



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 03:59 PM EST

PDB ID : 2CJA  
Title : Crystal structure of Methanosarcina barkeri seryl-tRNA synthetase complexed with ATP  
Authors : Bilokapic, S.; Maier, T.; Ahel, D.; Gruic-Sovulj, I.; Soll, D.; Weygand-Durasevic, I.; Ban, N.  
Deposited on : 2006-03-30  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

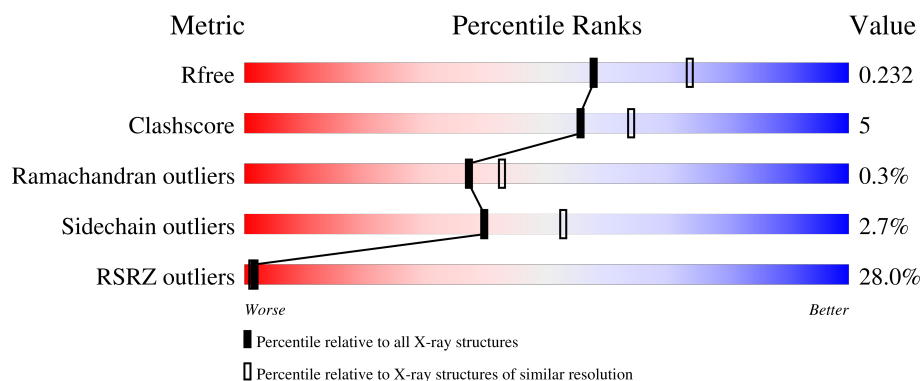
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	522	
1	B	522	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8418 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 SERYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	Se	0	2	0
			3916	2517	674	705	6	14			
1	B	489	Total	C	N	O	S	Se	0	1	0
			3982	2555	682	725	6	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 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>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0

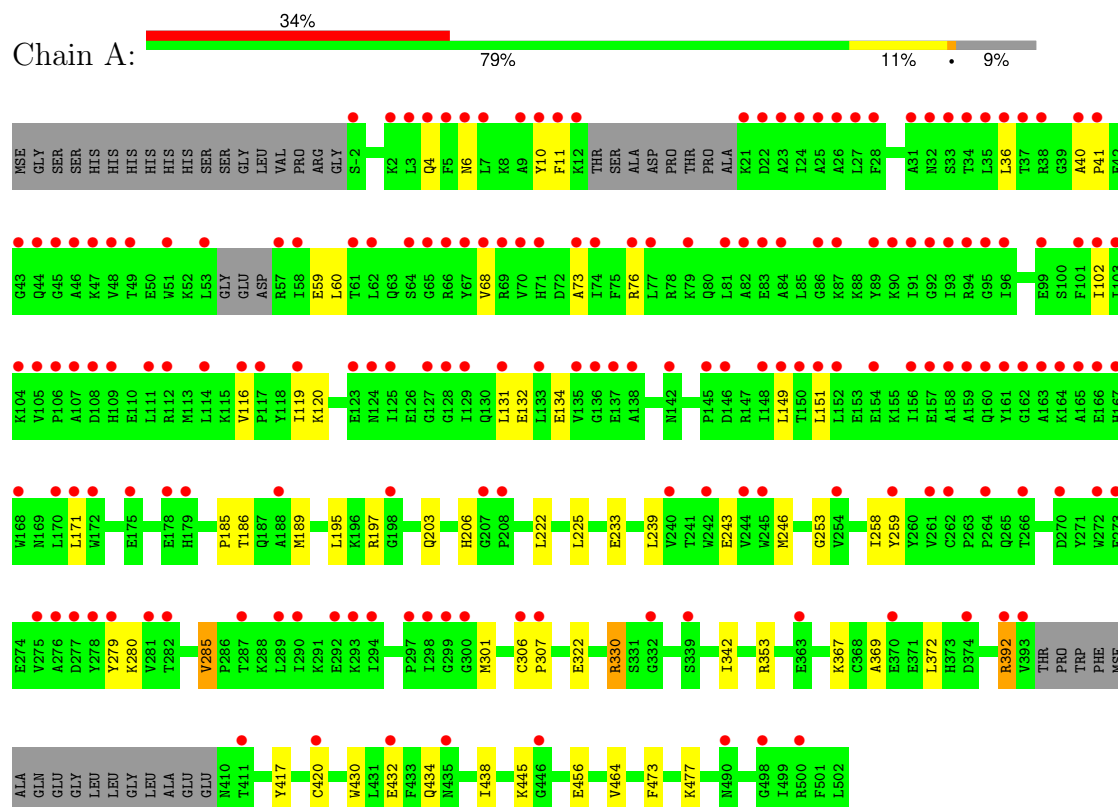
- Molecule 6 is water.

