



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 10:49 AM EST

PDB ID : 9YS2 / pdb_00009ys2
Title : Crystal structure of Cysteinyl-tRNA synthetase (CysRS) from Plasmodium falciparum in complex with cysteinyl-AMP
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-10-17
Resolution : 2.22 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	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

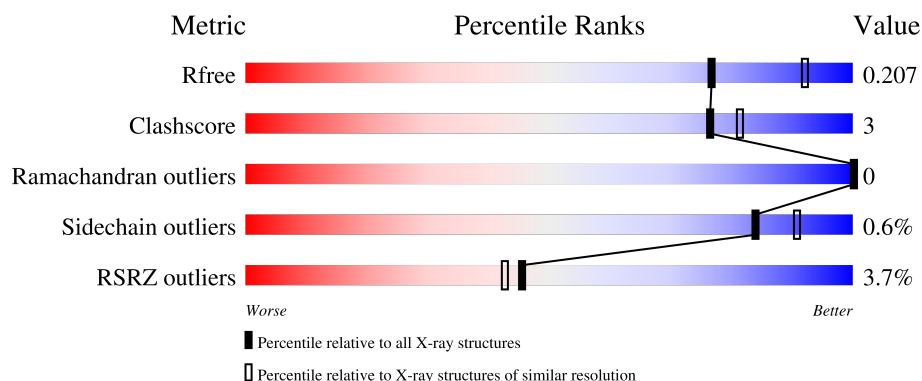
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	466	<div> <div>3%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	B	466	<div> <div>4%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7509 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 Cysteine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3546	2305	582	645	14			
1	B	430	Total	C	N	O	S	0	0	0
			3547	2307	583	643	14			

There are 42 discrepancies between the modelled and reference sequences:

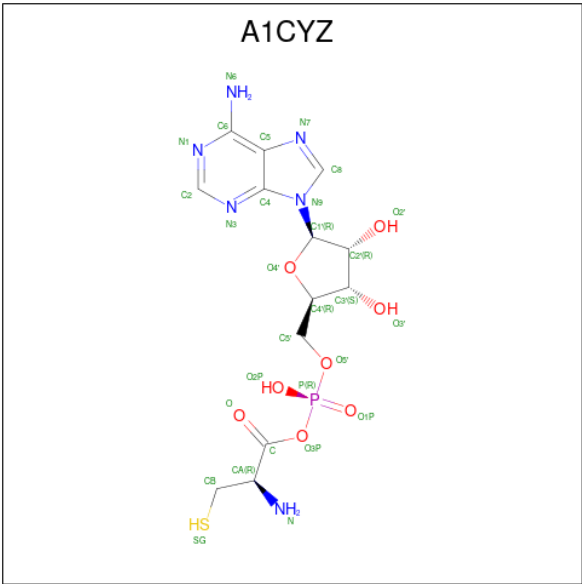
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8IJP3
A	-6	ALA	-	expression tag	UNP Q8IJP3
A	-5	HIS	-	expression tag	UNP Q8IJP3
A	-4	HIS	-	expression tag	UNP Q8IJP3
A	-3	HIS	-	expression tag	UNP Q8IJP3
A	-2	HIS	-	expression tag	UNP Q8IJP3
A	-1	HIS	-	expression tag	UNP Q8IJP3
A	0	HIS	-	expression tag	UNP Q8IJP3
A	1	MET	-	expression tag	UNP Q8IJP3
A	2	GLY	-	expression tag	UNP Q8IJP3
A	3	THR	-	expression tag	UNP Q8IJP3
A	4	LEU	-	expression tag	UNP Q8IJP3
A	5	GLU	-	expression tag	UNP Q8IJP3
A	6	ALA	-	expression tag	UNP Q8IJP3
A	7	GLN	-	expression tag	UNP Q8IJP3
A	8	THR	-	expression tag	UNP Q8IJP3
A	9	GLN	-	expression tag	UNP Q8IJP3
A	10	GLY	-	expression tag	UNP Q8IJP3
A	11	PRO	-	expression tag	UNP Q8IJP3
A	12	GLY	-	expression tag	UNP Q8IJP3
A	13	SER	-	expression tag	UNP Q8IJP3
B	-7	MET	-	initiating methionine	UNP Q8IJP3
B	-6	ALA	-	expression tag	UNP Q8IJP3
B	-5	HIS	-	expression tag	UNP Q8IJP3
B	-4	HIS	-	expression tag	UNP Q8IJP3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q8IJP3
B	-2	HIS	-	expression tag	UNP Q8IJP3
B	-1	HIS	-	expression tag	UNP Q8IJP3
B	0	HIS	-	expression tag	UNP Q8IJP3
B	1	MET	-	expression tag	UNP Q8IJP3
B	2	GLY	-	expression tag	UNP Q8IJP3
B	3	THR	-	expression tag	UNP Q8IJP3
B	4	LEU	-	expression tag	UNP Q8IJP3
B	5	GLU	-	expression tag	UNP Q8IJP3
B	6	ALA	-	expression tag	UNP Q8IJP3
B	7	GLN	-	expression tag	UNP Q8IJP3
B	8	THR	-	expression tag	UNP Q8IJP3
B	9	GLN	-	expression tag	UNP Q8IJP3
B	10	GLY	-	expression tag	UNP Q8IJP3
B	11	PRO	-	expression tag	UNP Q8IJP3
B	12	GLY	-	expression tag	UNP Q8IJP3
B	13	SER	-	expression tag	UNP Q8IJP3

- Molecule 2 is 5'-O-[(R)-{[(2R)-2-amino-3-sulfanylpropanoyl]oxy}(hydroxy)phosphoryl]adenosine (CCD ID: A1CYZ) (formula: C₁₃H₁₉N₆O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			29	13	6	8	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			29	13	6	8	1	1		

