



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 12:09 PM JST

PDB ID : 7VHV  
Title : Crystal structure of S. aureus D-alanine alanyl carrier protein ligase  
Authors : Lee, B.J.; Lee, I.-G.; Im, H.G.; Yoon, H.J.  
Deposited on : 2021-09-23  
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

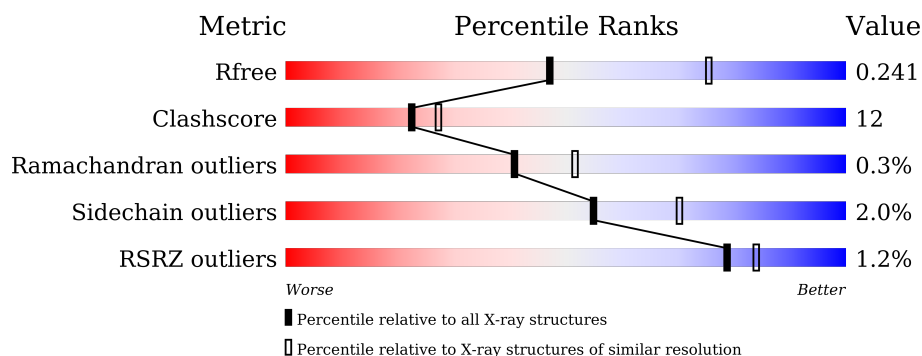
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	485	
1	B	485	
1	C	485	
1	D	485	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15795 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.

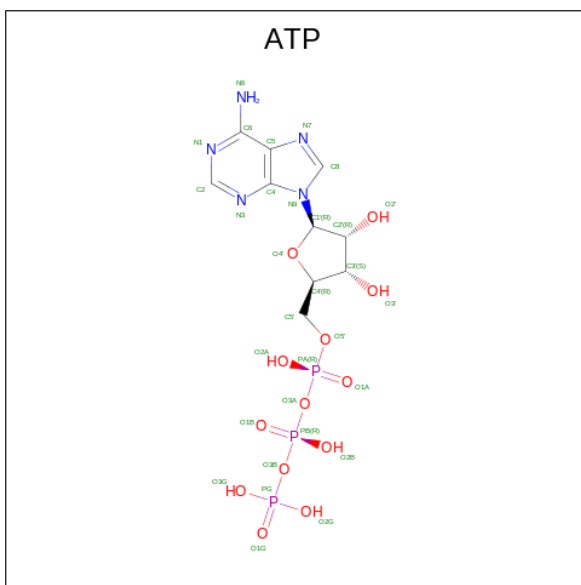
- Molecule 1 is a protein called D-alanine-D-alanyl carrier protein ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	480	Total	C	N	O	S	0	0	0
			3804	2426	621	737	20			
1	C	480	Total	C	N	O	S	0	0	0
			3804	2426	621	737	20			
1	A	485	Total	C	N	O	S	0	0	0
			3839	2447	626	745	21			
1	B	485	Total	C	N	O	S	0	0	0
			3839	2447	626	745	21			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

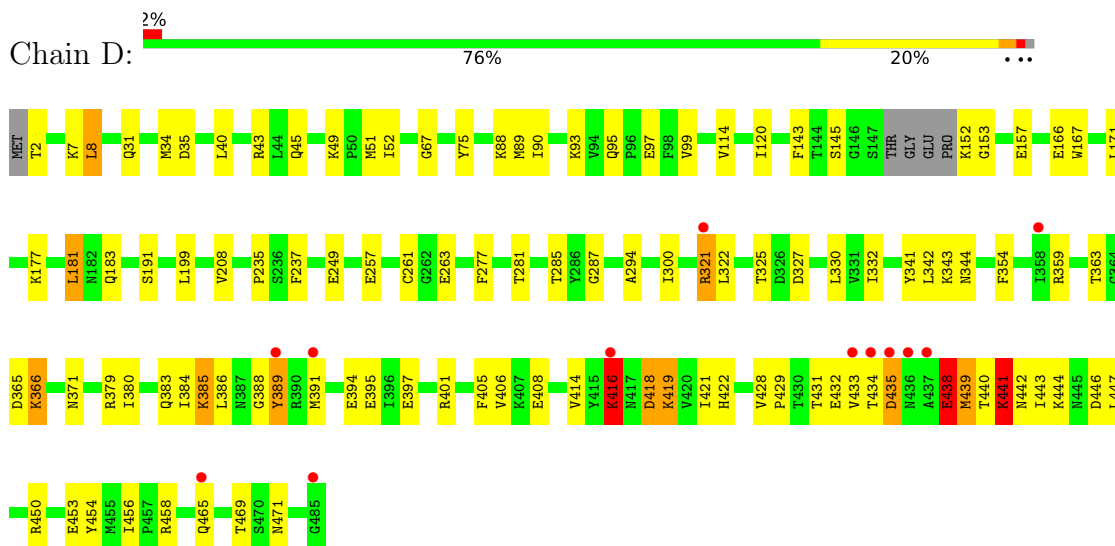
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	79	Total O 79 79	0	0
4	C	89	Total O 89 89	0	0
4	A	101	Total O 101 101	0	0
4	B	112	Total O 112 112	0	0

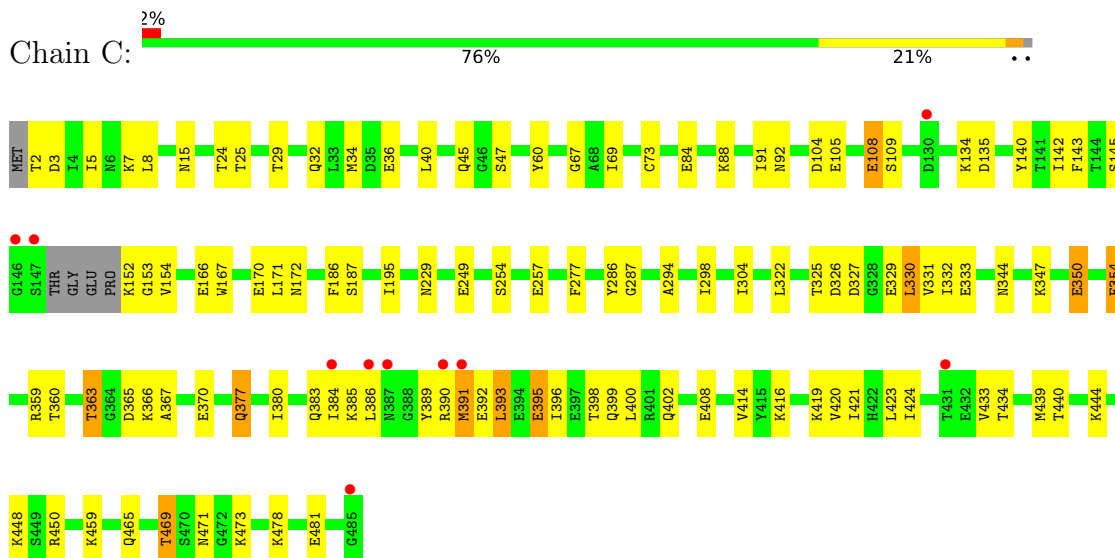
### 3 Residue-property plots

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.

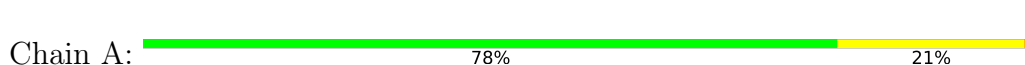
- Molecule 1: D-alanine-D-alanyl carrier protein ligase

