



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:46 pm BST

PDB ID : 4DQW
Title : Crystal Structure Analysis of PA3770
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 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 : 2.11
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) : 2.11

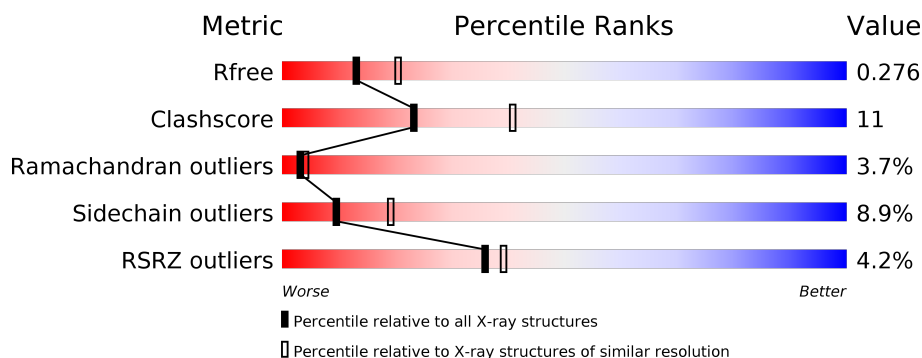
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>16%</div> <div>5%</div> <div>18%</div> </div> </div>
1	B	509	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>15%</div> <div>• •</div> <div>21%</div> </div> </div>

2 Entry composition

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:

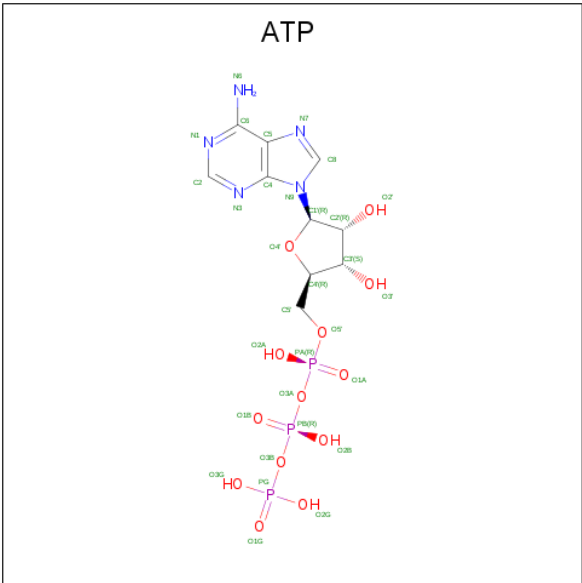
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9HXM5
A	-18	GLY	-	EXPRESSION TAG	UNP Q9HXM5
A	-17	SER	-	EXPRESSION TAG	UNP Q9HXM5
A	-16	SER	-	EXPRESSION TAG	UNP Q9HXM5
A	-15	HIS	-	EXPRESSION TAG	UNP Q9HXM5
A	-14	HIS	-	EXPRESSION TAG	UNP Q9HXM5
A	-13	HIS	-	EXPRESSION TAG	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 (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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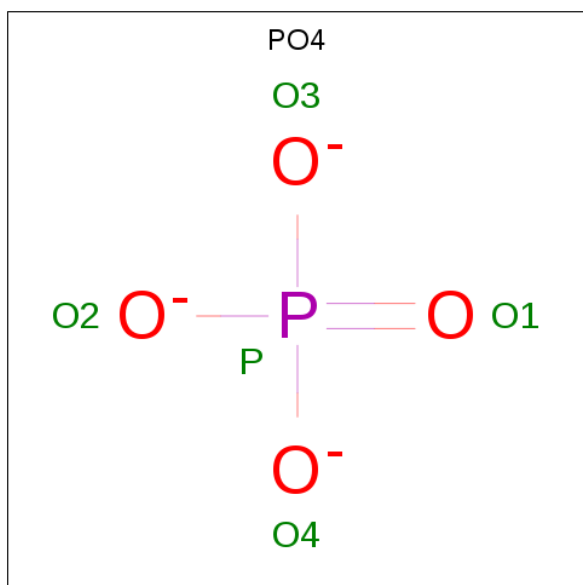
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

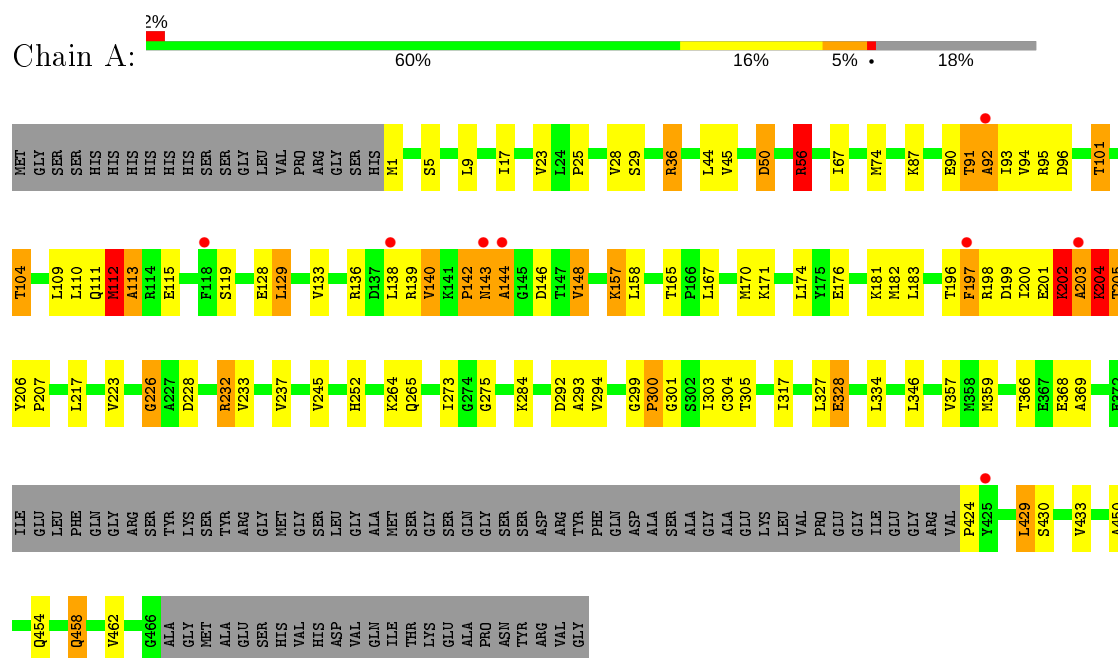
- Molecule 6 is water.

