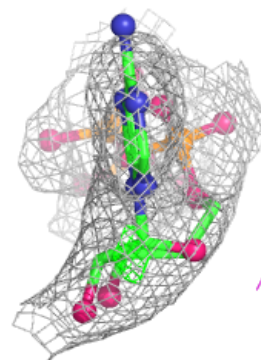
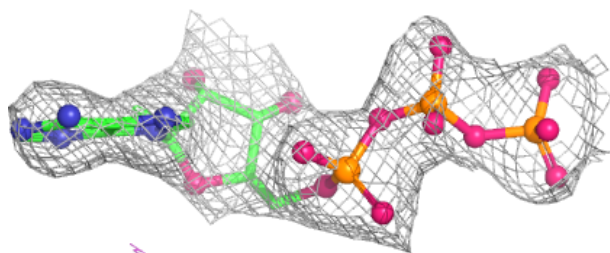
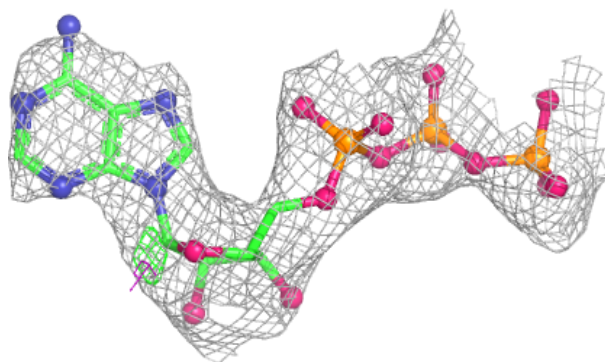
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	506	6/6	0.85	0.12	34,36,37,37	0
4	PO4	A	505	5/5	0.95	0.12	38,40,40,41	5
2	ATP	B	503	31/31	0.96	0.08	44,59,70,72	31
2	ATP	B	501	31/31	0.97	0.07	45,50,54,56	0
2	ATP	A	503	31/31	0.97	0.06	36,48,56,60	0
2	ATP	A	501	31/31	0.98	0.05	27,31,48,51	0
3	MN	A	504	1/1	0.98	0.04	49,49,49,49	0
3	MN	B	504	1/1	0.99	0.01	53,53,53,53	0
3	MN	A	502	1/1	0.99	0.02	38,38,38,38	0
3	MN	B	502	1/1	0.99	0.02	55,55,55,55	0

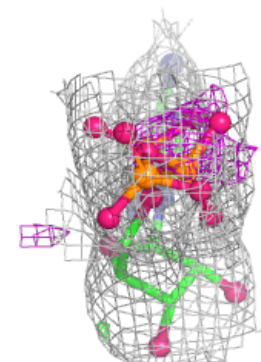
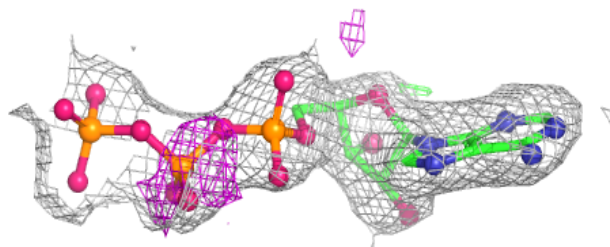
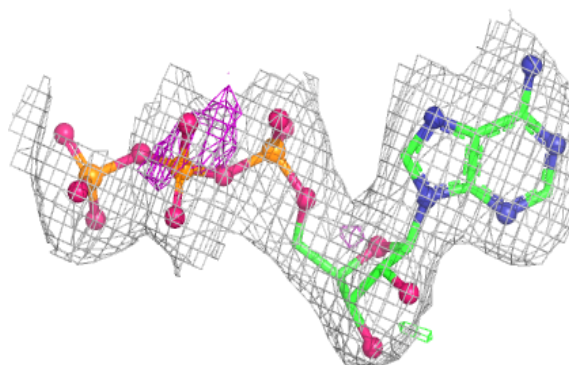
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 503:

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

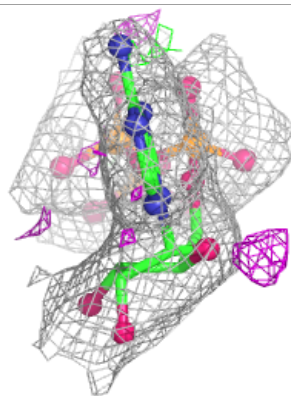
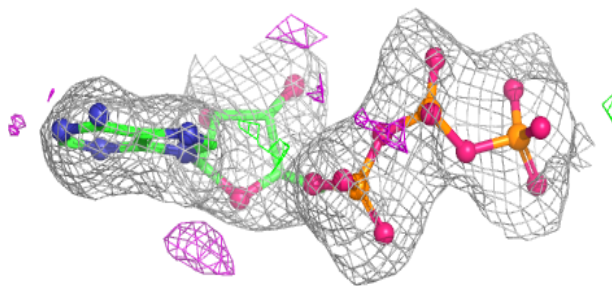
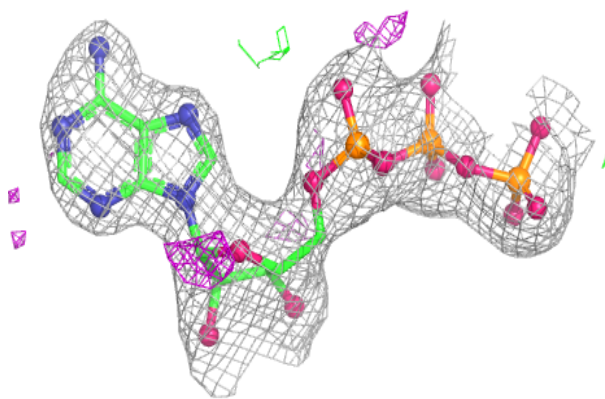
**Electron density around ATP B 501:**

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

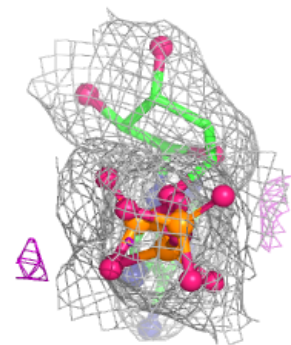
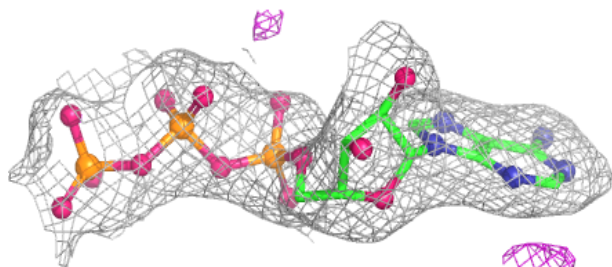
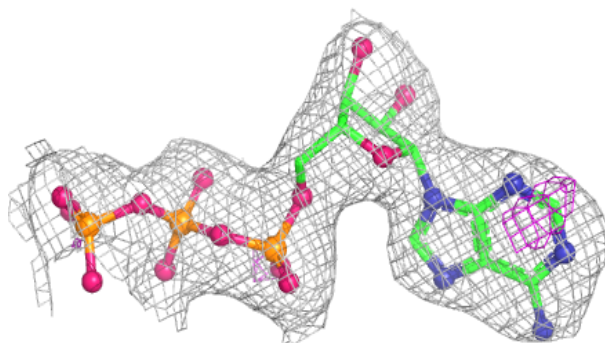


Electron density around ATP A 503:

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

**Electron density around ATP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.