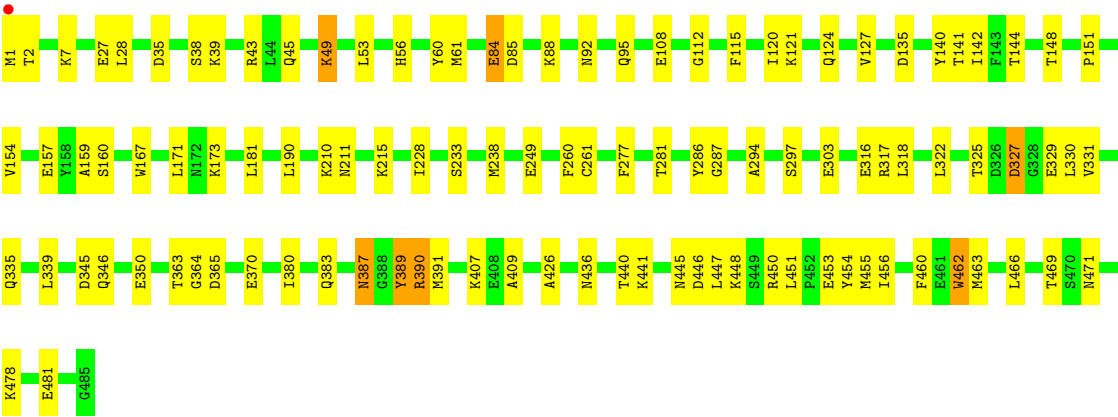


- Molecule 1: D-alanine-D-alanyl carrier protein ligase

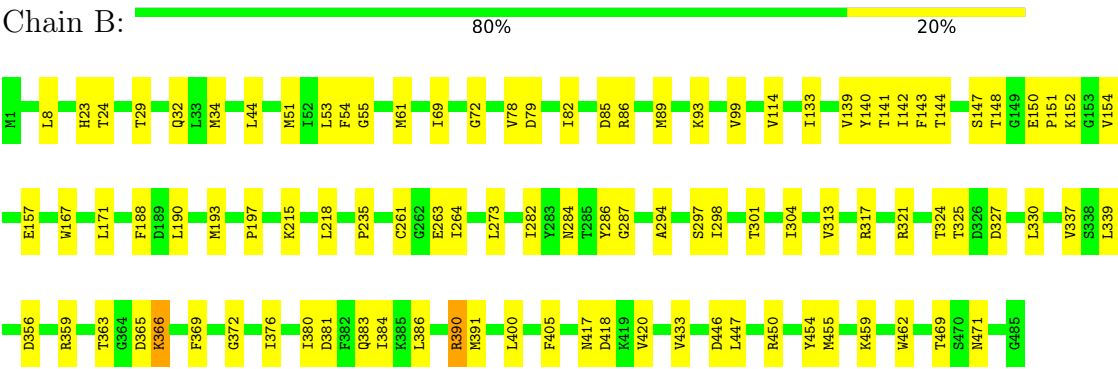


- Molecule 1: D-alanine-D-alanyl carrier protein ligase





● Molecule 1: D-alanine-D-alanyl carrier protein ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.47Å 88.51Å 130.85Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	39.91 – 2.55 44.71 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.91-2.55) 88.0 (44.71-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.189 , 0.240 0.190 , 0.241	Depositor DCC
$R_{free}$ test set	2004 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 22.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l 0.024 for -k,-h,-l 0.197 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.55	1/3916 (0.0%)	0.75	6/5308 (0.1%)
1	B	0.56	1/3916 (0.0%)	0.72	2/5308 (0.0%)
1	C	0.55	2/3879 (0.1%)	0.75	6/5256 (0.1%)
1	D	0.65	8/3879 (0.2%)	0.90	14/5256 (0.3%)
All	All	0.58	12/15590 (0.1%)	0.79	28/21128 (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	D	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	438	GLU	CD-OE1	-7.65	1.17	1.25
1	D	441	LYS	CE-NZ	-7.46	1.30	1.49
1	D	366	LYS	CD-CE	6.44	1.67	1.51
1	C	408	GLU	CD-OE1	-6.44	1.18	1.25
1	D	441	LYS	CD-CE	-6.37	1.35	1.51
1	D	389	TYR	CD1-CE1	-5.88	1.30	1.39
1	D	441	LYS	CG-CD	-5.55	1.33	1.52
1	D	389	TYR	CD2-CE2	-5.52	1.31	1.39
1	B	366	LYS	CB-CG	-5.41	1.38	1.52
1	D	419	LYS	CG-CD	5.34	1.70	1.52
1	C	350	GLU	CD-OE2	5.32	1.31	1.25
1	A	462	TRP	CB-CG	-5.26	1.40	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	441	LYS	CD-CE-NZ	-16.34	74.11	111.70
1	D	8	LEU	CB-CG-CD2	-14.69	86.03	111.00
1	D	416	LYS	CD-CE-NZ	13.64	143.07	111.70
1	D	438	GLU	CA-CB-CG	10.69	136.92	113.40
1	C	393	LEU	CB-CG-CD1	8.85	126.04	111.00
1	C	391	MET	CB-CG-SD	8.44	137.71	112.40
1	D	416	LYS	CB-CG-CD	7.87	132.07	111.60
1	B	390	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	C	408	GLU	CG-CD-OE2	7.59	133.48	118.30
1	D	321	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	D	321	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	390	ARG	NE-CZ-NH2	7.05	123.82	120.30
1	D	435	ASP	N-CA-C	-6.94	92.25	111.00
1	D	418	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	389	TYR	CD1-CE1-CZ	-6.69	113.78	119.80
1	D	366	LYS	CG-CD-CE	6.42	131.16	111.90
1	A	478	LYS	CD-CE-NZ	6.25	126.08	111.70
1	C	408	GLU	CG-CD-OE1	-5.83	106.64	118.30
1	A	390	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	181	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	A	478	LYS	CG-CD-CE	5.48	128.34	111.90
1	A	49	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	C	408	GLU	CA-CB-CG	5.21	124.86	113.40
1	B	390	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	D	8	LEU	CB-CG-CD1	5.19	119.83	111.00
1	A	462	TRP	CA-CB-CG	-5.12	103.96	113.70
1	C	370	GLU	CA-CB-CG	5.05	124.50	113.40
1	D	438	GLU	CB-CG-CD	5.02	127.76	114.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	438	GLU	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	3839	0	3825	81	0
1	B	3839	0	3827	76	1
1	C	3804	0	3791	93	0
1	D	3804	0	3788	110	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
3	C	31	0	12	1	0
3	D	31	0	12	2	0
4	A	101	0	0	12	0
4	B	112	0	0	9	3
4	C	89	0	0	9	3
4	D	79	0	0	9	0
All	All	15795	0	15279	357	4