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

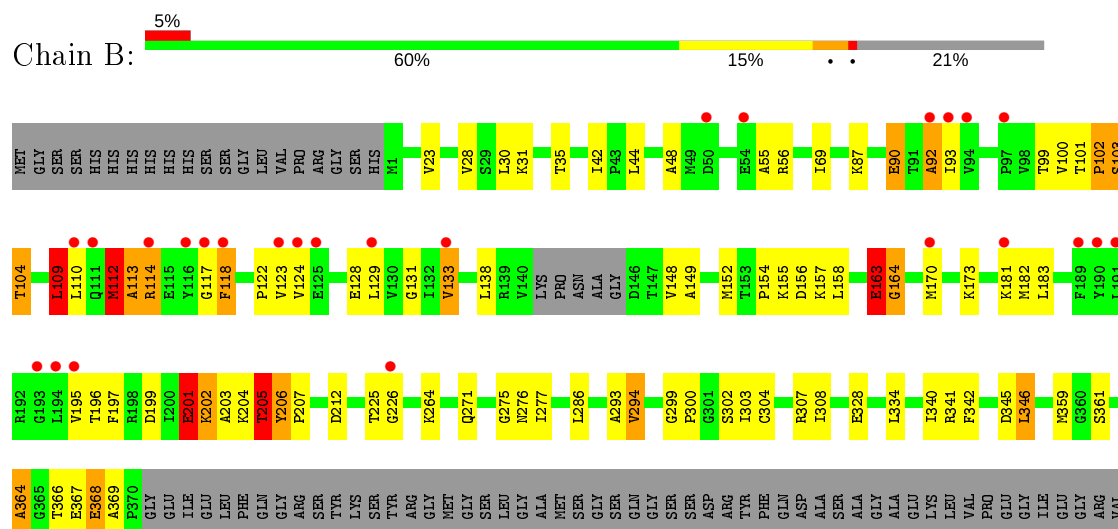
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



PRO	TYR	LYS	GLY	A428	I429	S430	V433	I452	Q453	Q458	P459	G466	ALA	GLY	MET	ALA	GLU	SER	HIS	VAL	HIS	ASP	VAL	GLN	ILE	THR	LYS	GLU	ALA	PRO	ASN	TYR	ARG	VAL	GLY
-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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 95.05 – 2.51	Depositor EDS
% Data completeness (in resolution range)	88.8 (54.92-2.51) 88.8 (95.05-2.51)	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)	0.32 , 42.2	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, MN, 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	0.51	0/3123	0.69	2/4224 (0.0%)
1	B	0.47	0/3005	0.71	1/4068 (0.0%)
All	All	0.49	0/6128	0.70	3/8292 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ASN	N-CA-C	-5.25	96.83	111.00
1	A	56[A]	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	56[B]	ARG	NE-CZ-NH1	5.06	122.83	120.30

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

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Mol	Chain	Res	Type	Group
1	A	202	LYS	Peptide
1	A	204	LYS	Peptide
1	A	226	GLY	Peptide
1	A	275	GLY	Mainchain,Peptide
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 ⓘ

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	70	0
1	B	2967	0	3043	71	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
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	141	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 11.