-
- The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (a purine ring system with an amino group at the 6-position) attached to a ribose sugar (a five-membered ring with hydroxyl groups at the 2' and 3' positions). The ribose is linked to a chain of three phosphate groups (labeled alpha, beta, and gamma) via phosphodiester bonds. The alpha phosphate is directly attached to the 5' carbon of the ribose. The beta and gamma phosphates are linked in series. The structure is shown with stereochemistry, including wedge and dash bonds to indicate the 3D arrangement of atoms. Various atoms are labeled with numbers (e.g., N1, N3, N7, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801

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

- MLI
-
- The diagram shows the chemical structure of Malic acid (MLI). It consists of a three-carbon chain. The central carbon (C1) is bonded to two hydroxyl groups (O6 and O8). The rightmost carbon (C2) is bonded to a carboxylate group (O7 and O9). The leftmost carbon (C3) is bonded to a carboxylate group (O6 and O8). The atoms are labeled as follows: C1, C2, C3, O6, O7, O8, and O9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Na 2 2	0	0
6	B	2	Total Na 2 2	0	0

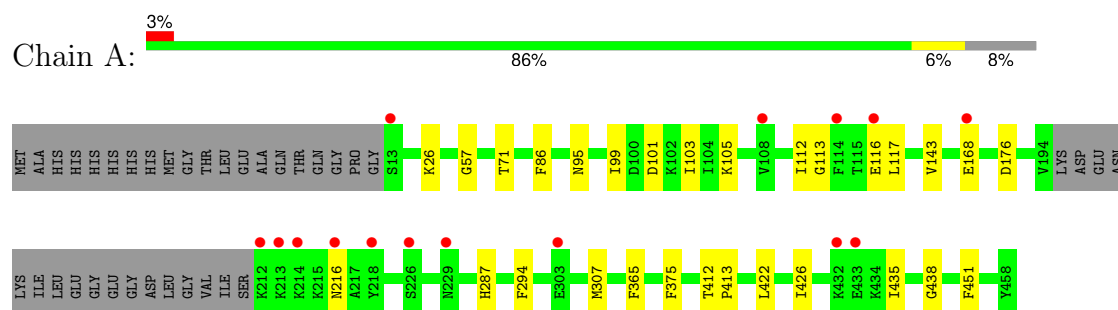
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	152	Total O 152 152	0	0
7	B	103	Total O 103 103	0	0

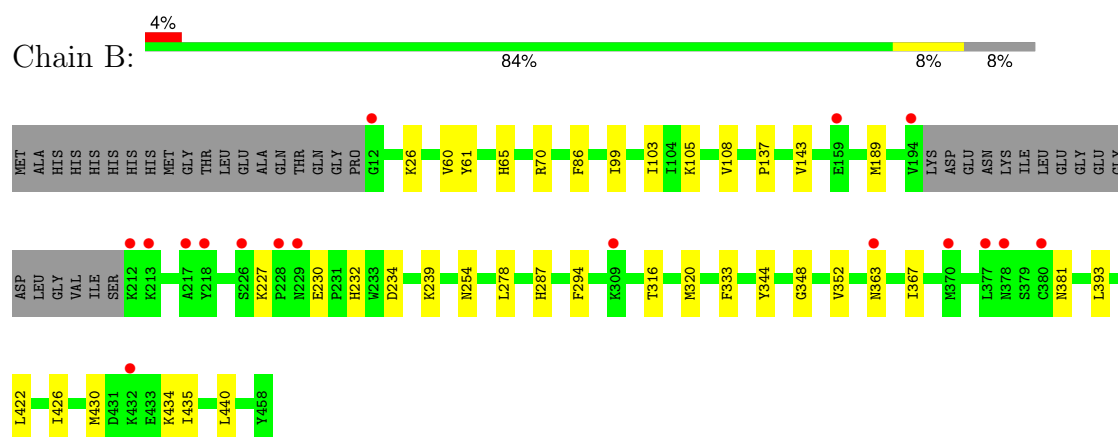
3 Residue-property plots [i](#)

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: Cysteine-tRNA ligase



• Molecule 1: Cysteine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.04Å 120.04Å 365.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.82 – 2.22 47.82 – 2.22	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.82-2.22) 100.0 (47.82-2.22)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.22Å)	Xtriage
Refinement program	PHENIX (2.0_5847: ???)	Depositor
R, R_{free}	0.176 , 0.205 0.179 , 0.207	Depositor DCC
R_{free} test set	3949 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7509	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: MLI, NA, ZN, ATP, A1CYZ

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	0.36	0/3643	0.54	0/4928
1	B	0.35	0/3644	0.53	0/4928
All	All	0.35	0/7287	0.53	0/9856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3546	0	3455	20	0
1	B	3547	0	3461	20	0
2	A	29	0	0	1	0
2	B	29	0	0	0	0
3	A	62	0	24	0	0
4	A	14	0	4	1	0
4	B	21	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	152	0	0	0	0
7	B	103	0	0	0	0
All	All	7509	0	6950	39	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 3.