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 (357) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LYS:O	1:D:343:LYS:NZ	1.65	1.27
1:C:383:GLN:HE21	1:C:392:GLU:HG3	1.24	1.02
1:B:321:ARG:NH1	4:B:602:HOH:O	1.91	1.01
1:A:383:GLN:HB3	1:A:390:ARG:HH12	1.24	1.00
1:B:363:THR:HG23	1:B:365:ASP:H	1.27	0.99
1:B:325:THR:HG22	1:B:327:ASP:H	1.28	0.95
1:A:436:ASN:HD22	1:A:462:TRP:HZ3	1.13	0.94
1:D:8:LEU:HD12	1:D:199:LEU:HB3	1.48	0.94
1:D:152:LYS:N	4:D:605:HOH:O	2.01	0.93
1:D:8:LEU:CD1	1:D:199:LEU:HB3	1.98	0.92
1:D:166:GLU:OE2	4:D:601:HOH:O	1.87	0.91
1:C:40:LEU:HD23	1:C:67:GLY:HA3	1.52	0.89
1:D:8:LEU:HD23	1:D:34:MET:HE1	1.52	0.88
1:D:325:THR:HG22	1:D:327:ASP:H	1.34	0.88
1:A:363:THR:HG23	1:A:365:ASP:H	1.39	0.88
1:B:321:ARG:NH2	4:B:607:HOH:O	2.08	0.87
1:D:177:LYS:O	4:D:602:HOH:O	1.91	0.87
1:A:469:THR:HG22	1:A:471:ASN:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:PRO:HD2	1:B:263:GLU:HG3	1.56	0.87
1:D:469:THR:HG22	1:D:471:ASN:H	1.39	0.87
1:A:390:ARG:O	4:A:601:HOH:O	1.91	0.86
1:A:383:GLN:CB	1:A:390:ARG:HH12	1.87	0.86
1:A:383:GLN:HB3	1:A:390:ARG:NH1	1.90	0.85
1:C:15:ASN:OD1	4:C:601:HOH:O	1.94	0.84
1:C:363:THR:HG22	1:C:365:ASP:H	1.41	0.84
1:B:337:VAL:O	1:B:359:ARG:NH1	2.09	0.84
1:C:465:GLN:NE2	4:C:603:HOH:O	2.09	0.83
1:B:86:ARG:HH12	1:B:150:GLU:HG2	1.43	0.83
1:A:303:GLU:OE1	1:A:303:GLU:N	2.13	0.81
1:D:300:ILE:O	4:D:604:HOH:O	1.96	0.81
1:A:325:THR:HG23	1:A:327:ASP:H	1.44	0.80
1:B:417:ASN:O	4:B:603:HOH:O	1.98	0.79
1:C:424:ILE:HD12	1:C:459:LYS:HB2	1.63	0.79
1:B:446:ASP:O	1:B:450:ARG:NH1	2.16	0.78
1:A:211:ASN:OD1	1:A:215:LYS:NZ	2.14	0.78
1:C:469:THR:HG22	1:C:473:LYS:H	1.49	0.77
1:D:438:GLU:O	1:D:440:THR:N	2.18	0.77
1:A:345:ASP:OD1	4:A:602:HOH:O	2.01	0.77
1:D:8:LEU:HD23	1:D:34:MET:CE	2.15	0.77
1:A:88:LYS:NZ	1:A:108:GLU:O	2.18	0.76
1:A:330:LEU:HB3	1:A:363:THR:HG21	1.66	0.76
1:A:325:THR:HG22	1:A:329:GLU:H	1.51	0.76
1:C:152:LYS:N	4:C:604:HOH:O	2.17	0.76
1:D:385:LYS:CD	1:D:385:LYS:H	1.95	0.75
1:C:469:THR:HG23	1:C:471:ASN:H	1.52	0.75
1:D:8:LEU:CD2	1:D:34:MET:CE	2.65	0.75
1:B:469:THR:HG22	1:B:471:ASN:H	1.52	0.74
1:C:187:SER:O	4:C:602:HOH:O	2.05	0.74
1:A:318:LEU:O	4:A:603:HOH:O	2.05	0.74
1:B:85:ASP:OD2	4:B:606:HOH:O	2.05	0.73
1:D:379:ARG:NH2	3:D:502:ATP:O2B	2.22	0.73
1:A:387:ASN:ND2	1:A:387:ASN:O	2.22	0.73
1:A:446:ASP:OD1	1:A:450:ARG:NH1	2.21	0.73
1:C:8:LEU:HD23	1:C:34:MET:HE1	1.71	0.73
1:D:432:GLU:HG2	1:D:434:THR:HB	1.71	0.72
1:A:316:GLU:OE1	4:A:605:HOH:O	2.07	0.72
1:D:385:LYS:H	1:D:385:LYS:CE	2.02	0.72
1:A:112:GLY:O	4:A:604:HOH:O	2.06	0.72
1:D:8:LEU:CD2	1:D:34:MET:HE2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:GLU:N	1:C:105:GLU:OE1	2.23	0.71
1:B:86:ARG:NH1	1:B:150:GLU:HG2	2.05	0.71
1:D:465:GLN:HG3	4:D:613:HOH:O	1.89	0.71
1:B:264:ILE:HD12	1:B:264:ILE:H	1.56	0.71
1:B:418:ASP:OD1	4:B:608:HOH:O	2.08	0.71
1:B:157:GLU:HG3	1:B:339:LEU:HD21	1.73	0.70
1:C:385:LYS:HA	1:C:389:TYR:O	1.91	0.70
1:C:325:THR:HG23	1:C:327:ASP:H	1.56	0.70
1:D:429:PRO:HG2	1:D:432:GLU:HG3	1.73	0.69
1:D:434:THR:O	1:D:435:ASP:OD1	2.11	0.69
1:D:429:PRO:CG	1:D:432:GLU:HG3	2.24	0.68
1:C:2:THR:HB	1:C:7:LYS:HE3	1.75	0.68
1:B:391:MET:HE3	1:B:455:MET:HG3	1.74	0.68
1:B:330:LEU:O	1:B:363:THR:HG22	1.94	0.67
1:A:330:LEU:O	1:A:363:THR:HG22	1.94	0.66
1:B:23:HIS:O	1:B:24:THR:OG1	2.11	0.66
1:A:469:THR:HG22	1:A:471:ASN:N	2.11	0.66
1:D:416:LYS:HE2	1:D:419:LYS:HE3	1.78	0.65
1:C:322:LEU:HB3	1:C:330:LEU:HD11	1.77	0.65
1:B:330:LEU:HB3	1:B:363:THR:HG21	1.79	0.65
1:D:40:LEU:HD12	1:D:120:ILE:HD11	1.77	0.64
1:D:384:ILE:HA	1:D:385:LYS:HE3	1.78	0.64
1:C:350:GLU:HB3	4:C:612:HOH:O	1.98	0.64
1:D:416:LYS:HE3	1:D:419:LYS:N	2.12	0.63
1:D:440:THR:HG22	1:D:444:LYS:HE3	1.79	0.63
1:C:399:GLN:NE2	1:C:450:ARG:O	2.31	0.63
1:D:394:GLU:OE1	4:D:606:HOH:O	2.15	0.63
1:A:453:GLU:HA	1:A:456:ILE:HD12	1.81	0.63
1:B:143:PHE:HA	1:B:152:LYS:O	1.98	0.63
1:B:86:ARG:HH22	1:B:150:GLU:HG2	1.64	0.62
1:D:8:LEU:HD21	1:D:34:MET:HE2	1.80	0.62
1:A:85:ASP:O	4:A:609:HOH:O	2.16	0.62
1:B:380:ILE:O	1:B:383:GLN:HG2	1.99	0.61
1:D:8:LEU:CD2	1:D:34:MET:HE1	2.27	0.61
1:D:439:MET:HA	1:D:441:LYS:NZ	2.15	0.60
1:C:322:LEU:HD22	1:C:332:ILE:HG12	1.82	0.60
1:B:363:THR:HG23	1:B:365:ASP:N	2.09	0.60
1:C:287:GLY:HA3	1:C:294:ALA:HA	1.82	0.60
1:C:24:THR:OG1	1:C:25:THR:N	2.35	0.60
1:C:325:THR:HG22	1:C:329:GLU:H	1.65	0.59
1:A:27:GLU:O	1:A:28:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LEU:HD22	1:A:451:LEU:HD12	1.84	0.59
1:D:435:ASP:HB3	1:D:438:GLU:HB3	1.83	0.59
1:D:435:ASP:CB	1:D:438:GLU:HB3	2.32	0.59
1:D:379:ARG:HH22	3:D:502:ATP:PB	2.25	0.59
1:C:366:LYS:HE3	1:C:377:GLN:HB2	1.85	0.58
1:C:330:LEU:O	1:C:363:THR:HB	2.03	0.58
1:A:287:GLY:HA3	1:A:294:ALA:HA	1.85	0.58
1:C:390:ARG:NH2	1:A:389:TYR:CD2	2.71	0.58
1:A:144:THR:O	1:A:151:PRO:HB3	2.02	0.58
1:A:35:ASP:HA	1:A:127:VAL:HG13	1.85	0.58
1:D:416:LYS:HG3	1:D:419:LYS:HB2	1.87	0.57
1:C:8:LEU:HB3	1:C:34:MET:HE1	1.87	0.57
1:A:140:TYR:CD1	1:A:142:ILE:HG13	2.39	0.57
1:D:52:ILE:HB	1:D:99:VAL:HG12	1.87	0.57
1:D:342:LEU:HG	1:D:343:LYS:HG3	1.87	0.57
1:A:88:LYS:N	4:A:609:HOH:O	2.39	0.56
1:B:327:ASP:O	1:B:366:LYS:NZ	2.27	0.56
1:D:235:PRO:HD2	1:D:263:GLU:HG3	1.87	0.56
1:D:434:THR:C	1:D:435:ASP:OD1	2.44	0.56
1:B:72:GLY:HA2	1:B:133:ILE:HD12	1.88	0.56
1:A:238:MET:HE3	1:A:260:PHE:HZ	1.71	0.56
1:D:287:GLY:HA3	1:D:294:ALA:HA	1.87	0.56
1:B:86:ARG:NH2	1:B:150:GLU:HG2	2.20	0.56
1:C:385:LYS:HG3	1:C:385:LYS:O	2.04	0.56
1:D:330:LEU:O	1:D:363:THR:HB	2.05	0.55
1:B:190:LEU:HD13	1:B:261:CYS:HB3	1.86	0.55
1:C:469:THR:HG23	1:C:471:ASN:N	2.19	0.55
1:A:407:LYS:CE	4:A:608:HOH:O	2.51	0.55
1:C:440:THR:HG22	1:C:444:LYS:HE3	1.88	0.55
1:D:322:LEU:HD22	1:D:332:ILE:HG12	1.89	0.55
1:A:249:GLU:HB2	1:A:277:PHE:HA	1.89	0.55
1:C:478:LYS:NZ	1:C:481:GLU:OE1	2.33	0.55
1:D:90:ILE:HG12	1:D:143:PHE:CZ	2.43	0.54
1:C:108:GLU:OE2	1:C:109:SER:N	2.40	0.54
1:D:380:ILE:HA	1:D:383:GLN:HG3	1.89	0.54
1:A:364:GLY:HA2	1:A:380:ILE:HD12	1.90	0.54
1:B:287:GLY:HA3	1:B:294:ALA:HA	1.89	0.54
1:A:325:THR:HG22	1:A:329:GLU:N	2.23	0.54
1:D:414:VAL:HG21	1:D:422:HIS:NE2	2.22	0.54
1:B:325:THR:HG22	1:B:327:ASP:N	2.11	0.54
1:C:8:LEU:HB3	1:C:34:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:THR:OG1	1:C:32:GLN:HG3	2.08	0.53
1:A:390:ARG:HH11	1:A:390:ARG:HG2	1.73	0.53
1:D:40:LEU:HD12	1:D:120:ILE:CD1	2.37	0.53
1:A:325:THR:HG23	1:A:327:ASP:N	2.19	0.53
1:A:56:HIS:NE2	1:A:210:LYS:HG2	2.23	0.53
1:A:115:PHE:CE2	1:A:120:ILE:HD11	2.43	0.53
1:A:160:SER:OG	1:A:335:GLN:O	2.22	0.52
1:A:167:TRP:CD2	1:A:317:ARG:HD3	2.44	0.52
1:A:463:MET:HE2	1:A:466:LEU:CD2	2.39	0.52
1:A:436:ASN:ND2	1:A:462:TRP:CZ3	2.63	0.52
1:C:433:VAL:HG22	1:C:439:MET:HG3	1.91	0.52
1:C:167:TRP:CZ2	1:C:171:LEU:HD11	2.45	0.52
1:B:215:LYS:HB2	1:B:218:LEU:HD23	1.90	0.52
1:C:383:GLN:HE21	1:C:392:GLU:CG	2.10	0.52
1:A:322:LEU:HD13	1:A:330:LEU:HD11	1.91	0.52
1:B:53:LEU:CD1	1:B:61:MET:HE1	2.40	0.51
1:B:148:THR:HG21	1:B:381:ASP:OD2	2.11	0.51
1:C:414:VAL:O	1:C:421:ILE:HG12	2.10	0.51
1:D:99:VAL:CG2	1:D:114:VAL:HG22	2.40	0.51
1:C:392:GLU:OE1	1:A:389:TYR:HE2	1.94	0.51
1:B:167:TRP:CD2	1:B:317:ARG:HD3	2.46	0.51
1:C:344:ASN:OD1	1:C:347:LYS:HG3	2.10	0.51
1:C:391:MET:SD	1:C:395:GLU:HB3	2.51	0.51
1:D:431:THR:O	1:D:431:THR:OG1	2.25	0.51
1:C:143:PHE:HA	1:C:153:GLY:HA2	1.92	0.51
1:C:384:ILE:HG23	1:C:393:LEU:HD21	1.93	0.51
1:A:181:LEU:HB2	1:A:228:ILE:HG21	1.93	0.51
1:C:45:GLN:O	4:C:605:HOH:O	2.19	0.51
1:D:446:ASP:OD1	1:D:450:ARG:HD2	2.11	0.50
1:B:147:SER:OG	4:B:609:HOH:O	2.19	0.50
1:B:61:MET:HE2	1:B:61:MET:HA	1.93	0.50
1:C:3:ASP:O	1:C:7:LYS:HG3	2.12	0.50
1:D:354:PHE:CD1	1:D:359:ARG:HG2	2.47	0.50
1:D:363:THR:HG22	1:D:365:ASP:H	1.76	0.50
1:D:439:MET:HG2	1:D:442:ASN:OD1	2.12	0.50
1:A:380:ILE:HG23	1:A:383:GLN:NE2	2.27	0.50
1:B:86:ARG:CZ	1:B:150:GLU:HG2	2.41	0.50
1:B:469:THR:HG22	1:B:471:ASN:N	2.25	0.50
1:D:181:LEU:HD21	1:D:208:VAL:CG2	2.42	0.50
1:C:344:ASN:OD1	1:C:347:LYS:HB2	2.11	0.50