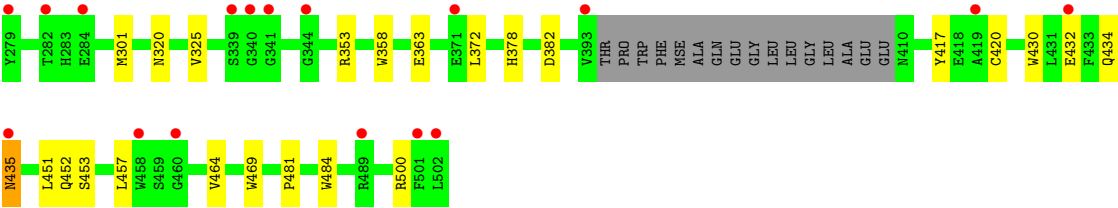
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	221	Total O 221 221	0	0
6	B	231	Total O 231 231	0	0

### 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. 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. 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: SERYL-TRNA SYNTHETASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.31Å 97.31Å 270.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.74 – 2.20 19.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.74-2.20) 98.9 (19.74-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.203 , 0.233 0.204 , 0.232	Depositor DCC
$R_{free}$ test set	3781 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/4005	0.52	0/5385
1	B	0.39	0/4075	0.53	0/5487
All	All	0.39	0/8080	0.52	0/10872

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

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	3916	0	3870	37	0
1	B	3982	0	3923	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	B	2	0	0	0	0
6	A	221	0	0	2	0
6	B	231	0	0	1	0
All	All	8418	0	7817	73	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 5.