All (141) 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:429:LEU:HD22	1:A:433:VAL:HG23	1.54	0.88
1:B:163:GLU:HG3	1:B:164:GLY:N	1.88	0.87
1:B:155:LYS:HA	1:B:158:LEU:HD13	1.57	0.86
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:HG22	1:B:303:ILE:O	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: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:149:ALA:HA	1:B:152:MET:HE2	1.74	0.67
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:A:357:VAL:HG23	1:A:359:MET:HE2	1.78	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:100:VAL:HG23	1:B:123:VAL:HG22	1.79	0.63
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:O	1:A:1:MET:CG	2.47	0.62
1:A:139:ARG:O	1:A:140:VAL:HB	2.00	0.61
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: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:44:LEU:HD22	1:A:359:MET:HE3	1.85	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:357:VAL:HG23	1:A:359:MET:CE	2.39	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:B:87:LYS:NZ	1:B:212:ASP:OD2	2.39	0.50
1:B:196:THR:OG1	1:B:199:ASP:OD2	2.29	0.50
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:A:56[A]:ARG:HH11	1:A:56[A]:ARG:HG3	1.78	0.48
1:B:277:ILE:HD11	1:B:294:VAL:CG1	2.43	0.48
1:A:205:THR:O	1:A:205:THR:OG1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:346:LEU:HD12	1:B:346:LEU:O	2.16	0.46
1:A:200:ILE:C	1:A:202:LYS:H	2.18	0.46
1:A:273:ILE:HG12	1:A:293:ALA:HB3	1.98	0.46
1:B:103:SER:O	1:B:104:THR:C	2.55	0.46
1:B:340:ILE:HG23	1:B:345:ASP:HB2	1.98	0.46
1:B:35:THR:HA	1:B:293:ALA:HB2	1.98	0.46
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:131:GLY:HA2	1:B:158:LEU:HD11	1.97	0.45
1:B:99:THR:HG22	1:B:122:PRO:HG2	1.98	0.44
1:B:44:LEU:CD2	1:B:359:MET:HE1	2.47	0.44
1:A:366:THR:CG2	1:A:369:ALA:H	2.30	0.44
1:A:90:GLU:HB2	1:A:93:ILE:HD12	1.99	0.44
1:B:109:LEU:O	1:B:112:MET:N	2.46	0.44
1:A:202:LYS:O	1:A:203:ALA:CB	2.65	0.44
1:B:366:THR:O	1:B:367:GLU:C	2.56	0.44
1:B:429:LEU:HD22	1:B:429:LEU:O	2.18	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:B:42:ILE:HD12	1:B:44:LEU:HD12	2.01	0.43
1:B:155:LYS:C	1:B:157:LYS:H	2.23	0.43
1:A:87:LYS:NZ	1:A:217:LEU:O	2.45	0.42
1:A:303:ILE:O	1:A:303:ILE:HG22	2.19	0.42
1:B:100:VAL:HG21	1:B:133:VAL:HG21	2.01	0.42
1:B:170:MET:HE1	1:B:195:VAL:HG21	2.00	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:170:MET:CG	1:A:182:MET:HG2	2.50	0.42
1:A:90:GLU:CB	1:A:93:ILE:HD12	2.50	0.42
1:A:109:LEU:O	1:A:113:ALA:CB	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:PRO:C	1:B:158:LEU:CD1	2.88	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:327:LEU:O	1:A:328:GLU:C	2.59	0.41
1:B:92:ALA:HB3	1:B:199:ASP:HB3	2.00	0.41
1:B:48:ALA:HB2	1:B:69:ILE:CG2	2.51	0.41
1:A:167:LEU:HD22	1:A:200:ILE:HG12	2.03	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:174:LEU:HD21	1:A:181:LYS:C	2.41	0.40
1:A:74:MET:O	1:A:232:ARG:NH1	2.54	0.40
1:A:9:LEU:O	1:A:317:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/509 (81%)	383 (93%)	17 (4%)	13 (3%)	4	5
1	B	399/509 (78%)	348 (87%)	34 (8%)	17 (4%)	2	3
All	All	812/1018 (80%)	731 (90%)	51 (6%)	30 (4%)	3	4

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ALA
1	A	140	VAL

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Mol	Chain	Res	Type
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
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%)	284 (89%)	34 (11%)	6	13
1	B	303/390 (78%)	281 (93%)	22 (7%)	14	27
All	All	621/780 (80%)	565 (91%)	56 (9%)	9	19

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
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	95	ARG
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	142	PRO
1	A	143	ASN
1	A	146	ASP
1	A	148	VAL
1	A	176	GLU
1	A	197	PHE
1	A	202	LYS
1	A	204	LYS
1	A	232	ARG
1	A	264	LYS
1	A	265	GLN
1	A	284	LYS
1	A	294	VAL
1	A	300	PRO
1	A	305	THR
1	A	334	LEU
1	A	429	LEU
1	A	430	SER
1	B	31	LYS
1	B	114	ARG
1	B	118	PHE
1	B	128	GLU
1	B	133	VAL
1	B	163	GLU
1	B	173	LYS
1	B	197	PHE

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Mol	Chain	Res	Type
1	B	201	GLU
1	B	202	LYS
1	B	205	THR
1	B	225	THR
1	B	264	LYS
1	B	294	VAL
1	B	334	LEU
1	B	342	PHE
1	B	346	LEU
1	B	368	GLU
1	B	429	LEU
1	B	430	SER
1	B	452	ILE
1	B	453	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	GLN
1	A	458	GLN
1	B	453	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	ATP	A	503	3	26,33,33	1.01	1 (3%)	31,52,52	1.36	3 (9%)
5	GOL	A	506	-	5,5,5	0.47	0	5,5,5	0.49	0
2	ATP	A	501	3	26,33,33	0.88	1 (3%)	31,52,52	1.39	6 (19%)
4	PO4	A	505	-	4,4,4	0.66	0	6,6,6	0.53	0
2	ATP	B	503	3	26,33,33	0.92	1 (3%)	31,52,52	1.42	6 (19%)
2	ATP	B	501	3	26,33,33	0.96	1 (3%)	31,52,52	1.41	4 (12%)