1:C:325:THR:HG22	1:C:329:GLU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:VAL:HG13	1:C:360:THR:HG23	1.93	0.50
1:A:387:ASN:OD1	1:A:454:TYR:HB2	2.12	0.50
1:A:407:LYS:NZ	4:A:608:HOH:O	2.15	0.50
1:D:440:THR:HA	1:D:443:ILE:HG22	1.93	0.50
1:B:400:LEU:CD2	1:B:447:LEU:HD11	2.42	0.50
1:D:325:THR:HG22	1:D:327:ASP:N	2.14	0.49
1:C:350:GLU:CG	4:C:612:HOH:O	2.60	0.49
1:A:85:ASP:C	4:A:609:HOH:O	2.50	0.49
1:D:385:LYS:CE	1:D:385:LYS:N	2.73	0.49
1:D:386:LEU:HB3	1:D:391:MET:SD	2.52	0.49
1:A:157:GLU:HG3	1:A:339:LEU:HD21	1.95	0.49
1:C:134:LYS:HG2	1:C:135:ASP:H	1.77	0.49
1:C:419:LYS:HD3	1:C:420:VAL:H	1.77	0.49
1:B:454:TYR:CD1	1:B:455:MET:HG2	2.47	0.49
1:C:166:GLU:O	1:C:170:GLU:HG3	2.12	0.49
1:A:380:ILE:HG23	1:A:383:GLN:HE22	1.76	0.49
1:C:145:SER:N	3:C:502:ATP:O1G	2.39	0.49
1:C:419:LYS:HD3	1:C:420:VAL:N	2.28	0.49
1:D:40:LEU:HD22	1:D:67:GLY:HA3	1.95	0.49
1:B:99:VAL:CG2	1:B:114:VAL:HG22	2.43	0.48
1:C:36:GLU:OE2	1:C:60:TYR:OH	2.29	0.48
1:D:43:ARG:O	1:D:43:ARG:HG2	2.12	0.48
1:D:435:ASP:HB2	1:D:438:GLU:HG3	1.94	0.48
1:C:433:VAL:CG2	1:C:439:MET:HG3	2.43	0.48
1:C:326:ASP:OD1	1:C:326:ASP:N	2.38	0.48
1:C:384:ILE:HD11	1:C:396:ILE:HD11	1.94	0.48
1:D:191:SER:OG	4:D:607:HOH:O	2.18	0.48
1:B:89:MET:SD	1:B:93:LYS:HE2	2.53	0.48
1:A:238:MET:HE3	1:A:260:PHE:CZ	2.48	0.48
1:B:356:ASP:OD2	4:B:610:HOH:O	2.20	0.48
1:B:369:PHE:CZ	1:B:372:GLY:HA2	2.49	0.48
1:D:371:ASN:O	4:D:608:HOH:O	2.20	0.47
1:B:78:VAL:HG13	1:B:82:ILE:HD12	1.95	0.47
1:B:366:LYS:HZ1	1:B:390:ARG:HH22	1.62	0.47
1:B:167:TRP:CZ2	1:B:171:LEU:HD11	2.49	0.47
1:C:396:ILE:O	1:C:400:LEU:HD13	2.14	0.47
1:B:69:ILE:HG12	1:B:139:VAL:HG23	1.95	0.47
1:D:385:LYS:O	1:D:385:LYS:HG2	2.13	0.47
1:D:429:PRO:HG3	1:D:432:GLU:HG3	1.94	0.47
1:C:380:ILE:O	1:C:383:GLN:HG3	2.14	0.47
1:A:463:MET:CE	1:A:466:LEU:CD2	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLU:HB2	1:C:277:PHE:HA	1.96	0.47
1:D:397:GLU:O	1:D:401:ARG:HG3	2.15	0.47
1:D:167:TRP:CZ2	1:D:171:LEU:HD11	2.50	0.47
1:C:47:SER:O	1:C:73:CYS:HB3	2.15	0.47
1:A:330:LEU:O	1:A:363:THR:CG2	2.62	0.47
1:D:342:LEU:C	1:D:344:ASN:H	2.17	0.46
1:C:433:VAL:HG12	1:C:433:VAL:O	2.15	0.46
1:C:433:VAL:HG13	1:C:439:MET:HG3	1.96	0.46
1:B:8:LEU:HD23	1:B:34:MET:HE1	1.98	0.46
1:A:167:TRP:CE2	1:A:171:LEU:HD11	2.51	0.46
1:D:416:LYS:NZ	1:D:419:LYS:HG3	2.30	0.46
1:A:190:LEU:HD13	1:A:261:CYS:HB3	1.97	0.46
1:D:414:VAL:HG23	1:D:421:ILE:HG13	1.96	0.46
1:B:54:PHE:O	1:B:61:MET:HE3	2.16	0.46
1:D:325:THR:CG2	1:D:327:ASP:H	2.18	0.46
1:D:257:GLU:HA	1:D:281:THR:O	2.16	0.46
1:C:91:ILE:HD12	1:C:92:ASN:N	2.31	0.46
1:B:86:ARG:HH22	1:B:150:GLU:CG	2.27	0.46
1:B:167:TRP:HZ2	1:B:297:SER:HB3	1.80	0.46
1:C:186:PHE:CD1	1:C:195:ILE:HD11	2.50	0.46
1:C:186:PHE:CE1	1:C:195:ILE:HD11	2.51	0.45
1:D:2:THR:HB	1:D:166:GLU:OE1	2.17	0.45
1:C:390:ARG:NH2	1:A:389:TYR:HD2	2.15	0.45
1:C:416:LYS:HD2	1:C:416:LYS:HA	1.74	0.45
1:A:53:LEU:HD11	1:A:61:MET:HA	1.98	0.45
1:D:49:LYS:HE2	1:D:95:GLN:O	2.17	0.45
1:D:456:ILE:O	4:D:609:HOH:O	2.21	0.45
1:A:391:MET:SD	1:A:455:MET:HG3	2.57	0.45
1:B:313:VAL:HG21	1:B:376:ILE:HG12	1.99	0.45
1:C:330:LEU:HG	1:C:331:VAL:N	2.32	0.45
1:B:215:LYS:CB	1:B:218:LEU:HD23	2.46	0.45
1:D:8:LEU:HD21	1:D:34:MET:CE	2.40	0.45
1:D:447:LEU:HB3	1:D:456:ILE:HG12	1.97	0.45
1:D:458:ARG:HD3	1:D:458:ARG:HA	1.78	0.45
1:D:261:CYS:HB2	1:D:285:THR:OG1	2.17	0.44
1:D:416:LYS:HG3	1:D:419:LYS:H	1.82	0.44
1:B:284:ASN:HB3	1:B:298:ILE:CG2	2.47	0.44
1:D:31:GLN:NE2	1:D:35:ASP:OD2	2.50	0.44
1:C:354:PHE:HB3	1:C:359:ARG:HA	2.00	0.44
1:D:416:LYS:HE3	1:D:419:LYS:HB2	1.99	0.44
1:C:229:ASN:HA	1:C:254:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LEU:HD22	1:C:423:LEU:HD21	2.00	0.44
1:B:264:ILE:H	1:B:264:ILE:CD1	2.26	0.44
1:B:264:ILE:HG13	3:B:502:ATP:H2	1.82	0.44
1:C:459:LYS:HB3	1:C:459:LYS:HE2	1.76	0.44
1:A:173:LYS:HD2	1:A:281:THR:HG21	1.99	0.44
1:D:99:VAL:HG21	1:D:114:VAL:HG22	1.99	0.44
1:C:384:ILE:CG2	1:C:393:LEU:HD21	2.48	0.44
1:B:454:TYR:HD1	1:B:455:MET:HG2	1.82	0.44
1:B:140:TYR:CD1	1:B:142:ILE:HG13	2.53	0.44
1:A:1:MET:H2	1:A:2:THR:HA	1.82	0.44
1:D:416:LYS:HE3	1:D:419:LYS:CB	2.48	0.43
1:C:398:THR:HG22	1:C:402:GLN:OE1	2.19	0.43
1:D:408:GLU:HB2	1:D:428:VAL:HB	2.01	0.43
1:C:142:ILE:O	1:C:154:VAL:N	2.29	0.43
1:A:60:TYR:OH	1:A:121:LYS:HE3	2.18	0.43
1:A:84:GLU:O	1:A:88:LYS:HG2	2.17	0.43
1:A:445:ASN:HA	1:A:448:LYS:HD2	2.01	0.43
1:D:249:GLU:HB2	1:D:277:PHE:HA	2.00	0.43
1:B:144:THR:O	1:B:151:PRO:HB3	2.18	0.43
1:B:193:MET:O	1:B:197:PRO:HG2	2.19	0.43
1:D:153:GLY:O	1:D:341:TYR:HA	2.19	0.43
1:D:157:GLU:OE2	1:D:359:ARG:NH1	2.49	0.43
1:A:440:THR:HG23	1:A:460:PHE:CD2	2.53	0.43
1:A:445:ASN:HA	1:A:448:LYS:CD	2.49	0.43
1:C:363:THR:HG22	1:C:365:ASP:N	2.21	0.43
1:C:330:LEU:HB2	1:C:367:ALA:HB3	2.01	0.43
1:C:333:GLU:HA	1:C:359:ARG:O	2.19	0.43
1:B:273:LEU:HD23	1:B:282:ILE:HG12	2.00	0.43
1:C:84:GLU:HG2	4:C:610:HOH:O	2.19	0.43
1:C:350:GLU:CB	4:C:612:HOH:O	2.64	0.43
1:A:141:THR:HA	1:A:154:VAL:O	2.19	0.43
1:B:141:THR:HA	1:B:154:VAL:O	2.19	0.43
1:C:40:LEU:CD2	1:C:67:GLY:HA3	2.36	0.42
1:C:167:TRP:CE2	1:C:171:LEU:HD11	2.54	0.42
1:D:88:LYS:HA	1:D:88:LYS:HD2	1.69	0.42
1:C:384:ILE:HG12	1:C:393:LEU:HD23	2.00	0.42
1:A:409:ALA:HA	1:A:426:ALA:O	2.19	0.42
1:A:39:LYS:NZ	4:A:613:HOH:O	2.51	0.42
1:A:167:TRP:CZ2	1:A:297:SER:HB3	2.55	0.42
1:B:384:ILE:O	1:B:390:ARG:HA	2.19	0.42
1:D:386:LEU:HD21	1:D:454:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:GLN:NE2	4:B:620:HOH:O	2.43	0.42
1:D:49:LYS:HG3	1:D:97:GLU:HG3	2.02	0.42
1:C:298:ILE:HD11	1:C:304:ILE:HD12	2.02	0.42
1:B:188:PHE:CD2	1:B:471:ASN:HB3	2.54	0.42
1:C:140:TYR:CD1	1:C:142:ILE:HG13	2.54	0.42
1:D:7:LYS:HE2	1:D:7:LYS:HB2	1.71	0.42
1:A:387:ASN:ND2	1:A:387:ASN:C	2.72	0.42
1:B:167:TRP:CZ2	1:B:297:SER:HB3	2.55	0.42
1:D:453:GLU:OE2	1:D:458:ARG:NH2	2.52	0.42
1:C:84:GLU:O	1:C:88:LYS:HG2	2.20	0.42
1:A:390:ARG:NH1	1:A:390:ARG:HG2	2.34	0.42
1:B:55:GLY:O	1:B:79:ASP:HA	2.20	0.42
1:B:235:PRO:HD2	1:B:263:GLU:CG	2.39	0.42
1:A:1:MET:H2	1:A:7:LYS:HD2	1.84	0.41
1:A:43:ARG:O	1:A:43:ARG:HG2	2.20	0.41
1:A:481:GLU:HG3	4:A:661:HOH:O	2.20	0.41
1:B:386:LEU:HD13	1:B:420:VAL:HG12	2.02	0.41
1:D:49:LYS:HG2	1:D:97:GLU:OE1	2.19	0.41
1:B:324:THR:HG22	4:B:612:HOH:O	2.19	0.41
1:B:400:LEU:HD21	1:B:447:LEU:HD11	2.02	0.41
1:B:433:VAL:HG21	1:B:462:TRP:CD2	2.55	0.41
1:D:8:LEU:HD13	1:D:199:LEU:HB3	1.95	0.41
1:D:405:PHE:CD1	1:D:405:PHE:N	2.88	0.41
1:A:135:ASP:HB3	1:A:159:ALA:HB2	2.02	0.41
1:B:301:THR:OG1	1:B:304:ILE:HG12	2.20	0.41
1:D:183:GLN:HG3	1:D:237:PHE:CD1	2.56	0.41
1:D:440:THR:CG2	1:D:444:LYS:HE3	2.47	0.41
1:C:354:PHE:HB3	1:C:359:ARG:HG2	2.03	0.41
1:D:416:LYS:HE2	1:D:419:LYS:CE	2.49	0.41
1:C:384:ILE:HG12	1:C:393:LEU:CD2	2.51	0.41
1:D:385:LYS:HB3	1:D:385:LYS:HE2	1.67	0.41
1:C:104:ASP:HB2	1:C:105:GLU:OE1	2.21	0.41
1:A:157:GLU:HG3	1:A:339:LEU:HD11	2.03	0.41
1:B:44:LEU:HD21	1:B:51:MET:SD	2.60	0.41
1:D:143:PHE:HA	1:D:152:LYS:O	2.20	0.41
1:D:406:VAL:HG23	1:D:443:ILE:HD11	2.03	0.41
1:D:440:THR:O	1:D:444:LYS:HG3	2.20	0.41
1:A:346:GLN:O	1:A:350:GLU:HG3	2.20	0.41
1:B:29:THR:OG1	1:B:32:GLN:HG3	2.21	0.41
1:D:181:LEU:HD21	1:D:208:VAL:HG23	2.02	0.40
1:D:416:LYS:CE	1:D:419:LYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:PRO:CD	1:B:263:GLU:HG3	2.39	0.40
1:D:388:GLY:O	1:D:389:TYR:CG	2.75	0.40
1:D:321:ARG:HH11	1:D:321:ARG:HD2	1.54	0.40
1:D:435:ASP:CB	1:D:438:GLU:CG	2.99	0.40
1:C:433:VAL:CG1	1:C:439:MET:HG3	2.51	0.40
1:A:92:ASN:O	1:A:95:GLN:HG2	2.21	0.40
1:D:435:ASP:HB2	1:D:438:GLU:HB3	2.02	0.40
1:D:441:LYS:HD3	1:D:442:ASN:N	2.36	0.40
1:C:5:ILE:HD11	1:C:69:ILE:CG2	2.51	0.40
1:C:172:ASN:ND2	1:C:257:GLU:OE1	2.51	0.40
1:D:51:MET:O	1:D:75:TYR:HA	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:TYR:CE1	1:B:390:ARG:NH2[2_444]	1.75	0.45
4:C:628:HOH:O	4:B:668:HOH:O[2_444]	2.02	0.18
4:C:685:HOH:O	4:B:707:HOH:O[2_444]	2.07	0.13
4:C:675:HOH:O	4:B:685:HOH:O[2_444]	2.16	0.04