All (73) 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:A:259:TYR:HB3	1:A:301[B]:MSE:HE2	1.48	0.94
1:B:186:THR:HA	1:B:189:MSE:HE2	1.54	0.89
1:B:186:THR:HA	1:B:189:MSE:CE	2.04	0.87
1:B:259:TYR:HB3	1:B:301[B]:MSE:HE2	1.59	0.84
1:A:186:THR:HA	1:A:189:MSE:HE3	1.69	0.75
1:A:243:GLU:HA	1:A:246:MSE:HE3	1.73	0.70
1:A:259:TYR:CB	1:A:301[B]:MSE:HE2	2.21	0.70
1:A:301[B]:MSE:HE1	1:B:239:LEU:HD12	1.74	0.69
1:A:186:THR:HA	1:A:189:MSE:CE	2.23	0.67
1:B:4:GLN:HG3	1:B:104:LYS:HB2	1.78	0.65
1:B:259:TYR:CB	1:B:301[B]:MSE:CE	2.74	0.65
1:B:417:TYR:HB2	1:B:434:GLN:HB3	1.79	0.64
1:B:186:THR:CA	1:B:189:MSE:HE2	2.29	0.61
1:B:18:THR:N	1:B:19:PRO:HD2	2.16	0.61
1:B:259:TYR:CB	1:B:301[B]:MSE:HE2	2.31	0.61
1:A:197[B]:ARG:HH12	1:A:203:GLN:H	1.49	0.60
1:A:417:TYR:HB2	1:A:434:GLN:HB3	1.83	0.60
1:A:102:ILE:HG12	1:A:132:GLU:HG3	1.87	0.57
1:A:171:LEU:HD11	1:A:392:ARG:HG3	1.87	0.56
1:A:259:TYR:CB	1:A:301[B]:MSE:CE	2.82	0.56
1:A:280:LYS:HD2	1:B:151:LEU:HD13	1.88	0.56
1:B:259:TYR:HB3	1:B:301[B]:MSE:CE	2.29	0.55
1:A:68:VAL:HG12	6:A:2016:HOH:O	2.06	0.55
1:B:1:MSE:HE3	6:B:2005:HOH:O	2.07	0.55
1:A:369:ALA:HB2	1:A:438:ILE:HD11	1.88	0.55
1:B:13:THR:HG21	1:B:17:PRO:HG3	1.89	0.55
1:A:259:TYR:HB3	1:A:301[B]:MSE:CE	2.30	0.54
1:A:206:HIS:HB2	1:B:235:ILE:HB	1.90	0.54
1:B:11:PHE:CD1	1:B:93:ILE:HD11	2.43	0.53
1:B:259:TYR:CB	1:B:301[B]:MSE:HE3	2.38	0.53
1:A:11:PHE:HE2	1:A:60:LEU:HD11	1.73	0.53
1:B:320:ASN:HD21	1:B:453:SER:H	1.57	0.52
1:A:258:ILE:O	1:B:264:PRO:HD3	2.10	0.52
1:B:259:TYR:HB2	1:B:301[B]:MSE:HE3	1.92	0.52
1:B:122:MSE:HG3	1:B:131:LEU:HD23	1.92	0.51
1:B:81:LEU:HD22	1:B:93:ILE:HD12	1.92	0.51
1:B:181:PHE:CZ	1:B:183:GLU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:THR:HA	1:B:189:MSE:HE3	1.90	0.50
1:A:445:LYS:NZ	1:A:456:GLU:OE1	2.45	0.49
1:B:131:LEU:HD11	1:B:152:LEU:HD22	1.95	0.48
1:A:4:GLN:HE21	1:A:6:ASN:HD21	1.60	0.48
1:A:233:GLU:OE2	1:A:330:ARG:HD2	2.14	0.48
1:B:451:LEU:HB2	1:B:457:LEU:HG	1.95	0.48
1:A:120:LYS:HB2	1:A:134:GLU:HG3	1.96	0.47
1:A:116:VAL:HB	1:A:119:ILE:HD12	1.97	0.46
1:B:78:ARG:HD2	1:B:96:ILE:HD11	1.97	0.46
1:A:306:CYS:SG	1:A:307:PRO:HD3	2.56	0.46
1:B:320:ASN:HD22	1:B:452:GLN:HB3	1.81	0.46
1:B:3:LEU:HD23	1:B:66:ARG:HB3	1.98	0.46
1:A:36:LEU:HD23	1:A:76:ARG:HD2	1.97	0.45
1:A:285:VAL:HG11	1:B:242:TRP:HB3	1.97	0.45
1:A:185:PRO:O	1:A:189:MSE:HG3	2.17	0.45
1:A:11:PHE:CE2	1:A:60:LEU:HD11	2.52	0.45
1:A:40:ALA:HA	1:A:41:PRO:HD3	1.87	0.45
1:B:378:HIS:ND1	1:B:382:ASP:OD2	2.48	0.45
1:A:10:TYR:HB3	1:A:59:GLU:HG2	2.00	0.43
1:B:18:THR:N	1:B:19:PRO:CD	2.80	0.43
1:B:481:PRO:HA	1:B:484:TRP:CD2	2.53	0.43
1:A:225:LEU:HD21	1:A:372:LEU:HD23	2.00	0.43
1:B:109:HIS:ND1	1:B:160:GLN:HB3	2.34	0.42
1:A:473:PHE:CE1	1:A:477:LYS:HG3	2.54	0.42
1:B:215:ARG:HA	1:B:215:ARG:HD3	1.91	0.42
1:B:435:ASN:C	1:B:435:ASN:HD22	2.23	0.42
1:A:353:ARG:HA	1:A:464:VAL:O	2.19	0.41
1:B:464:VAL:HG13	1:B:469:TRP:CE2	2.55	0.41
1:B:420:CYS:HB3	1:B:430:TRP:CE2	2.56	0.41
1:B:325:VAL:O	1:B:358:TRP:HA	2.20	0.41
1:B:225:LEU:HD21	1:B:372:LEU:HD22	2.03	0.40
1:A:73:ALA:HB2	6:A:2016:HOH:O	2.21	0.40
1:A:322:GLU:OE1	1:B:500:ARG:NH1	2.54	0.40
1:A:420:CYS:HB3	1:A:430:TRP:CE2	2.56	0.40
1:A:279:TYR:CE1	1:B:246:MSE:HG2	2.57	0.40
1:B:353:ARG:HA	1:B:464:VAL:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/522 (90%)	451 (96%)	19 (4%)	1 (0%)	44	52
1	B	486/522 (93%)	466 (96%)	18 (4%)	2 (0%)	30	34
All	All	957/1044 (92%)	917 (96%)	37 (4%)	3 (0%)	37	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	ASP
1	B	253	GLY
1	A	253	GLY

### 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	411/429 (96%)	399 (97%)	12 (3%)	37	50
1	B	418/429 (97%)	408 (98%)	10 (2%)	44	57
All	All	829/858 (97%)	807 (97%)	22 (3%)	40	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	149	LEU
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	222	LEU
1	A	239	LEU
1	A	285	VAL
1	A	330	ARG
1	A	342	ILE
1	A	367	LYS
1	A	392	ARG
1	A	432	GLU
1	B	7	LEU
1	B	16	ASP
1	B	37	THR
1	B	47	LYS
1	B	113	MSE
1	B	170	LEU
1	B	195	LEU
1	B	363	GLU
1	B	432	GLU
1	B	435	ASN

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

Mol	Chain	Res	Type
1	A	4	GLN
1	B	320	ASN
1	B	435	ASN

### 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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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$
4	ATP	B	1507	5	28,33,33	0.98	2 (7%)	34,52,52	1.13	2 (5%)
4	ATP	A	1505	-	28,33,33	1.47	4 (14%)	34,52,52	1.08	1 (2%)

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
4	ATP	B	1507	5	-	3/18/38/38	0/3/3/3
4	ATP	A	1505	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1505	ATP	PA-O3A	4.47	1.64	1.59
4	A	1505	ATP	PB-O3A	3.67	1.63	1.59
4	A	1505	ATP	O4'-C1'	2.78	1.44	1.40
4	A	1505	ATP	PB-O3B	2.66	1.62	1.59
4	B	1507	ATP	PB-O3B	2.19	1.61	1.59
4	B	1507	ATP	O4'-C1'	2.18	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1505	ATP	N3-C2-N1	-4.05	123.18	128.67
4	B	1507	ATP	N3-C2-N1	-3.86	123.43	128.67
4	B	1507	ATP	C4-C5-N7	-2.38	106.82	109.34

There are no chirality outliers.