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	503	3	-	0/18/38/38	0/3/3/3
2	ATP	B	503	3	-	3/18/38/38	0/3/3/3
2	ATP	B	501	3	-	6/18/38/38	0/3/3/3
2	ATP	A	501	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	ATP	C5-C4	2.58	1.47	1.40
2	B	503	ATP	C5-C4	2.50	1.47	1.40
2	B	501	ATP	C5-C4	2.40	1.47	1.40
2	A	501	ATP	C5-C4	2.14	1.46	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ATP	N3-C2-N1	-3.87	122.64	128.68
2	A	501	ATP	N3-C2-N1	-3.71	122.88	128.68
2	B	503	ATP	N3-C2-N1	-3.56	123.11	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	ATP	C4-C5-N7	-3.14	106.13	109.40
2	A	503	ATP	N3-C2-N1	-3.01	123.97	128.68
2	B	501	ATP	C1'-N9-C4	-2.76	121.79	126.64
2	B	503	ATP	C3'-C2'-C1'	2.73	105.09	100.98
2	B	501	ATP	C4-C5-N7	-2.69	106.59	109.40
2	A	503	ATP	PB-O3B-PG	-2.65	123.74	132.83
2	B	503	ATP	PA-O3A-PB	-2.46	124.39	132.83
2	B	503	ATP	PB-O3B-PG	-2.43	124.48	132.83
2	B	501	ATP	C2-N1-C6	2.40	122.86	118.75
2	B	503	ATP	C4-C5-N7	-2.31	107.00	109.40
2	A	501	ATP	PA-O3A-PB	-2.28	125.00	132.83
2	A	501	ATP	PB-O3B-PG	-2.17	125.38	132.83
2	B	503	ATP	C2-N1-C6	2.15	122.44	118.75
2	A	501	ATP	C4-C5-N7	-2.14	107.17	109.40
2	A	501	ATP	C2-N1-C6	2.05	122.27	118.75
2	A	501	ATP	C1'-N9-C4	-2.04	123.05	126.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

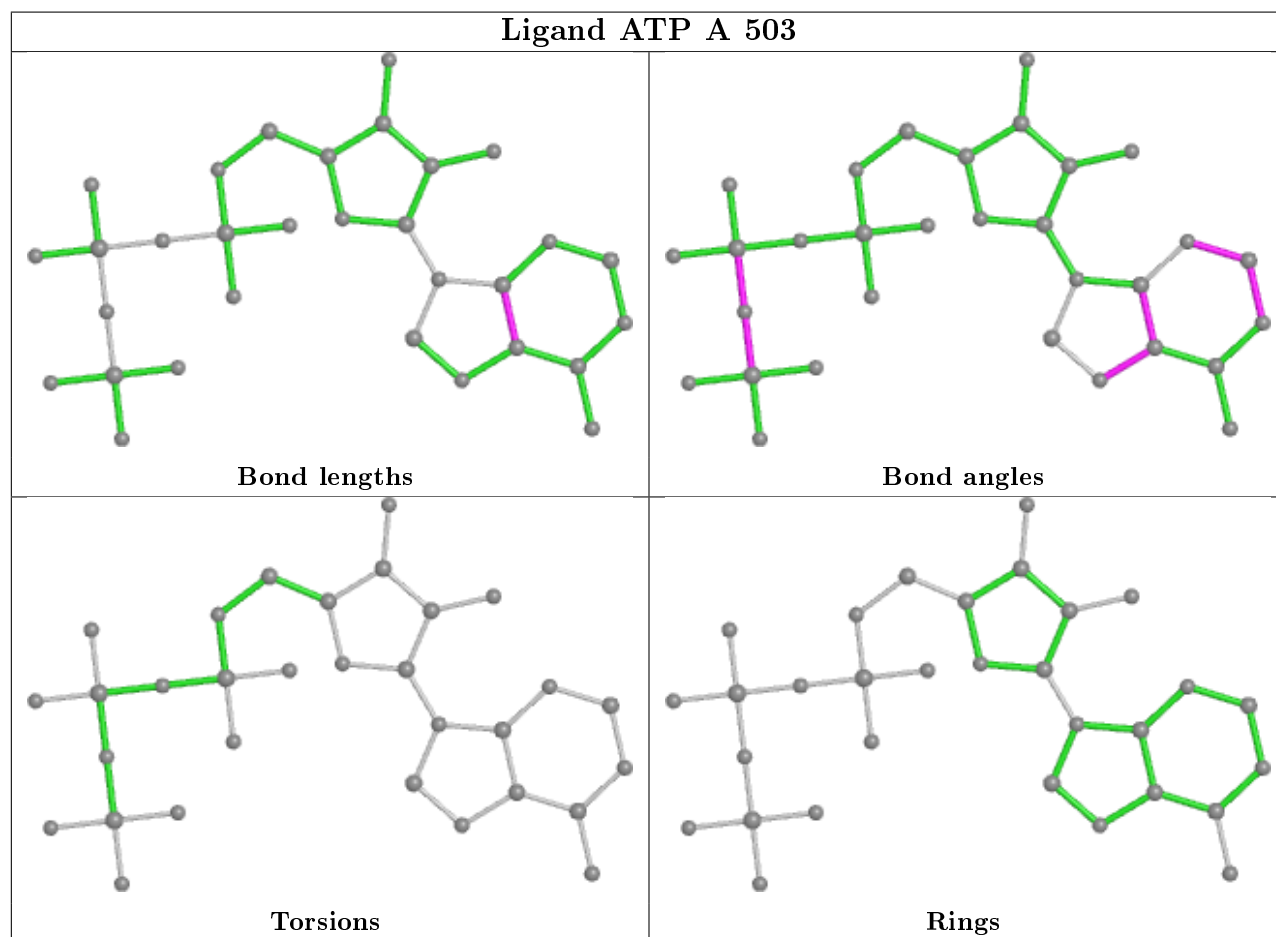
Mol	Chain	Res	Type	Atoms
2	B	503	ATP	C5'-O5'-PA-O2A
2	B	503	ATP	C5'-O5'-PA-O3A
5	A	506	GOL	O1-C1-C2-O2
5	A	506	GOL	O1-C1-C2-C3
2	B	501	ATP	C5'-O5'-PA-O3A
2	B	503	ATP	O4'-C4'-C5'-O5'
2	B	501	ATP	PB-O3A-PA-O1A
2	B	501	ATP	PG-O3B-PB-O2B
2	B	501	ATP	O4'-C4'-C5'-O5'
2	B	501	ATP	PG-O3B-PB-O1B
2	B	501	ATP	PB-O3A-PA-O2A