## 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	483/485 (100%)	467 (97%)	16 (3%)	0	100	100
1	B	483/485 (100%)	468 (97%)	15 (3%)	0	100	100
1	C	476/485 (98%)	458 (96%)	17 (4%)	1 (0%)	47	60
1	D	476/485 (98%)	456 (96%)	16 (3%)	4 (1%)	19	27
All	All	1918/1940 (99%)	1849 (96%)	64 (3%)	5 (0%)	41	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	438	GLU
1	D	418	ASP
1	D	439	MET
1	D	433	VAL
1	C	434	THR

### 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	431/431 (100%)	417 (97%)	14 (3%)	39	53
1	B	431/431 (100%)	428 (99%)	3 (1%)	84	90
1	C	427/431 (99%)	418 (98%)	9 (2%)	53	68
1	D	427/431 (99%)	419 (98%)	8 (2%)	57	72
All	All	1716/1724 (100%)	1682 (98%)	34 (2%)	55	70

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	45	GLN
1	D	89	MET
1	D	145	SER
1	D	366	LYS
1	D	385	LYS
1	D	395	GLU
1	D	416	LYS
1	D	441	LYS
1	C	108	GLU
1	C	286	TYR
1	C	330	LEU
1	C	354	PHE
1	C	363	THR
1	C	377	GLN
1	C	395	GLU

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Mol	Chain	Res	Type
1	C	448	LYS
1	C	469	THR
1	A	38	SER
1	A	45	GLN
1	A	49	LYS
1	A	84	GLU
1	A	124	GLN
1	A	148	THR
1	A	233	SER
1	A	286	TYR
1	A	327	ASP
1	A	331	VAL
1	A	370	GLU
1	A	387	ASN
1	A	389	TYR
1	A	441	LYS
1	B	286	TYR
1	B	405	PHE
1	B	459	LYS

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

Mol	Chain	Res	Type
1	D	377	GLN
1	D	465	GLN
1	D	484	ASN
1	C	15	ASN
1	C	383	GLN
1	A	383	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	C	502	2	26,33,33	1.07	3 (11%)	31,52,52	1.35	4 (12%)
3	ATP	D	502	2	26,33,33	0.99	1 (3%)	31,52,52	1.36	5 (16%)
3	ATP	B	502	2	26,33,33	0.90	2 (7%)	31,52,52	1.43	5 (16%)
3	ATP	A	502	2	26,33,33	0.97	2 (7%)	31,52,52	1.42	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	502	2	-	5/18/38/38	0/3/3/3
3	ATP	D	502	2	-	7/18/38/38	0/3/3/3
3	ATP	B	502	2	-	5/18/38/38	0/3/3/3
3	ATP	A	502	2	-	7/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ATP	C5-C4	2.71	1.48	1.40
3	D	502	ATP	C5-C4	2.70	1.48	1.40
3	C	502	ATP	C5-C4	2.66	1.48	1.40
3	B	502	ATP	C5-C4	2.24	1.46	1.40
3	C	502	ATP	O4'-C1'	2.15	1.44	1.41
3	A	502	ATP	O4'-C1'	2.08	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	ATP	C2-N3	2.03	1.35	1.32
3	B	502	ATP	O4'-C1'	2.01	1.43	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	ATP	N3-C2-N1	-3.94	122.52	128.68
3	B	502	ATP	PB-O3B-PG	-3.42	121.10	132.83
3	D	502	ATP	N3-C2-N1	-3.33	123.47	128.68
3	A	502	ATP	C4-C5-N7	-2.97	106.31	109.40
3	A	502	ATP	N3-C2-N1	-2.94	124.08	128.68
3	C	502	ATP	N3-C2-N1	-2.86	124.21	128.68
3	C	502	ATP	PB-O3B-PG	-2.80	123.21	132.83
3	C	502	ATP	C4-C5-N7	-2.78	106.50	109.40
3	A	502	ATP	PB-O3B-PG	-2.54	124.11	132.83
3	C	502	ATP	PA-O3A-PB	-2.51	124.21	132.83
3	D	502	ATP	C2-N1-C6	2.43	122.91	118.75
3	D	502	ATP	PA-O3A-PB	-2.25	125.12	132.83
3	B	502	ATP	C2-N1-C6	2.18	122.48	118.75
3	B	502	ATP	C4-C5-N7	-2.17	107.14	109.40
3	A	502	ATP	C2-N1-C6	2.16	122.45	118.75
3	A	502	ATP	O5'-C5'-C4'	-2.16	101.55	108.99
3	B	502	ATP	O2A-PA-O1A	2.08	122.55	112.24
3	D	502	ATP	O3'-C3'-C2'	2.03	118.38	111.82
3	A	502	ATP	O2G-PG-O1G	2.02	118.60	110.68
3	D	502	ATP	C4-C5-N7	-2.02	107.30	109.40

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	ATP	C5'-O5'-PA-O1A
3	D	502	ATP	C5'-O5'-PA-O2A
3	C	502	ATP	C5'-O5'-PA-O1A
3	C	502	ATP	C5'-O5'-PA-O2A
3	A	502	ATP	PB-O3A-PA-O5'
3	A	502	ATP	C5'-O5'-PA-O1A
3	A	502	ATP	C5'-O5'-PA-O2A
3	B	502	ATP	C5'-O5'-PA-O1A
3	B	502	ATP	C5'-O5'-PA-O2A
3	D	502	ATP	PB-O3A-PA-O5'
3	C	502	ATP	PB-O3A-PA-O5'

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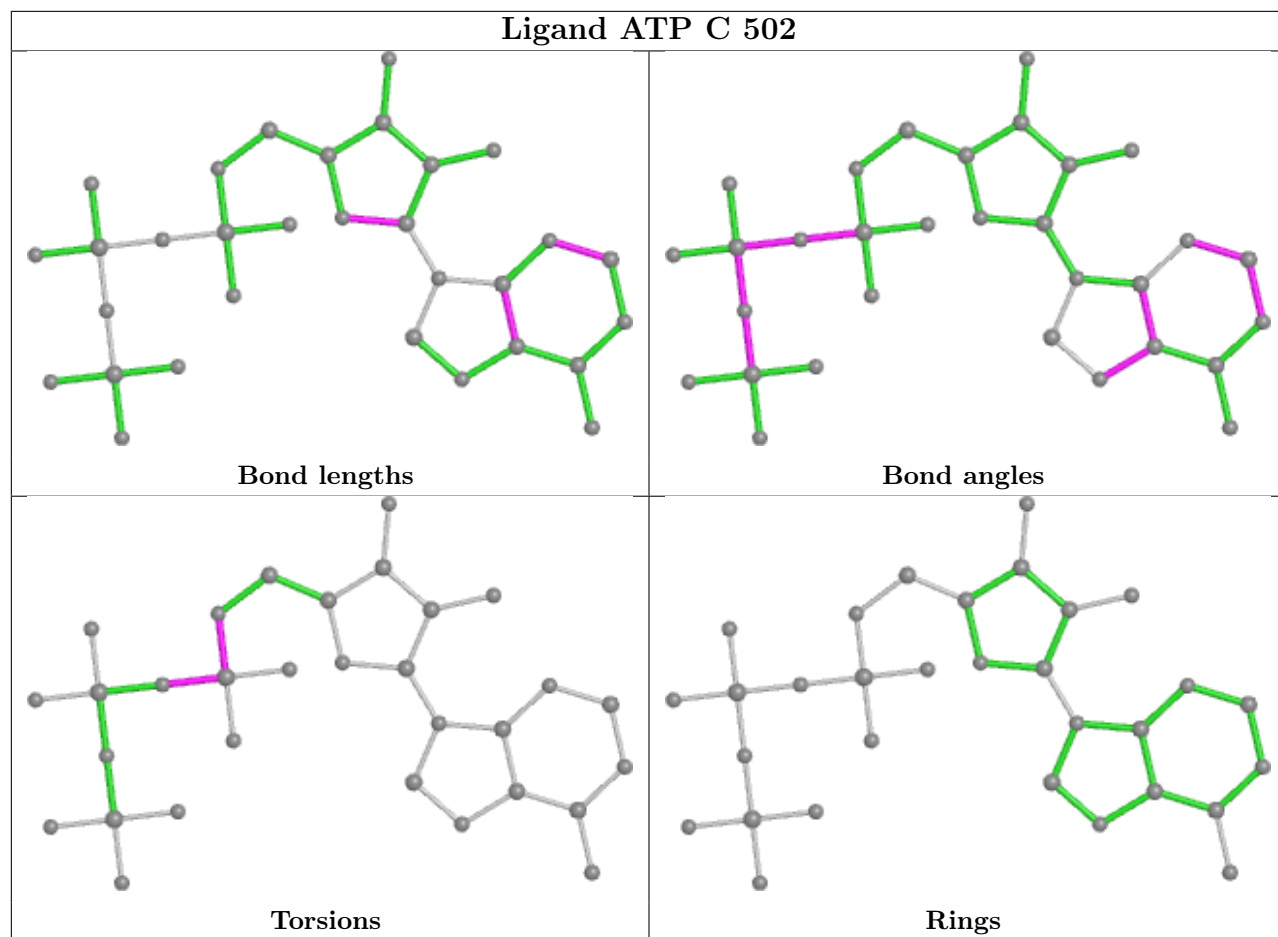
Mol	Chain	Res	Type	Atoms
3	B	502	ATP	PB-O3A-PA-O5'
3	D	502	ATP	PG-O3B-PB-O2B
3	B	502	ATP	PG-O3B-PB-O2B
3	D	502	ATP	PG-O3B-PB-O1B
3	A	502	ATP	PG-O3B-PB-O2B
3	C	502	ATP	PB-O3A-PA-O1A
3	D	502	ATP	C5'-O5'-PA-O3A
3	C	502	ATP	C5'-O5'-PA-O3A
3	A	502	ATP	C5'-O5'-PA-O3A
3	B	502	ATP	C5'-O5'-PA-O3A
3	D	502	ATP	PB-O3A-PA-O1A
3	A	502	ATP	PG-O3B-PB-O1B
3	A	502	ATP	PB-O3A-PA-O1A