All (39) 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:426:ILE:HG22	1:B:430:MET:HE2	1.66	0.77
1:A:168:GLU:N	1:A:168:GLU:OE1	2.32	0.61
1:A:113:GLY:N	1:A:116:GLU:OE1	2.34	0.61
1:A:112:ILE:HD11	1:A:117:LEU:HB2	1.81	0.60
1:B:435:ILE:HD13	1:B:440:LEU:HD12	1.86	0.58
4:A:504:MLI:H11	1:B:393:LEU:HD23	1.86	0.58
1:A:375:PHE:CD2	1:A:435:ILE:HD11	2.39	0.58
1:B:99:ILE:HD12	1:B:143:VAL:HG12	1.85	0.57
1:A:365:PHE:HE2	1:A:451:PHE:CE2	2.25	0.55
1:B:320:MET:HE1	1:B:344:TYR:OH	2.05	0.55
1:A:101:ASP:O	1:A:105:LYS:HG3	2.09	0.53
1:A:113:GLY:CA	1:A:116:GLU:OE1	2.57	0.51
1:A:26:LYS:HE2	1:A:86:PHE:O	2.12	0.50
1:A:422:LEU:HG	1:A:426:ILE:HD11	1.93	0.50
1:B:422:LEU:HG	1:B:426:ILE:HD11	1.95	0.49
1:B:227:LYS:CB	1:B:230:GLU:OE2	2.61	0.49
1:A:116:GLU:H	1:A:116:GLU:CD	2.21	0.49
1:B:348:GLY:O	1:B:352:VAL:HG23	2.13	0.48
1:B:26:LYS:HE2	1:B:86:PHE:O	2.13	0.48
1:B:232:HIS:CE1	1:B:239:LYS:HD3	2.49	0.47
1:A:99:ILE:HD12	1:A:143:VAL:HG12	1.95	0.47
1:A:113:GLY:O	1:A:116:GLU:OE1	2.32	0.47
1:A:438:GLY:HA3	1:B:137:PRO:O	2.14	0.47
1:B:381:ASN:OD1	1:B:434:LYS:HE2	2.17	0.44
1:A:412:THR:N	1:A:413:PRO:CD	2.81	0.44
1:B:60:VAL:O	1:B:60:VAL:HG23	2.17	0.44
1:B:189:MET:HE2	1:B:278:LEU:HD11	2.00	0.44
1:A:103:ILE:HG23	1:A:117:LEU:HD23	2.00	0.43
1:A:365:PHE:HE2	1:A:451:PHE:HE2	1.67	0.43
1:A:176:ASP:OD2	1:A:216:ASN:OD1	2.37	0.42
1:B:363:ASN:O	1:B:367:ILE:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:HB3	1:B:103:ILE:HG12	2.01	0.42
1:B:70:ARG:HG3	1:B:333:PHE:CD1	2.55	0.42
1:A:57:GLY:HA3	1:A:95:ASN:O	2.21	0.41
1:B:65:HIS:HA	1:B:316:THR:HA	2.02	0.41
1:B:234:ASP:OD1	1:B:239:LYS:HE2	2.20	0.41
1:A:71:THR:OG1	2:A:501:A1CYN:N3	2.54	0.41
1:A:307:MET:HE3	1:A:307:MET:HB2	2.01	0.40
1:B:105:LYS:O	1:B:108:VAL:HG22	2.22	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	425/466 (91%)	419 (99%)	6 (1%)	0	100	100
1	B	426/466 (91%)	419 (98%)	7 (2%)	0	100	100
All	All	851/932 (91%)	838 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/423 (92%)	386 (100%)	2 (0%)	86	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	387/423 (92%)	384 (99%)	3 (1%)	79	87
All	All	775/846 (92%)	770 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	A	294	PHE
1	B	254	ASN
1	B	287	HIS
1	B	294	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	ASN
1	B	378	ASN
1	B	400	ASN
1	B	405	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	A1CYZ	B	501	5	26,31,31	0.96	2 (7%)	27,46,46	0.92	1 (3%)
3	ATP	A	502	-	28,33,33	0.73	1 (3%)	34,52,52	0.89	1 (2%)
4	MLI	B	502	-	6,6,6	1.71	1 (16%)	7,7,7	1.13	0
4	MLI	A	504	-	6,6,6	1.80	1 (16%)	7,7,7	1.15	0
4	MLI	B	503	-	6,6,6	1.71	1 (16%)	7,7,7	1.15	1 (14%)
4	MLI	A	503	-	6,6,6	1.57	1 (16%)	7,7,7	1.51	1 (14%)
2	A1CYZ	A	501	5	26,31,31	0.90	0	27,46,46	0.91	1 (3%)
3	ATP	A	508	-	28,33,33	0.67	0	34,52,52	1.02	2 (5%)
4	MLI	B	504	-	6,6,6	1.81	1 (16%)	7,7,7	1.07	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
2	A1CYZ	B	501	5	-	2/15/37/37	0/3/3/3
3	ATP	A	502	-	-	5/18/38/38	0/3/3/3
4	MLI	B	502	-	-	0/4/4/4	-
4	MLI	A	504	-	-	2/4/4/4	-
4	MLI	B	503	-	-	4/4/4/4	-
4	MLI	A	503	-	-	0/4/4/4	-
2	A1CYZ	A	501	5	-	2/15/37/37	0/3/3/3
3	ATP	A	508	-	-	8/18/38/38	0/3/3/3
4	MLI	B	504	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	MLI	C1-C3	3.16	1.56	1.51
4	B	504	MLI	C1-C3	2.94	1.55	1.51
4	B	503	MLI	C1-C3	2.78	1.55	1.51
4	B	502	MLI	C1-C3	2.70	1.55	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	MLI	C1-C3	2.55	1.55	1.51
3	A	502	ATP	PA-O3A	2.55	1.62	1.59
2	B	501	A1CYZ	P-O5'	2.20	1.68	1.59
2	B	501	A1CYZ	P-O3P	2.10	1.64	1.60

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	ATP	O4'-C1'-N9	-3.09	104.65	108.75
3	A	502	ATP	C5-C6-N6	2.75	124.50	120.31
3	A	508	ATP	C5-C6-N6	2.41	123.98	120.31
2	B	501	A1CYZ	C5-C6-N6	2.30	123.81	120.31
4	A	503	MLI	O6-C2-C1	-2.24	115.74	122.11
4	B	503	MLI	O6-C2-C1	-2.13	116.04	122.11
2	A	501	A1CYZ	C5-C6-N6	2.11	123.53	120.31

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	ATP	PB-O3B-PG-O2G
3	A	508	ATP	C5'-O5'-PA-O1A
3	A	508	ATP	C5'-O5'-PA-O2A
3	A	508	ATP	C5'-O5'-PA-O3A
3	A	508	ATP	O4'-C4'-C5'-O5'
3	A	508	ATP	C3'-C4'-C5'-O5'
3	A	502	ATP	O4'-C4'-C5'-O5'
3	A	502	ATP	PB-O3B-PG-O1G
2	A	501	A1CYZ	O-C-CA-N
2	B	501	A1CYZ	O-C-CA-N
2	A	501	A1CYZ	O3P-C-CA-N
2	B	501	A1CYZ	O3P-C-CA-N
4	B	503	MLI	C3-C1-C2-O6
4	B	503	MLI	C3-C1-C2-O7
4	B	503	MLI	C2-C1-C3-O9
4	A	504	MLI	C3-C1-C2-O6
4	A	504	MLI	C3-C1-C2-O7
3	A	508	ATP	PB-O3B-PG-O1G
3	A	502	ATP	PB-O3B-PG-O2G
3	A	502	ATP	PB-O3B-PG-O3G
3	A	508	ATP	PB-O3B-PG-O3G
4	B	503	MLI	C2-C1-C3-O8

Continued on next page...