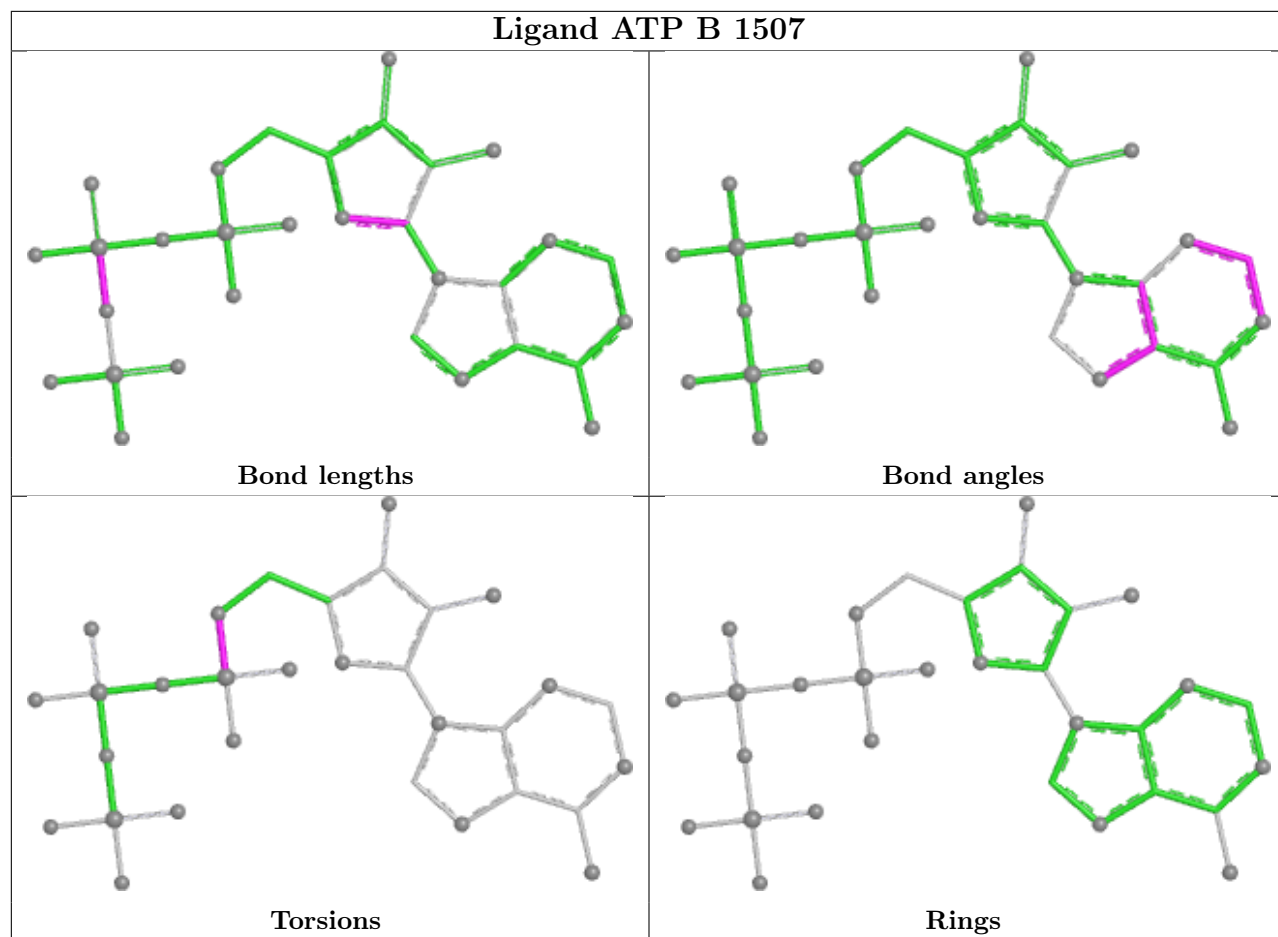
All (3) torsion outliers are listed below:

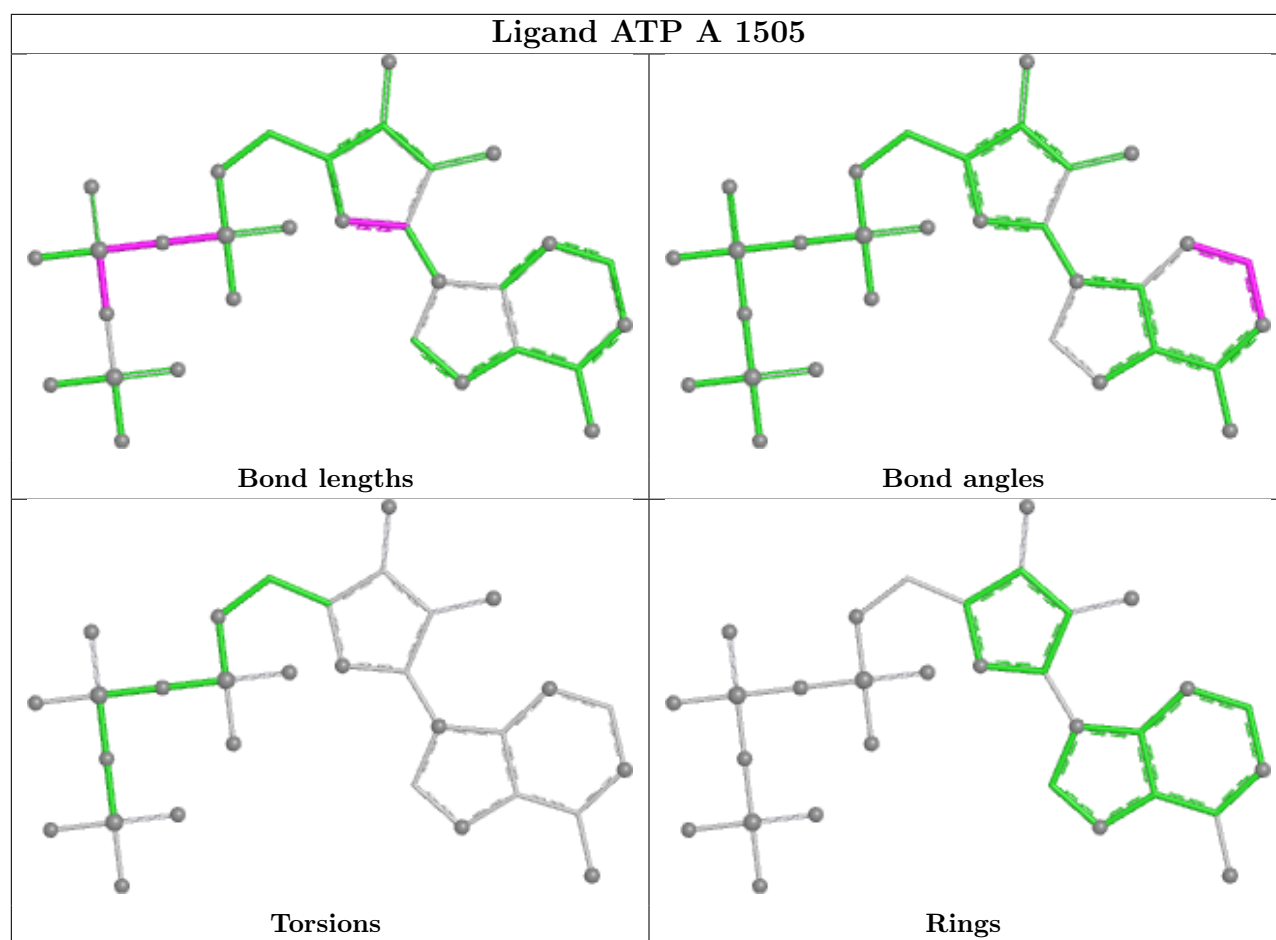
Mol	Chain	Res	Type	Atoms
4	B	1507	ATP	C5'-O5'-PA-O2A
4	B	1507	ATP	C5'-O5'-PA-O3A
4	B	1507	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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

**Warning:** The R factor obtained from EDS is 0.3114, which does not match the depositor's R factor of 0.203. Please interpret the results in this section carefully.