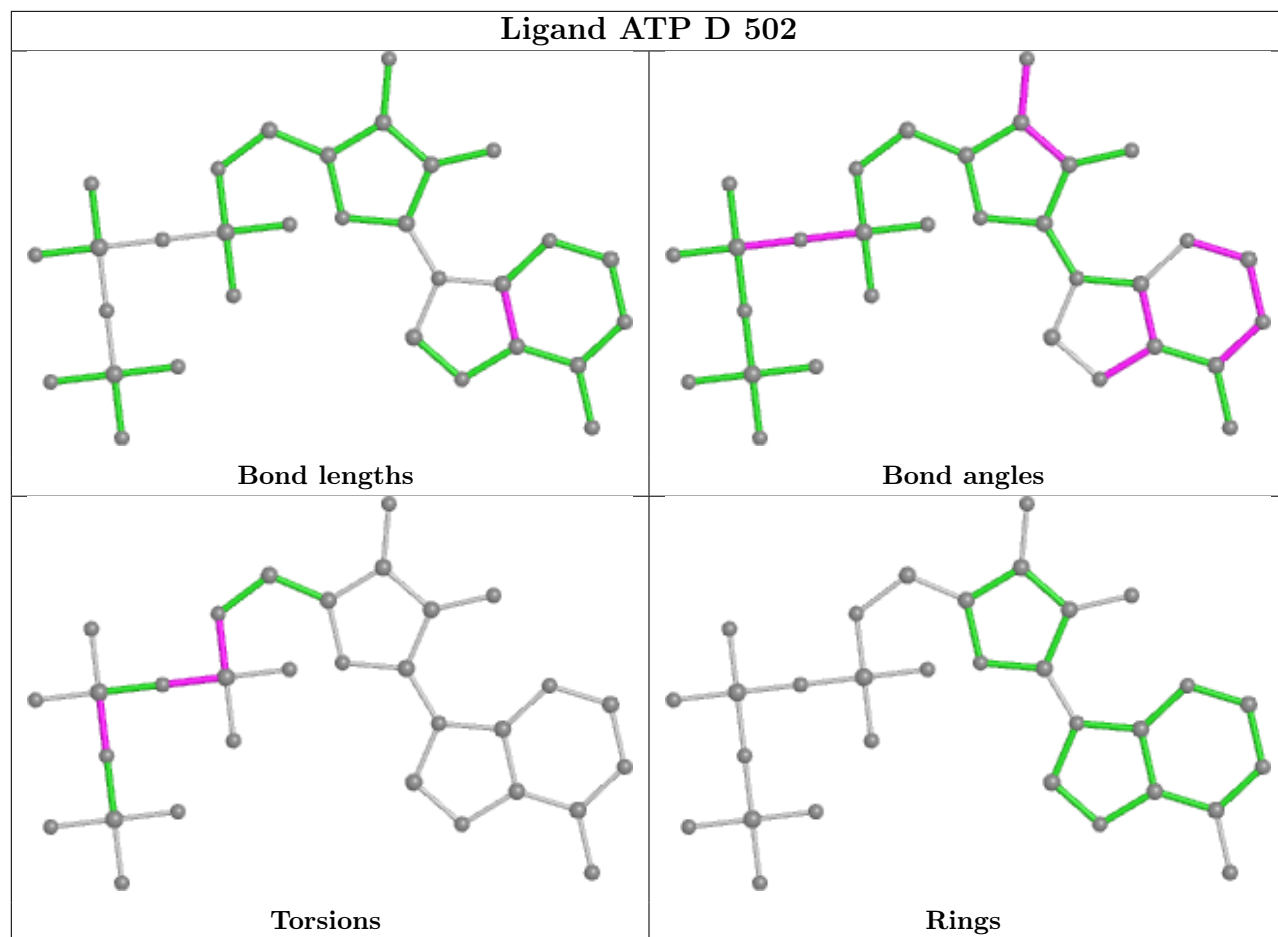
There are no ring outliers.

3 monomers are involved in 4 short contacts:

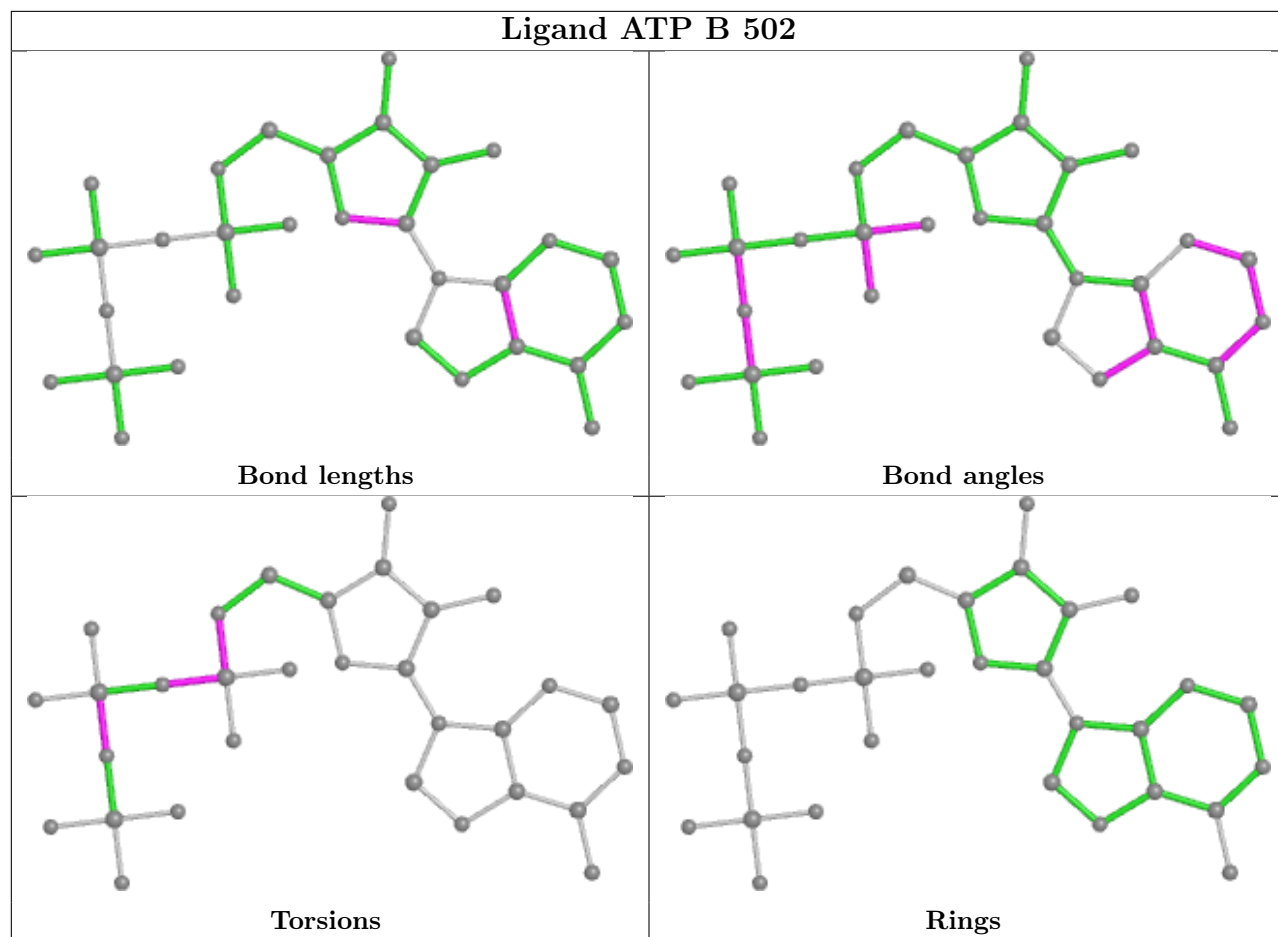
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	ATP	1	0
3	D	502	ATP	2	0
3	B	502	ATP	1	0

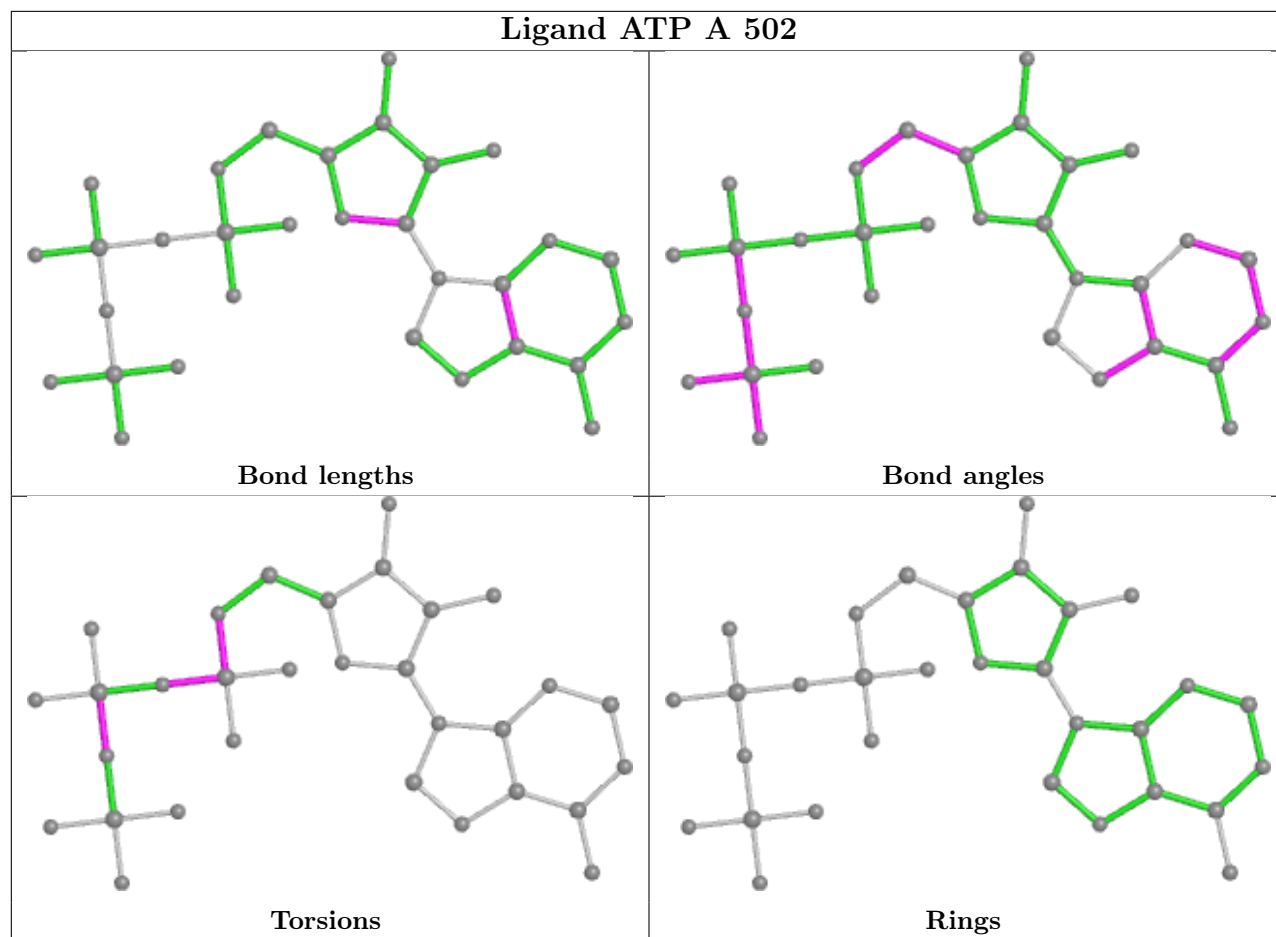
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