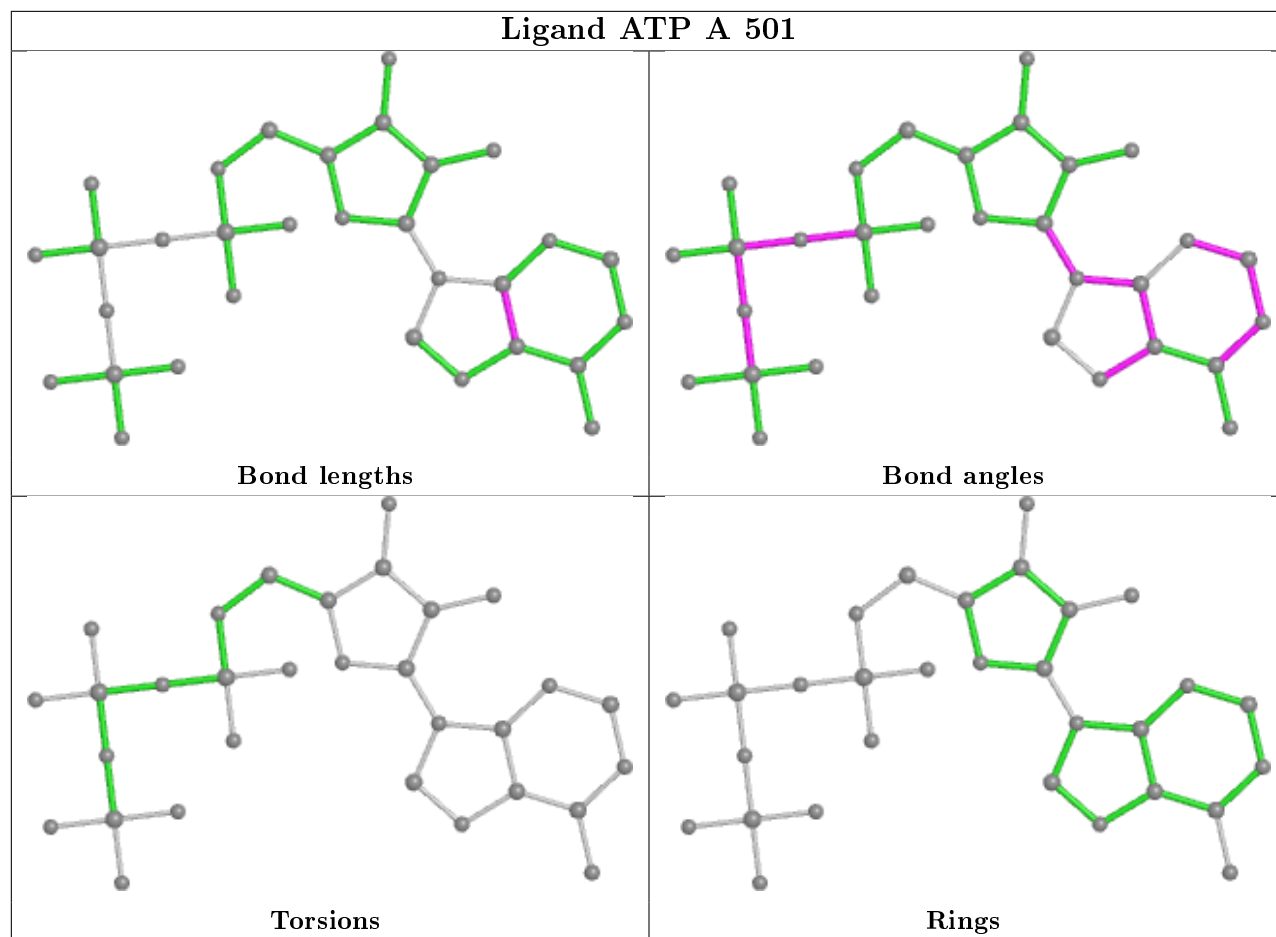
There are no ring outliers.