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	464/522 (88%)	1.82	176 (37%)  	30, 65, 140, 144	1 (0%)
1	B	476/522 (91%)	1.38	87 (18%)  	56, 64, 75, 95	0
All	All	940/1044 (90%)	1.60	263 (27%)  	30, 64, 122, 144	1 (0%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	ALA	8.4
1	A	65	GLY	7.8
1	B	161	TYR	7.8
1	A	68	VAL	7.3
1	B	165	ALA	7.1
1	A	165	ALA	6.9
1	B	162	GLY	6.2
1	A	92	GLY	5.9
1	B	167	HIS	5.9
1	A	128	GLY	5.9
1	A	46	ALA	5.9
1	A	23	ALA	5.6
1	A	158	ALA	5.4
1	A	3	LEU	5.2
1	A	167	HIS	5.1
1	A	82	ALA	5.0
1	B	164	LYS	5.0
1	A	53	LEU	5.0
1	B	27	LEU	4.9
1	A	156	ILE	4.6
1	A	161	TYR	4.6
1	A	276	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	119	ILE	4.4
1	A	136	GLY	4.3
1	A	107	ALA	4.2
1	A	70	VAL	4.2
1	B	57	ARG	4.2
1	B	82	ALA	4.1
1	A	106	PRO	4.1
1	A	129	ILE	4.0
1	A	90	LYS	4.0
1	B	51	TRP	3.9
1	B	107	ALA	3.9
1	A	64	SER	3.8
1	A	86	GLY	3.8
1	A	166	GLU	3.8
1	A	282	THR	3.7
1	B	15	ALA	3.7
1	B	84	ALA	3.6
1	B	150	THR	3.6
1	A	124	ASN	3.6
1	A	45	GLY	3.6
1	A	162	GLY	3.6
1	A	164	LYS	3.6
1	A	163	ALA	3.5
1	A	281	VAL	3.5
1	A	67	TYR	3.5
1	A	93	ILE	3.5
1	B	95	GLY	3.4
1	A	21	LYS	3.4
1	A	33	SER	3.4
1	A	36	LEU	3.4
1	A	289	LEU	3.4
1	A	490	ASN	3.4
1	A	26	ALA	3.4
1	A	9	ALA	3.3
1	A	6	ASN	3.3
1	A	299	GLY	3.3
1	A	35	LEU	3.2
1	A	135	VAL	3.2
1	A	84	ALA	3.2
1	B	10	TYR	3.2
1	A	500	ARG	3.2
1	A	103	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	3.2
1	A	171	LEU	3.2
1	A	339	SER	3.2
1	A	420	CYS	3.1
1	A	37	THR	3.1
1	A	5	PHE	3.1
1	B	502	LEU	3.1
1	A	10	TYR	3.1
1	A	117	PRO	3.1
1	B	158	ALA	3.1
1	B	276	ALA	3.1
1	A	76	ARG	3.1
1	B	-1	HIS	3.0
1	A	-2	SER	3.0
1	A	261	VAL	3.0
1	A	31	ALA	3.0
1	B	125	ILE	3.0
1	B	65	GLY	3.0
1	B	344	GLY	3.0
1	A	292	GLU	3.0
1	B	166	GLU	3.0
1	A	168	TRP	3.0
1	B	160	GLN	3.0
1	A	91	ILE	3.0
1	A	370	GLU	3.0
1	A	28	PHE	3.0
1	A	101	PHE	3.0
1	A	27	LEU	2.9
1	B	79	LYS	2.9
1	B	419	ALA	2.9
1	A	157	GLU	2.9
1	A	102	ILE	2.9
1	B	152	LEU	2.9
1	A	32	ASN	2.9
1	B	19	PRO	2.9
1	A	159	ALA	2.9
1	B	-3	GLY	2.9
1	A	66	ARG	2.9
1	A	374	ASP	2.9
1	A	2	LYS	2.9
1	A	34	THR	2.9
1	B	13	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	446	GLY	2.9
1	A	51	TRP	2.8
1	A	272	TRP	2.8
1	A	22	ASP	2.8
1	A	41	PRO	2.8
1	A	244	VAL	2.8
1	B	371	GLU	2.8
1	A	133	LEU	2.8
1	A	125	ILE	2.8
1	A	278	TYR	2.8
1	B	72	ASP	2.8
1	A	116	VAL	2.8
1	A	393	VAL	2.8
1	A	47	LYS	2.8
1	A	83	GLU	2.8
1	A	300	GLY	2.8
1	A	137	GLU	2.8
1	A	148	ILE	2.8
1	A	11	PHE	2.7
1	A	48	VAL	2.7
1	A	49	THR	2.7
1	A	94	ARG	2.7
1	A	392	ARG	2.7
1	B	25	ALA	2.7
1	B	46	ALA	2.7
1	A	95	GLY	2.7
1	B	340	GLY	2.7
1	B	341	GLY	2.7
1	A	69	ARG	2.7
1	A	74	ILE	2.7
1	B	156	ILE	2.7
1	A	264	PRO	2.7
1	A	25	ALA	2.7
1	B	154	GLU	2.7
1	A	277	ASP	2.7
1	A	275	VAL	2.7
1	A	79	LYS	2.7
1	A	43	GLY	2.6
1	B	92	GLY	2.6
1	A	287	THR	2.6
1	A	266	THR	2.6
1	A	432	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	432	GLU	2.6
1	A	262	CYS	2.6
1	B	93	ILE	2.6
1	A	105	VAL	2.6
1	A	240	VAL	2.6
1	B	275	VAL	2.6
1	A	294	ILE	2.6
1	B	58	ILE	2.6
1	A	127	GLY	2.6
1	A	89	TYR	2.6
1	A	151	LEU	2.6
1	B	17	PRO	2.6
1	A	109	HIS	2.6
1	B	99	GLU	2.5
1	A	61	THR	2.5
1	A	152	LEU	2.5
1	A	142	ASN	2.5
1	B	87	LYS	2.5
1	A	123	GLU	2.5
1	A	178	GLU	2.5
1	A	112	ARG	2.5
1	A	131	LEU	2.5
1	A	254	VAL	2.5
1	B	75	PHE	2.5
1	A	149	LEU	2.5
1	B	-2	SER	2.4
1	B	200	SER	2.4
1	B	126	GLU	2.4
1	A	114	LEU	2.4
1	B	98	VAL	2.4
1	A	273	GLU	2.4
1	B	91	ILE	2.4
1	B	123	GLU	2.4
1	A	293	LYS	2.4
1	A	81	LEU	2.4
1	A	170	LEU	2.4
1	B	435	ASN	2.4
1	A	298	ILE	2.4
1	A	146	ASP	2.4
1	A	188	ALA	2.4
1	A	24	ILE	2.4
1	B	268	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	71	HIS	2.4
1	A	207	GLY	2.4
1	A	242	TRP	2.3
1	A	245	TRP	2.3
1	B	282	THR	2.3
1	B	41	PRO	2.3
1	B	205	ILE	2.3
1	B	460	GLY	2.3
1	A	150	THR	2.3
1	B	489	ARG	2.3
1	A	160	GLN	2.3
1	A	279	TYR	2.3
1	B	50	GLU	2.3
1	A	297	PRO	2.3
1	A	498	GLY	2.3
1	A	175	GLU	2.3
1	A	363	GLU	2.3
1	A	306	CYS	2.3
1	A	38	ARG	2.3
1	A	57	ARG	2.3
1	A	172	TRP	2.3
1	B	168	TRP	2.3
1	A	4	GLN	2.3
1	B	56	ASP	2.3
1	A	77	LEU	2.2
1	A	307	PRO	2.2
1	B	209	GLN	2.2
1	A	290	ILE	2.2
1	B	339	SER	2.2
1	B	393	VAL	2.2
1	A	58	ILE	2.2
1	A	62	LEU	2.2
1	B	212	ARG	2.2
1	B	279	TYR	2.2
1	A	12	LYS	2.2
1	A	154	GLU	2.2
1	B	151	LEU	2.2
1	A	40	ALA	2.2
1	B	137	GLU	2.1
1	B	458	TRP	2.1
1	B	20	ALA	2.1
1	A	411	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	22	ASP	2.1
1	A	198	GLY	2.1
1	A	96	ILE	2.1
1	B	220	ILE	2.1
1	A	7	LEU	2.1
1	A	145	PRO	2.1
1	A	259	TYR	2.1
1	B	501	PHE	2.1
1	B	128	GLY	2.1
1	A	179	HIS	2.1
1	A	44	GLN	2.1
1	A	435	ASN	2.1
1	B	117	PRO	2.1
1	B	272	TRP	2.1
1	B	94	ARG	2.1
1	A	108	ASP	2.1
1	A	332	GLY	2.1
1	B	129	ILE	2.1
1	A	87	LYS	2.1
1	A	104	LYS	2.1
1	B	12	LYS	2.1
1	B	90	LYS	2.1
1	A	208	PRO	2.1
1	B	172	TRP	2.1
1	A	73	ALA	2.1
1	A	138	ALA	2.1
1	B	186	THR	2.1
1	A	270	ASP	2.0
1	A	99	GLU	2.0
1	B	284	GLU	2.0
1	B	106	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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.