## Ligand ATP B 502





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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	485/485 (100%)	-0.32	1 (0%) 95 97	28, 44, 67, 83	0
1	B	485/485 (100%)	-0.44	0 100 100	29, 42, 57, 77	0
1	C	480/485 (98%)	-0.11	10 (2%) 63 70	27, 51, 84, 110	0
1	D	480/485 (98%)	-0.21	12 (2%) 57 63	29, 47, 76, 107	0
All	All	1930/1940 (99%)	-0.27	23 (1%) 79 84	27, 45, 73, 110	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	433	VAL	12.1
1	C	386	LEU	6.5
1	C	485	GLY	4.6
1	C	390	ARG	4.3
1	D	485	GLY	4.3
1	D	436	ASN	4.2
1	C	387	ASN	3.4
1	C	147	SER	3.2
1	D	389	TYR	3.1
1	D	434	THR	3.0
1	D	437	ALA	2.8
1	C	384	ILE	2.7
1	D	321	ARG	2.6
1	A	1	MET	2.6
1	D	391	MET	2.5
1	C	431	THR	2.4
1	C	391	MET	2.3
1	C	146	GLY	2.3
1	D	435	ASP	2.3
1	C	130	ASP	2.3
1	D	416	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	358	ILE	2.2
1	D	465	GLN	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

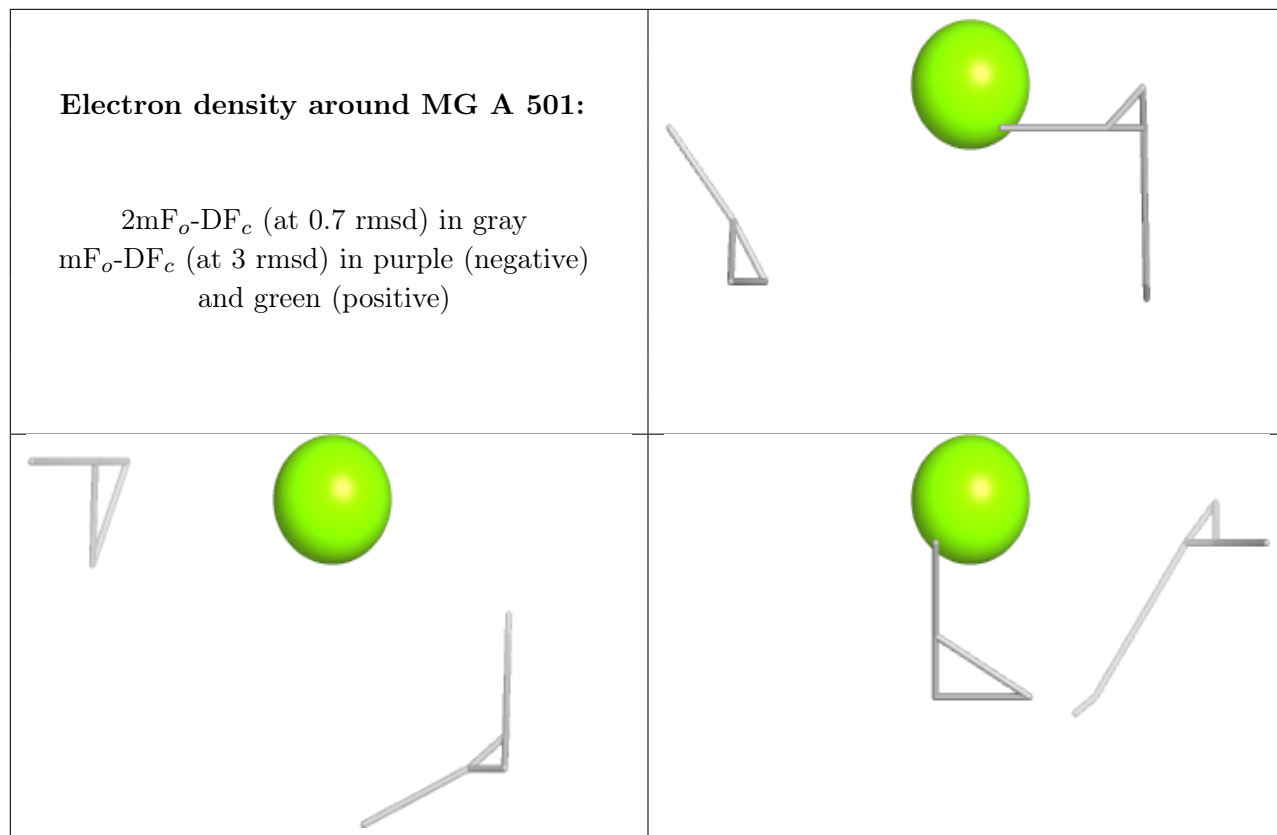
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	501	1/1	0.91	0.10	38,38,38,38	0
2	MG	B	501	1/1	0.94	0.14	49,49,49,49	0
2	MG	D	501	1/1	0.96	0.21	44,44,44,44	0
3	ATP	C	502	31/31	0.96	0.12	39,44,63,70	0
3	ATP	D	502	31/31	0.97	0.12	36,42,57,58	0
2	MG	C	501	1/1	0.97	0.22	55,55,55,55	0
3	ATP	A	502	31/31	0.97	0.12	29,36,46,51	0
3	ATP	B	502	31/31	0.97	0.11	32,37,47,52	0

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

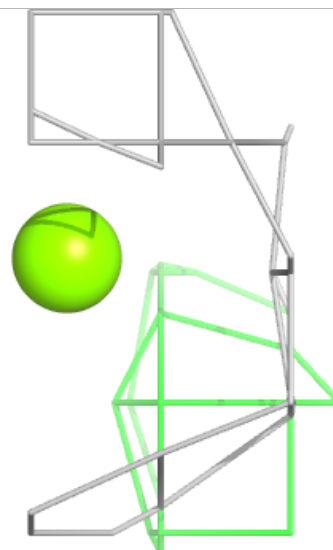
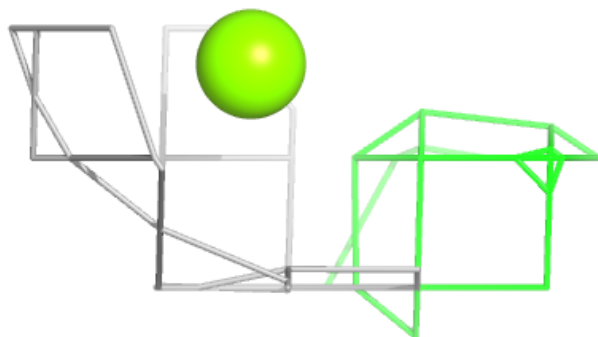
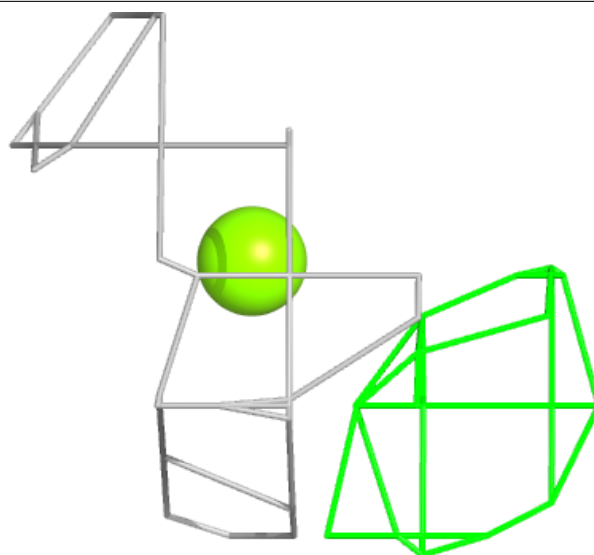
**Electron density around MG A 501:**

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



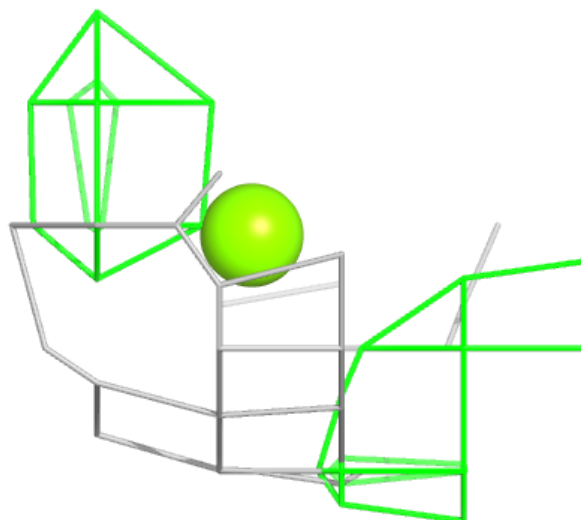
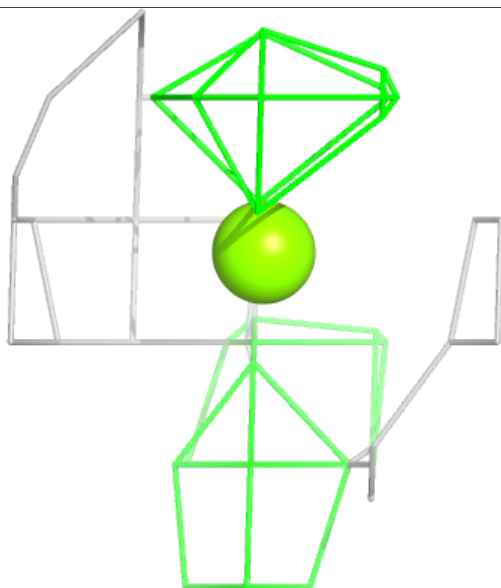
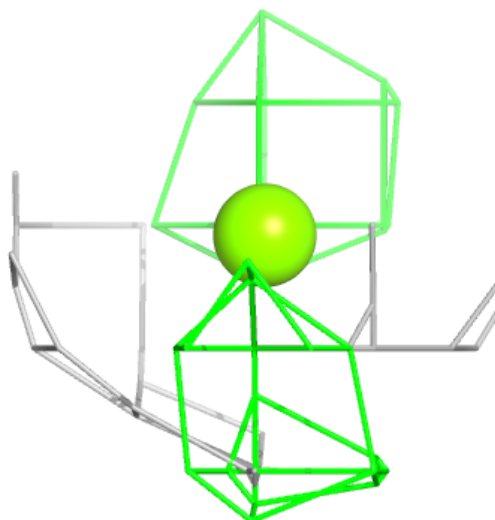
**Electron density around MG B 501:**