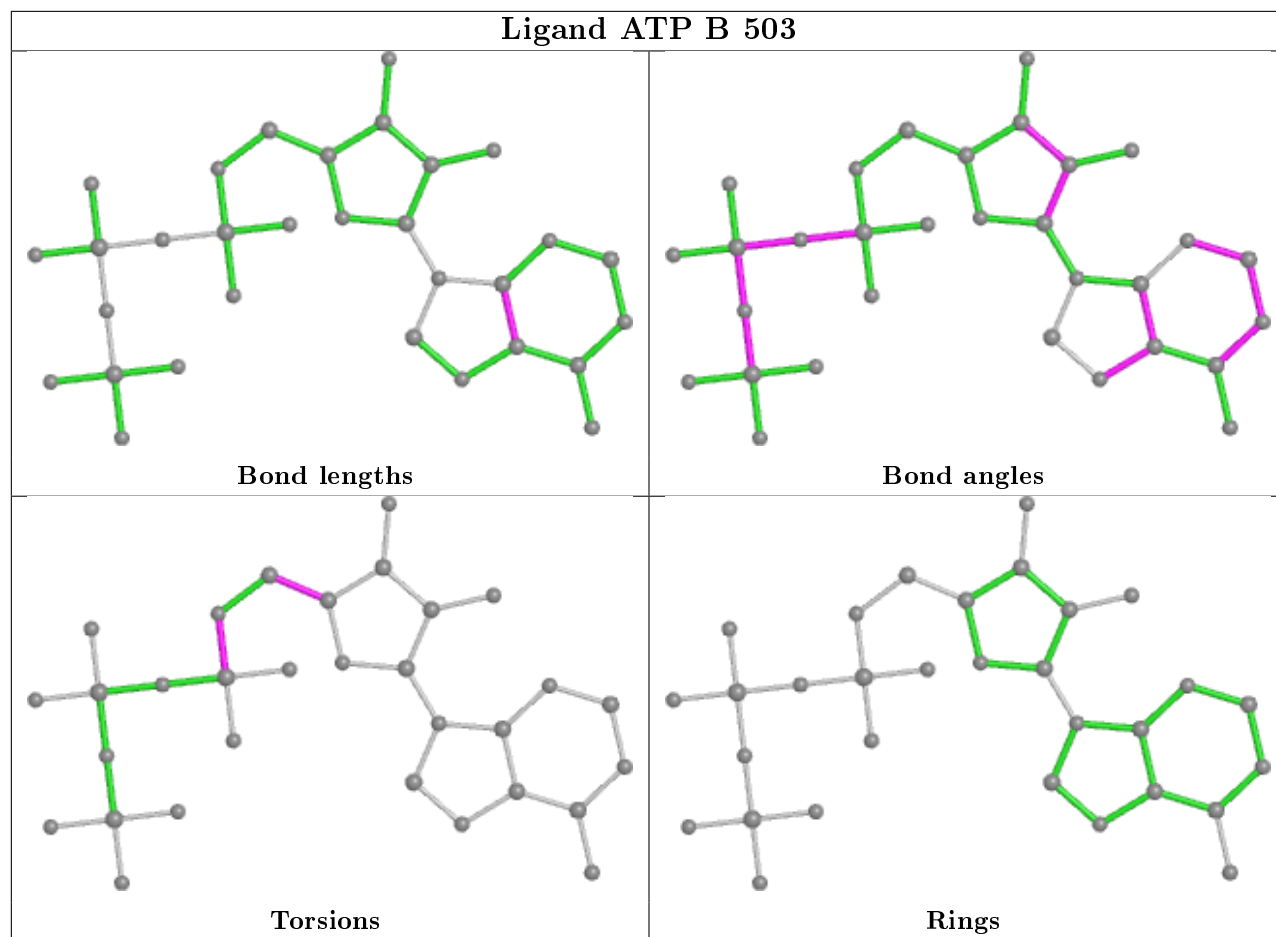
3 monomers are involved in 3 short contacts:

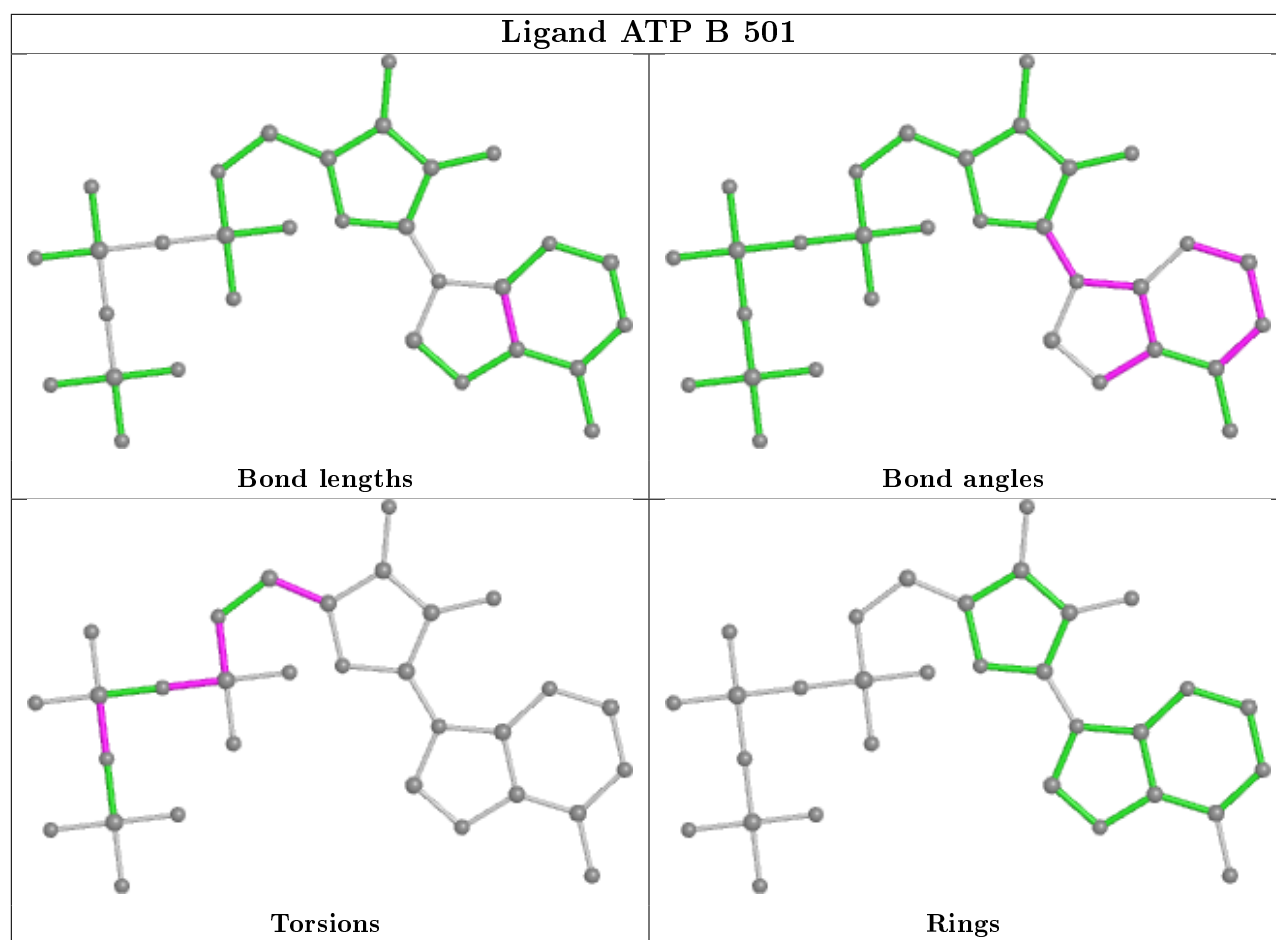
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	ATP	1	0
2	A	501	ATP	1	0
2	B	501	ATP	1	0