Continued from previous page...

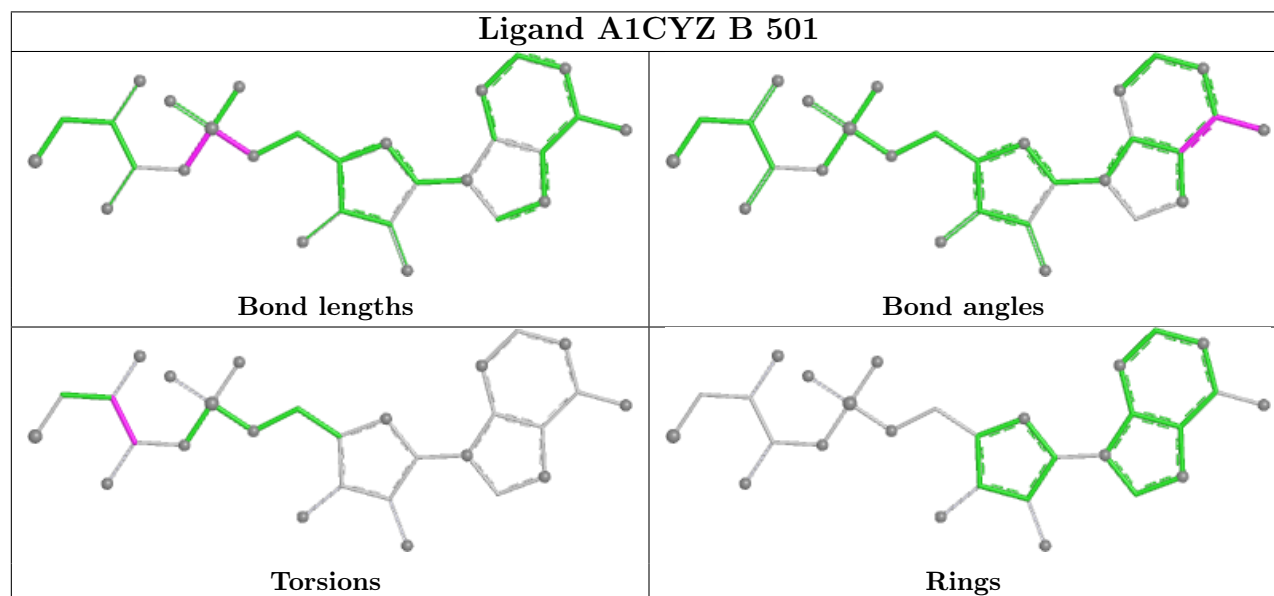
Mol	Chain	Res	Type	Atoms
3	A	502	ATP	PA-O3A-PB-O2B

There are no ring outliers.

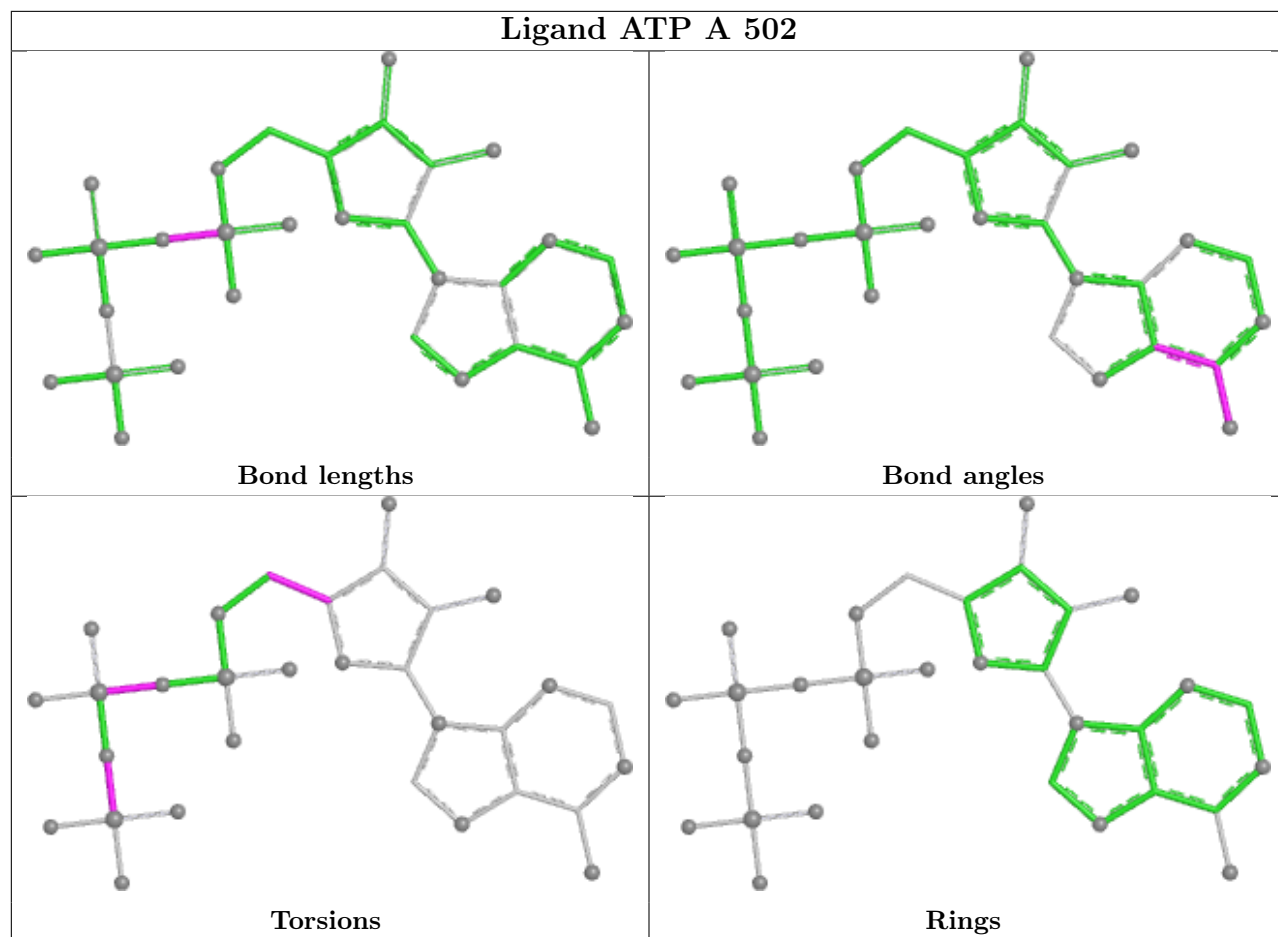
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	MLI	1	0
2	A	501	A1CYZ	1	0