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and green (positive)



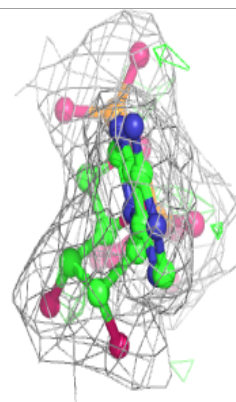
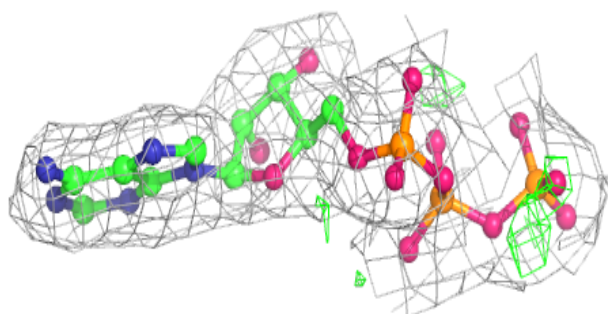
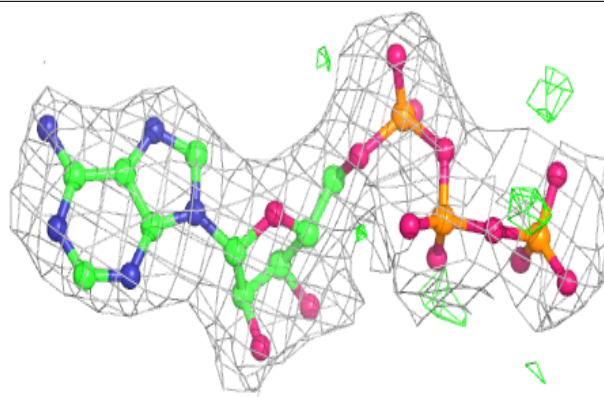
**Electron density around MG D 501:**

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

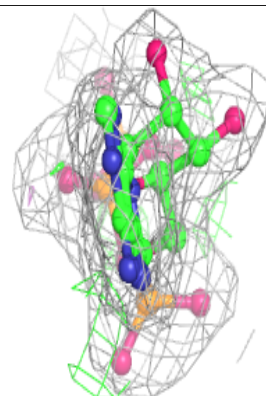
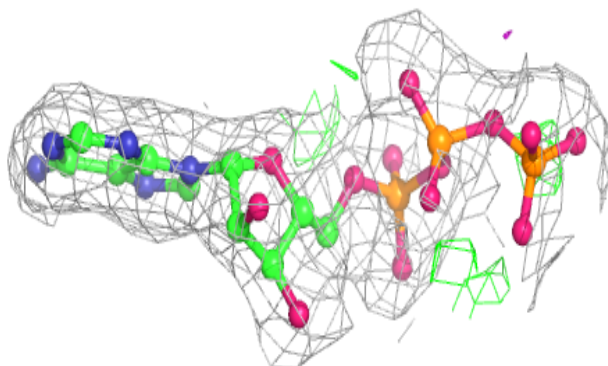
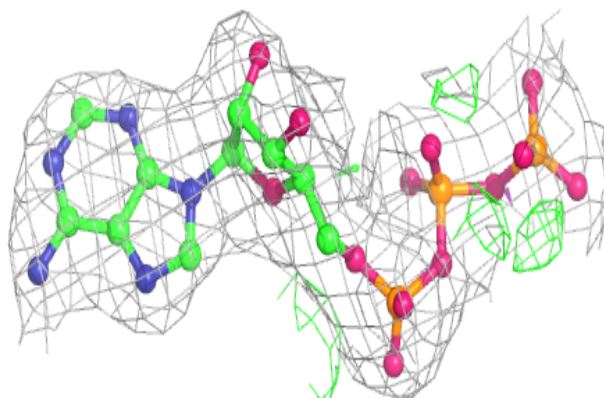


**Electron density around ATP C 502:**

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

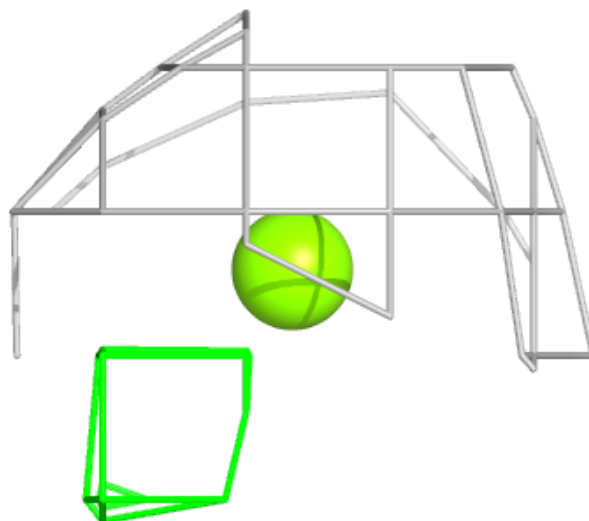
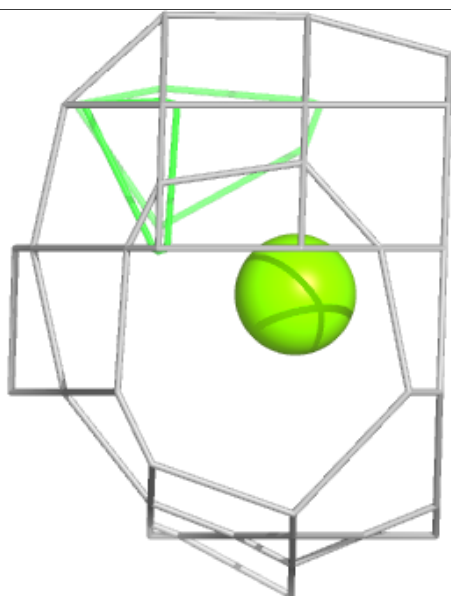
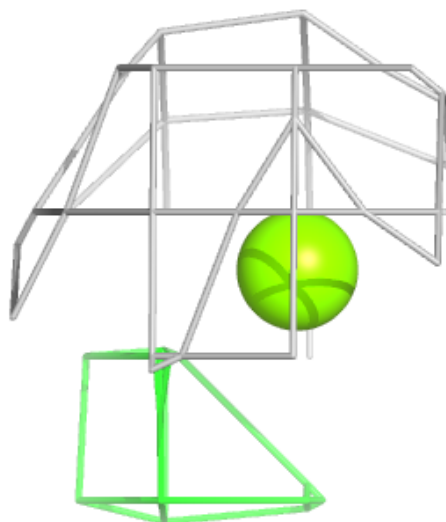
**Electron density around ATP D 502:**

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



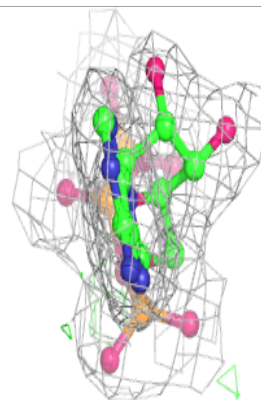
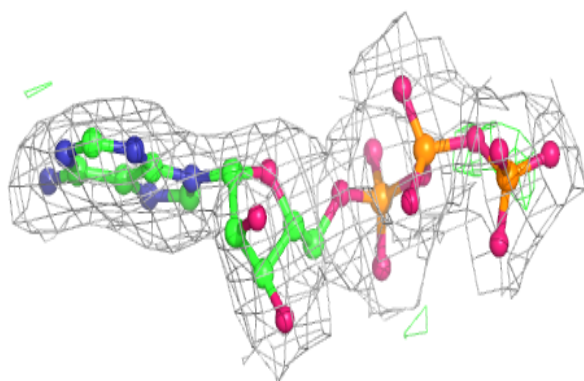
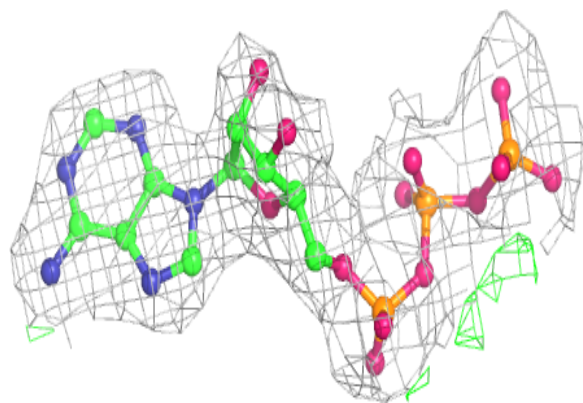
**Electron density around MG C 501:**

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

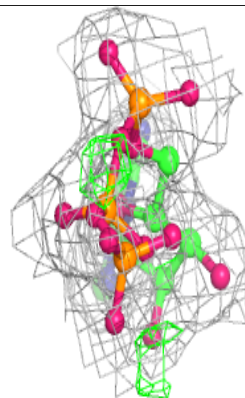
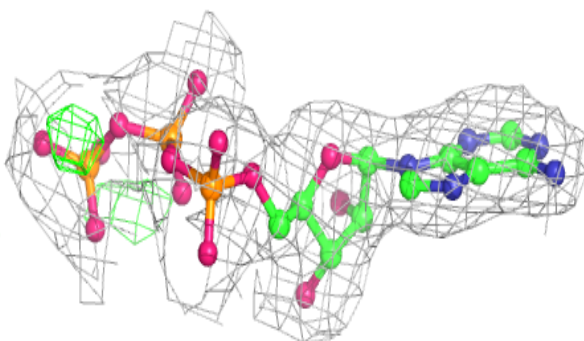
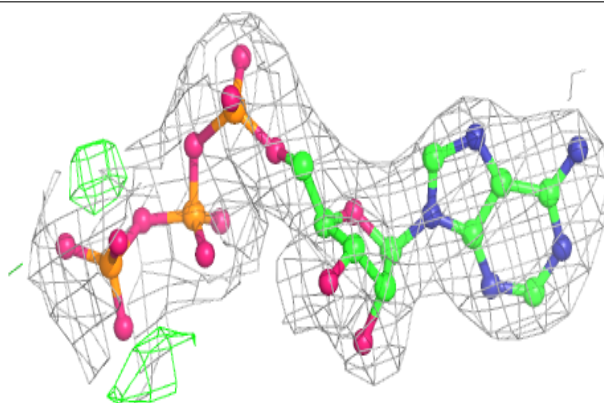


**Electron density around ATP A 502:**

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

**Electron density around ATP B 502:**

$2mF_o-DF_c$  (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.