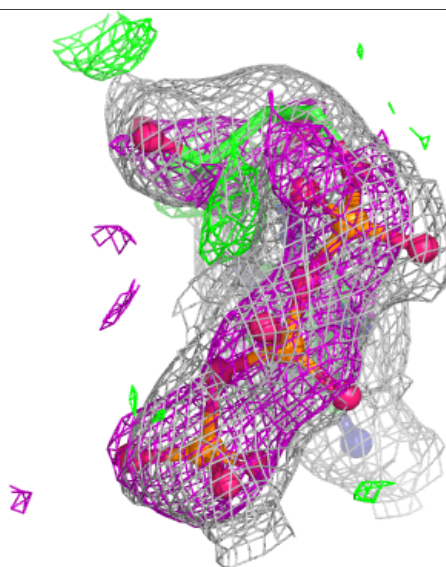
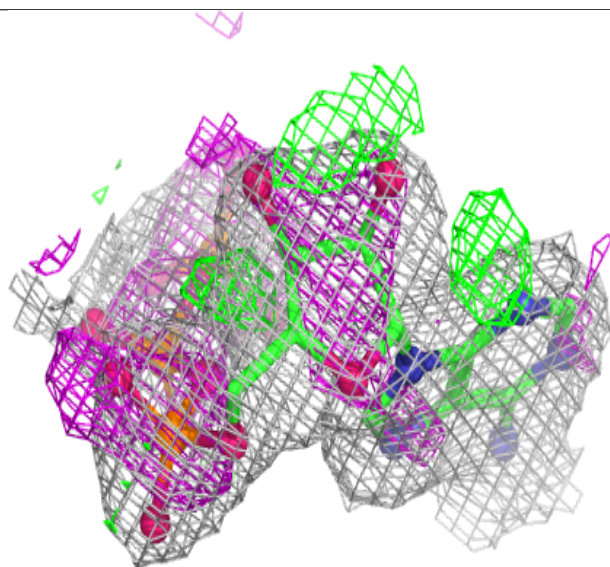
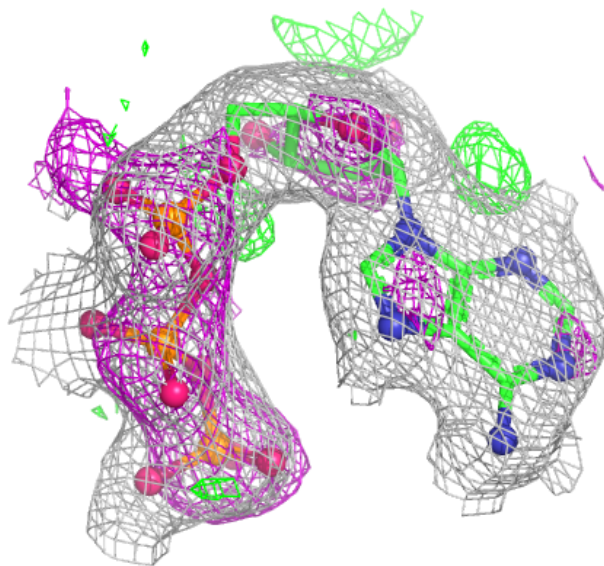
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	1506	1/1	0.81	0.22	76,76,76,76	0
5	MG	B	1505	1/1	0.83	0.22	70,70,70,70	0
4	ATP	B	1507	31/31	0.85	0.15	49,58,78,78	0
4	ATP	A	1505	31/31	0.86	0.15	41,47,65,66	0
3	CL	B	1504	1/1	0.97	0.23	37,37,37,37	0
3	CL	A	1504	1/1	0.98	0.19	34,34,34,34	0
2	ZN	B	1503	1/1	0.98	0.09	44,44,44,44	0
2	ZN	A	1503	1/1	0.99	0.10	39,39,39,39	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.