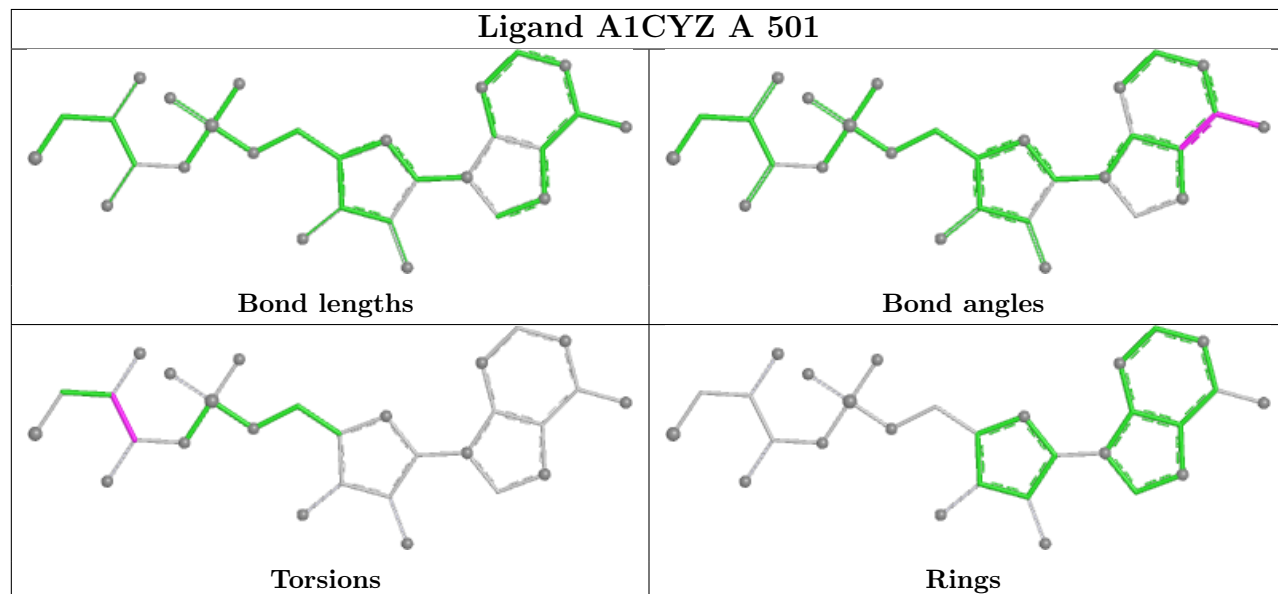
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