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%)	0.04	8 (1%) 66 69	21, 38, 67, 86	18 (4%)
1	B	404/509 (79%)	0.43	26 (6%) 19 20	23, 56, 105, 137	33 (8%)
All	All	819/1018 (80%)	0.23	34 (4%) 36 39	21, 44, 95, 137	51 (6%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	6.6
1	B	129	LEU	3.5
1	B	111	GLN	3.4
1	B	190	TYR	3.2
1	A	197	PHE	3.2
1	A	203	ALA	3.1
1	B	116	TYR	3.1
1	B	191	LEU	3.1
1	B	97	PRO	2.8
1	B	124	VAL	2.8
1	B	189	PHE	2.8
1	A	118	PHE	2.8
1	B	110	LEU	2.7
1	A	138	LEU	2.7
1	B	94	VAL	2.5
1	B	226	GLY	2.5
1	B	133	VAL	2.5
1	B	117	GLY	2.5
1	B	118	PHE	2.4
1	B	181	LYS	2.4
1	B	54	GLU	2.4
1	A	92	ALA	2.3
1	B	50	ASP	2.3
1	A	144	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	ALA	2.2
1	B	93	ILE	2.2
1	A	425	TYR	2.2
1	B	114	ARG	2.2
1	B	195	VAL	2.2
1	B	170	MET	2.1
1	B	125	GLU	2.1
1	A	143	ASN	2.1
1	B	123	VAL	2.1
1	B	194	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

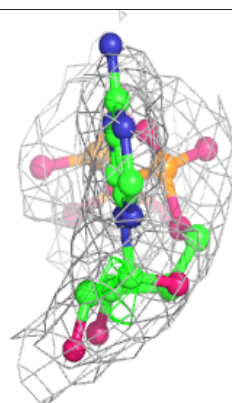
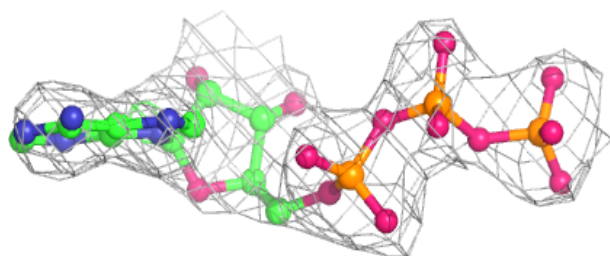
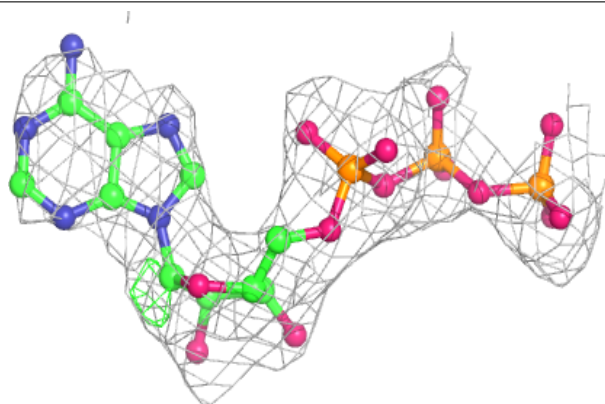
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	506	6/6	0.93	0.09	34,36,37,37	0
2	ATP	B	503	31/31	0.95	0.19	44,59,70,72	31
2	ATP	A	503	31/31	0.97	0.19	36,48,56,60	0
2	ATP	B	501	31/31	0.97	0.15	45,50,54,56	0
4	PO4	A	505	5/5	0.98	0.15	38,40,40,41	5
3	MN	A	502	1/1	0.98	0.11	38,38,38,38	0
3	MN	A	504	1/1	0.98	0.14	49,49,49,49	0
2	ATP	A	501	31/31	0.98	0.15	27,31,48,51	0
3	MN	B	504	1/1	0.99	0.10	53,53,53,53	0
3	MN	B	502	1/1	0.99	0.09	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.