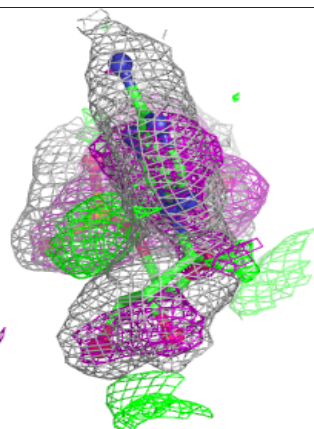
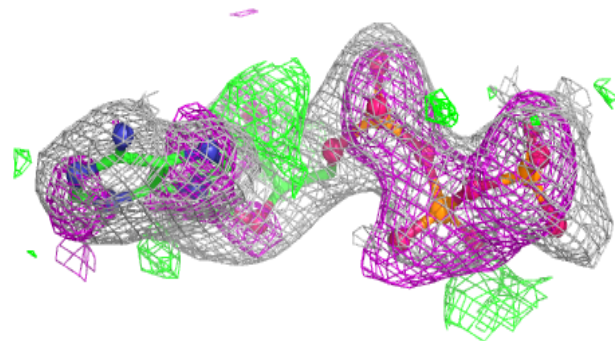
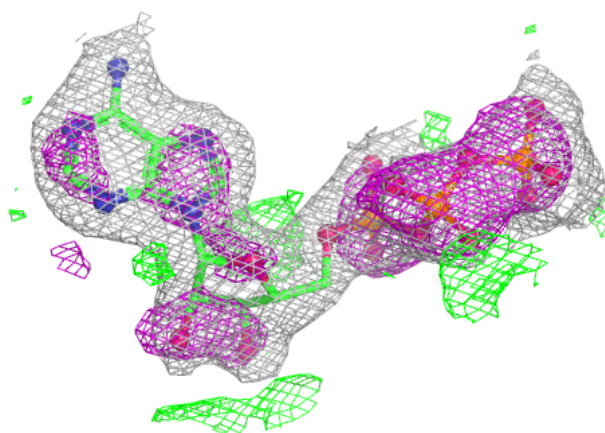
**Electron density around ATP B 1507:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 1505:**

$2mF_o-DF_c$  (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.