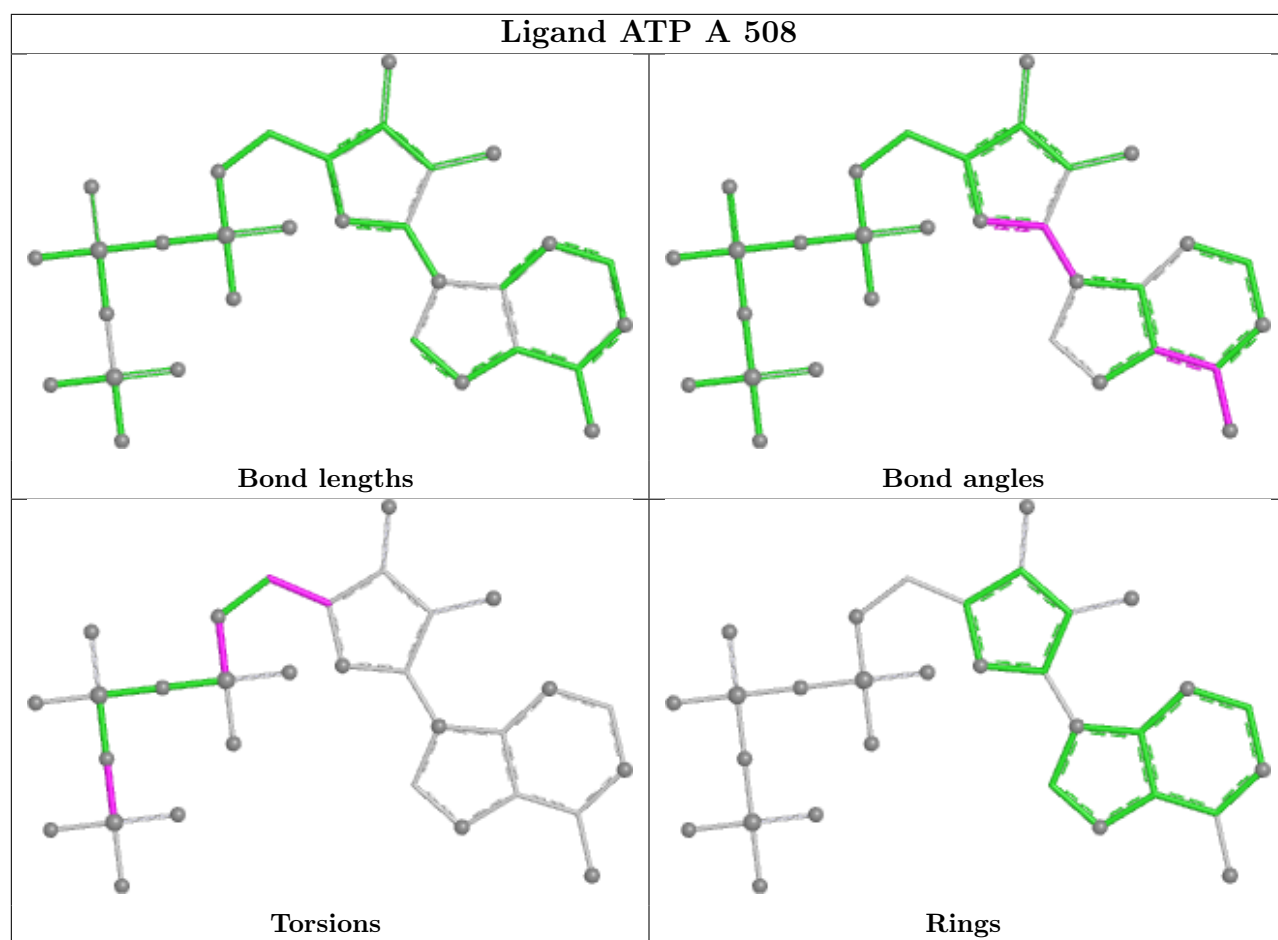


Ligand ATP A 502



Ligand A1CYZ A 501





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	429/466 (92%)	-0.01	15 (3%) 47 44	34, 47, 75, 187	0
1	B	430/466 (92%)	0.06	17 (3%) 43 40	37, 50, 81, 122	0
All	All	859/932 (92%)	0.02	32 (3%) 45 43	34, 48, 79, 187	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ASN	4.9
1	B	213	LYS	4.0
1	B	217	ALA	4.0
1	B	228	PRO	3.7
1	A	212	LYS	3.5
1	B	378	ASN	3.3
1	A	432	LYS	3.3
1	A	226	SER	3.2
1	A	116	GLU	3.1
1	A	114	PHE	3.0
1	B	370	MET	3.0
1	B	159	GLU	3.0
1	B	218	TYR	2.9
1	A	213	LYS	2.9
1	A	218	TYR	2.7
1	B	12	GLY	2.6
1	A	13	SER	2.6
1	B	363	ASN	2.6
1	A	108	VAL	2.5
1	A	214	LYS	2.4
1	B	432	LYS	2.3
1	B	377	LEU	2.3
1	A	168	GLU	2.2
1	A	229	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	309	LYS	2.2
1	B	194	VAL	2.1
1	B	226	SER	2.1
1	A	303	GLU	2.0
1	A	216	ASN	2.0
1	B	380	CYS	2.0
1	A	433	GLU	2.0
1	B	212	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

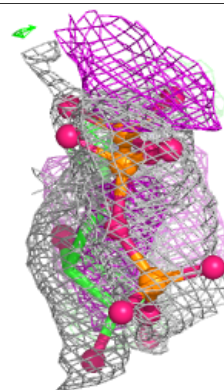
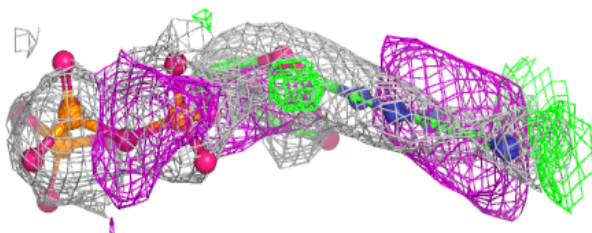
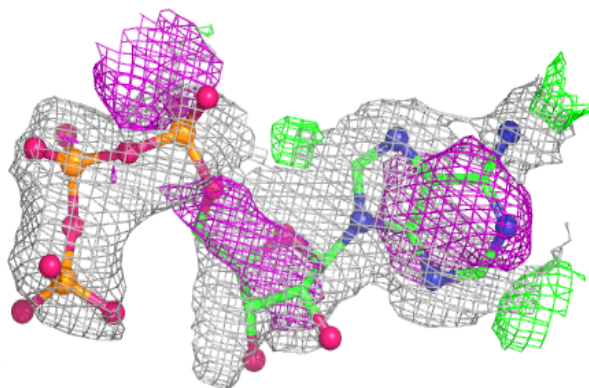
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ATP	A	502	31/31	0.59	0.15	67,94,176,237	0
3	ATP	A	508	31/31	0.61	0.15	67,97,196,242	0
6	NA	A	507	1/1	0.78	0.11	68,68,68,68	0
4	MLI	B	503	7/7	0.82	0.16	63,72,80,82	0
4	MLI	A	503	7/7	0.83	0.14	56,63,68,72	0
6	NA	B	507	1/1	0.84	0.14	70,70,70,70	0
4	MLI	B	502	7/7	0.87	0.13	66,72,77,79	0
6	NA	B	506	1/1	0.92	0.12	59,59,59,59	0
6	NA	A	506	1/1	0.94	0.10	57,57,57,57	0
4	MLI	B	504	7/7	0.95	0.08	54,64,66,69	0
4	MLI	A	504	7/7	0.96	0.07	58,62,67,73	0
2	A1CYZ	B	501	29/29	0.97	0.07	39,51,56,65	0
2	A1CYZ	A	501	29/29	0.97	0.07	33,45,52,64	0
5	ZN	A	505	1/1	0.99	0.02	44,44,44,44	0
5	ZN	B	505	1/1	1.00	0.02	44,44,44,44	0