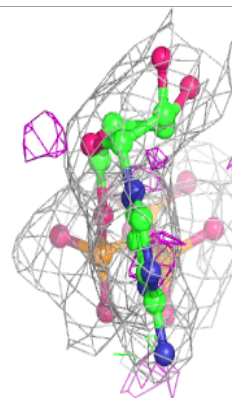
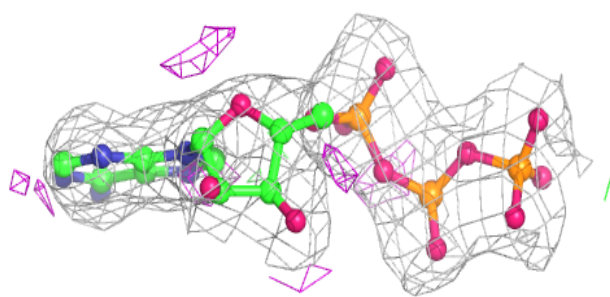
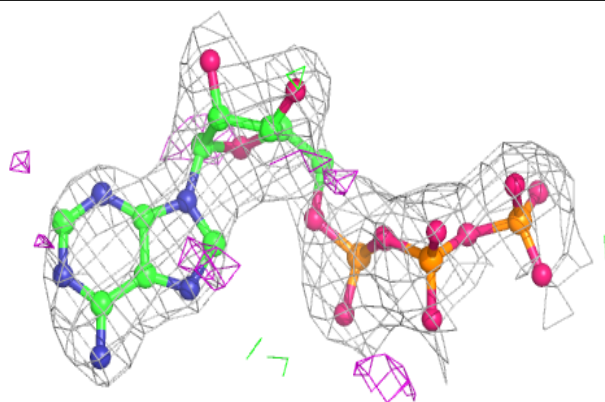
Electron density around ATP B 503:

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



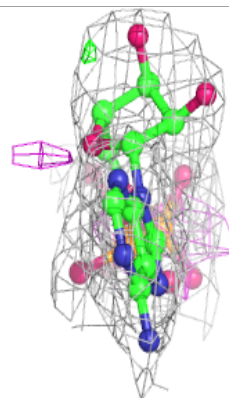
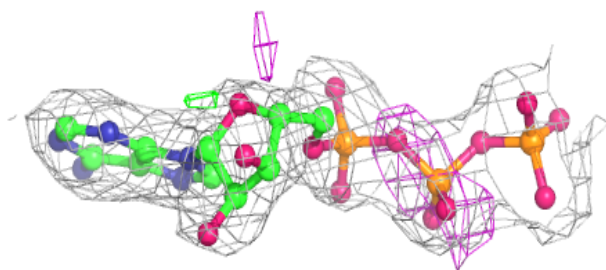
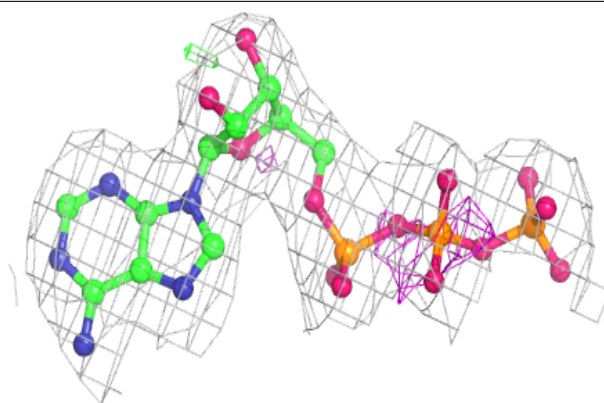
Electron density around ATP A 503:

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

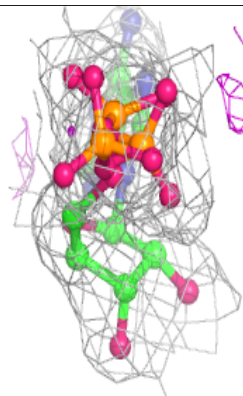
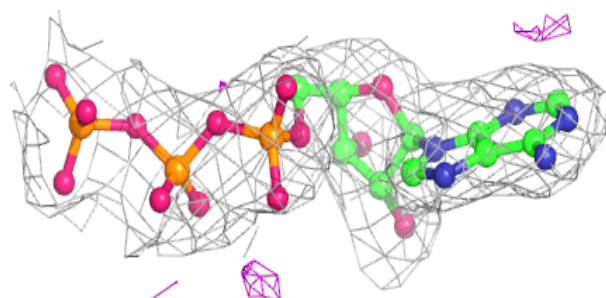
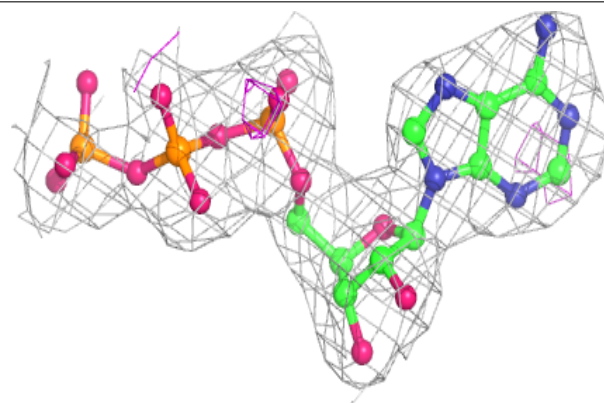


Electron density around ATP B 501:

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

**Electron density around ATP A 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

There are no such residues in this entry.