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

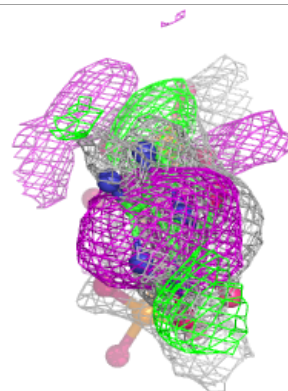
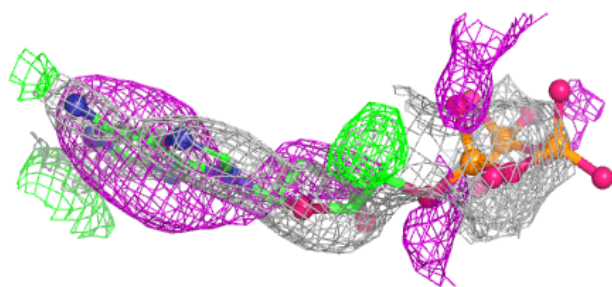
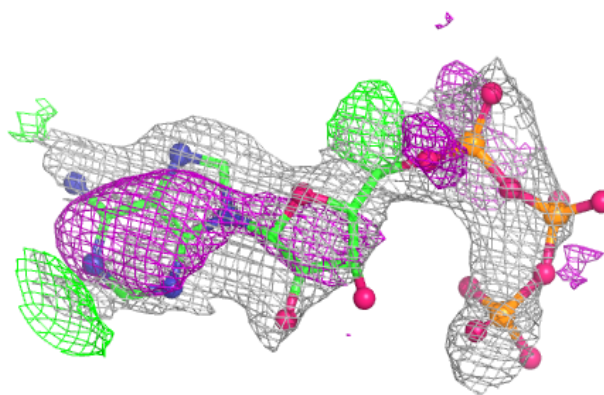
Electron density around ATP A 502:

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

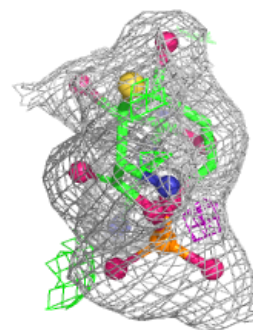
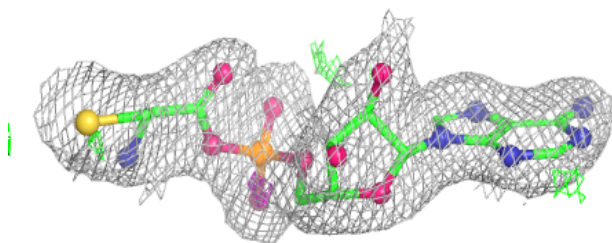
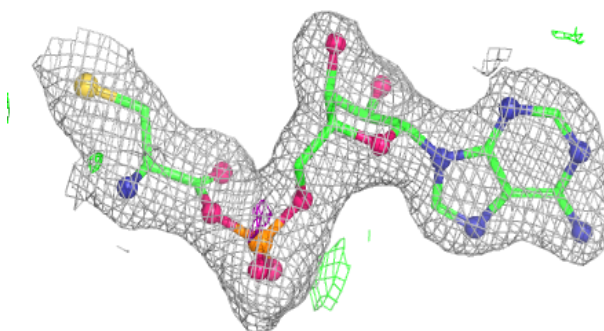


Electron density around ATP A 508:

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

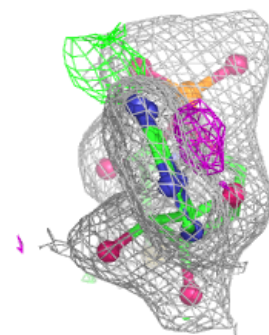
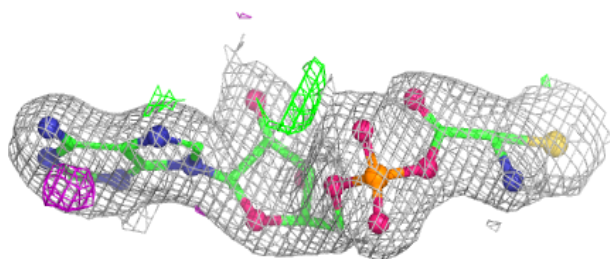
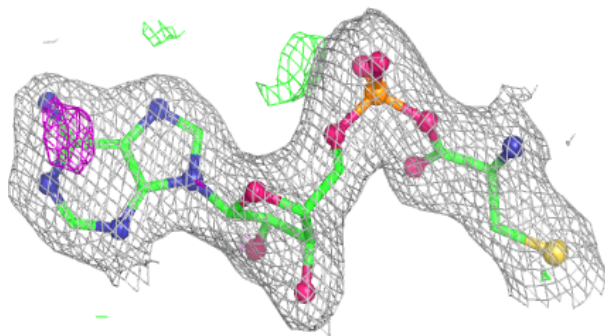
**Electron density around A1CYZ B 501:**

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



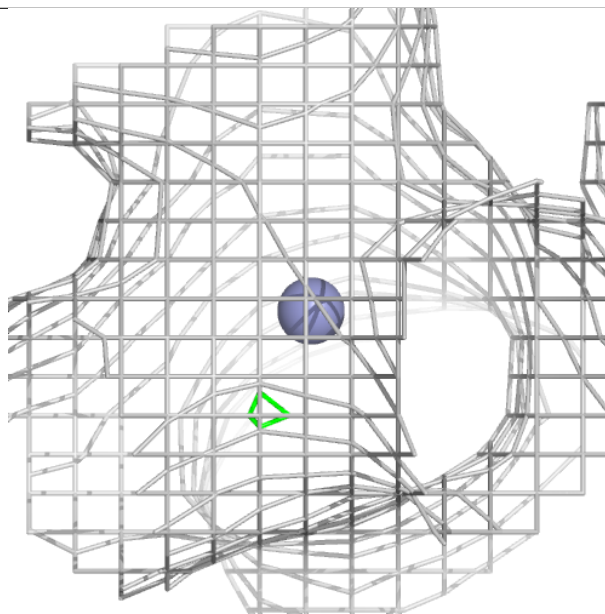
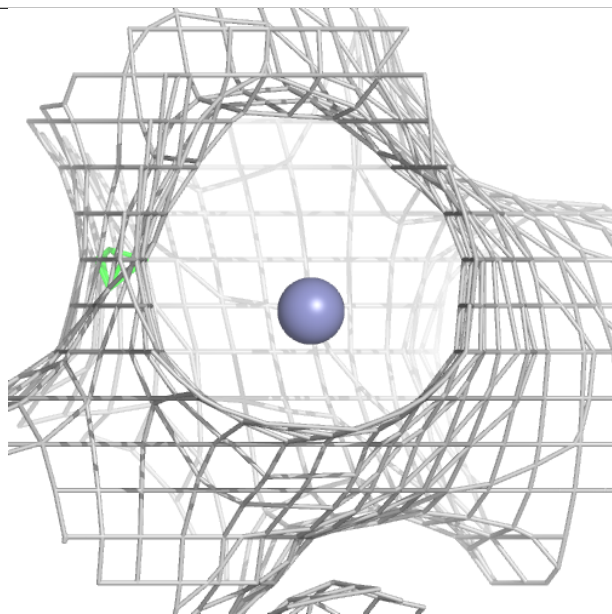
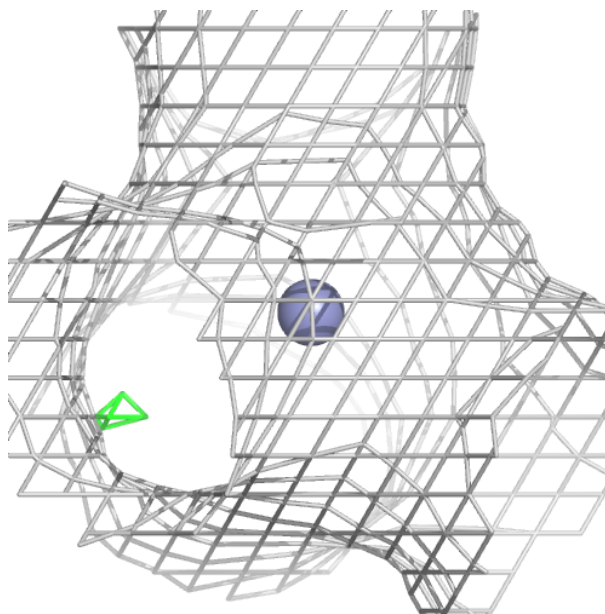
Electron density around A1CYZ A 501:

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



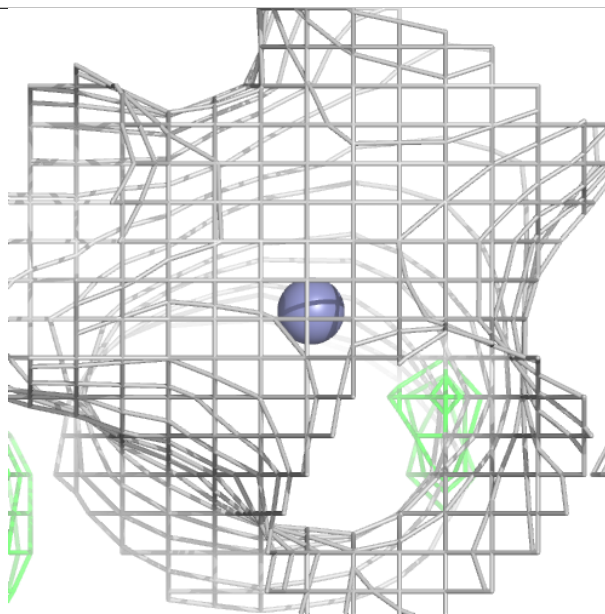
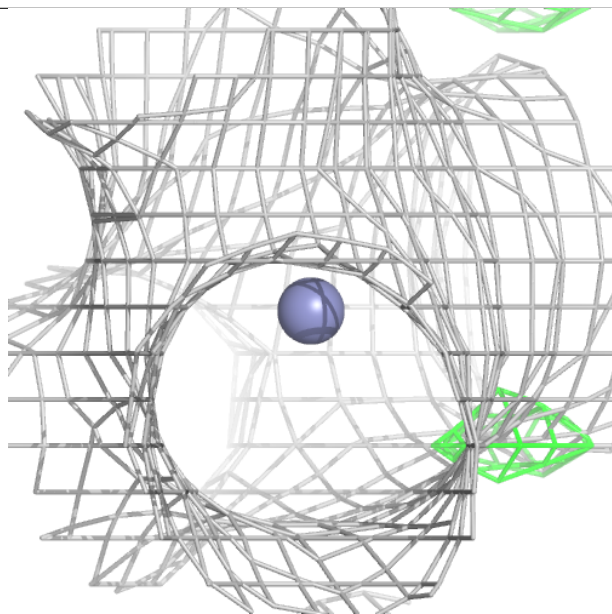
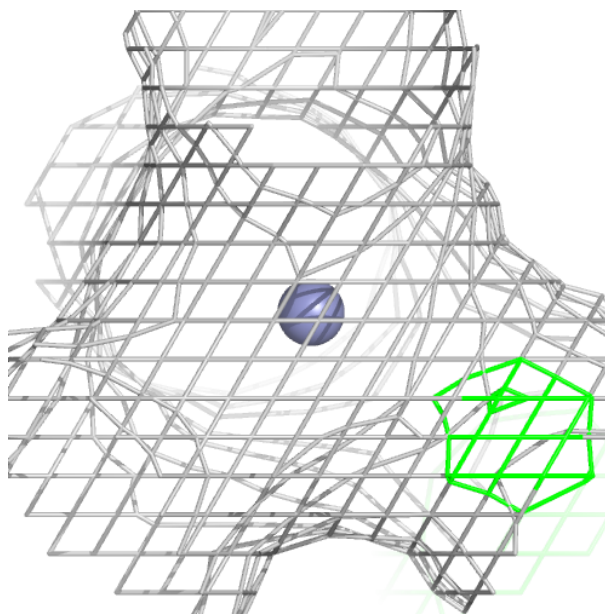
Electron density around ZN A 505:

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



Electron density around ZN B 505:

$2mF_o-DF_c$ (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.