



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 06:23 PM EDT

PDB ID : 2CJA / pdb_00002cja
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

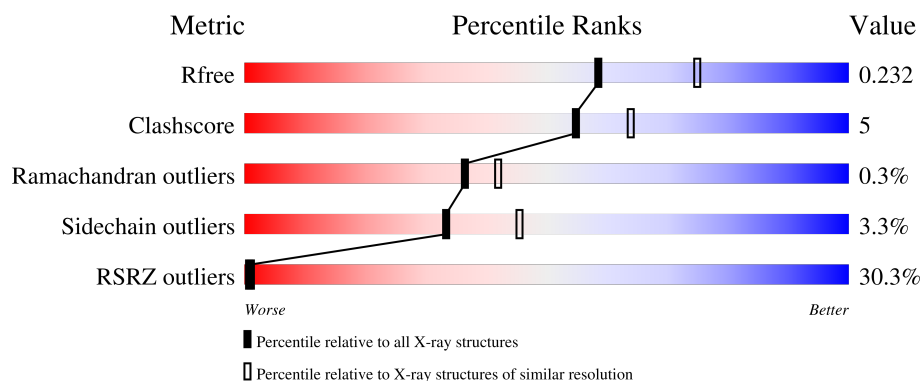
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 ≥ 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	522	36% 79% 12% 9%
1	B	522	19% 80% 13% 6%

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 (CCD ID: 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 (CCD ID: 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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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 (CCD ID: 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

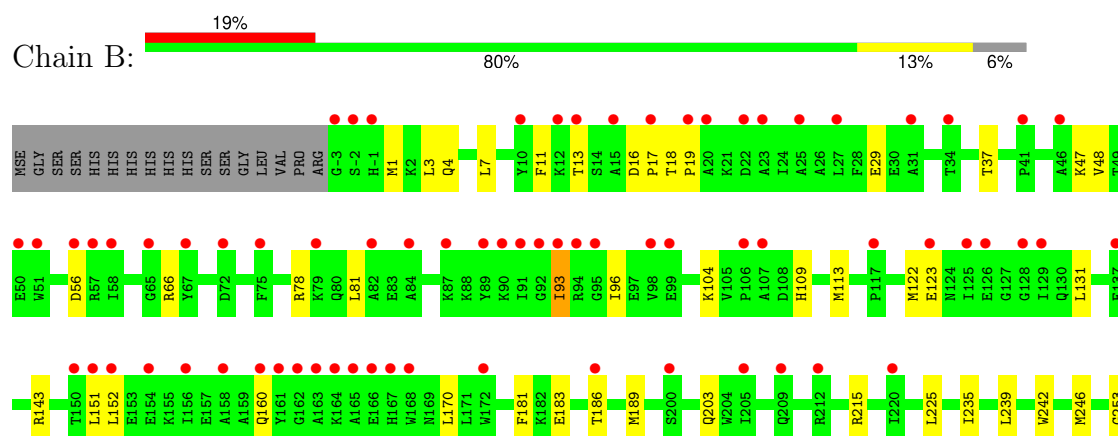
3 Residue-property plots

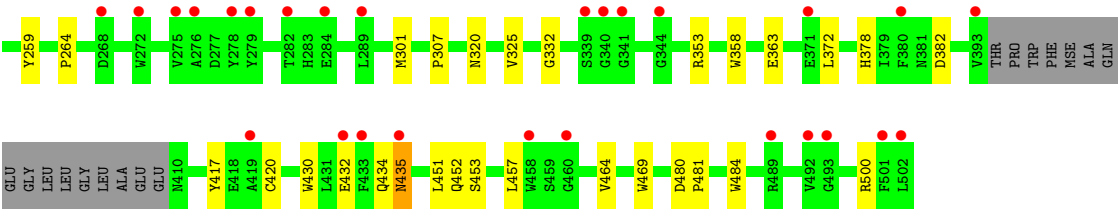
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	43.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: ATP, CL, MG, 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	0.51	0/4005	0.75	1/5385 (0.0%)
1	B	0.50	0/4075	0.76	6/5487 (0.1%)
All	All	0.50	0/8080	0.75	7/10872 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	PRO	N-CA-C	5.51	117.42	110.70
1	B	332	GLY	N-CA-C	5.48	118.24	110.74
1	A	332	GLY	N-CA-C	5.25	117.93	110.74
1	B	480	ASP	CA-C-N	5.16	124.96	119.28
1	B	480	ASP	C-N-CA	5.16	124.96	119.28
1	B	143	ARG	CA-C-N	5.02	123.40	120.24
1	B	143	ARG	C-N-CA	5.02	123.40	120.24

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	3916	0	3870	38	0
1	B	3982	0	3923	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	75	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 (75) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:186:THR:HA	1:B:189:MSE:HE3	1.90	0.50
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:B:435:ASN:C	1:B:435:ASN:HD22	2.23	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:A:445:LYS:NZ	1:A:456:GLU:OE1	2.45	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:ND2	2.76	0.42
1:A:353:ARG:HA	1:A:464:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:237:PRO:HB3	1:B:203:GLN:CD	2.45	0.40
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%)	43	51
1	B	486/522 (93%)	466 (96%)	18 (4%)	2 (0%)	30	34
All	All	957/1044 (92%)	917 (96%)	37 (4%)	3 (0%)	36	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%)	397 (97%)	14 (3%)	32	44
1	B	418/429 (97%)	405 (97%)	13 (3%)	35	48
All	All	829/858 (97%)	802 (97%)	27 (3%)	33	45

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	131	LEU
1	A	149	LEU
1	A	151	LEU
1	A	195	LEU
1	A	215	ARG
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	29	GLU
1	B	37	THR
1	B	47	LYS
1	B	48	VAL
1	B	93	ILE
1	B	113	MSE
1	B	123	GLU
1	B	170	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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	B	209	GLN
1	B	283	HIS
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	32,33,33	1.41	5 (15%)	48,52,52	1.70	10 (20%)
4	ATP	A	1505	-	32,33,33	1.69	7 (21%)	48,52,52	1.72	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	1507	5	-	3/22/38/38	0/3/3/3
4	ATP	A	1505	-	-	0/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1507	ATP	C5-C4	4.75	1.47	1.39
4	A	1505	ATP	C5-C4	4.54	1.47	1.39
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	B	1507	ATP	C5-C6	2.77	1.48	1.41
4	A	1505	ATP	C5-C6	2.75	1.48	1.41
4	A	1505	ATP	PB-O3B	2.66	1.62	1.59
4	B	1507	ATP	C5-N7	-2.32	1.34	1.39
4	B	1507	ATP	C8-N7	2.24	1.36	1.31
4	A	1505	ATP	C5-N7	-2.23	1.35	1.39
4	B	1507	ATP	PB-O3B	2.19	1.61	1.59
4	A	1505	ATP	C8-N7	2.04	1.35	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1505	ATP	C5-C4-N3	-5.75	118.80	126.72
4	B	1507	ATP	C5-C4-N3	-5.58	119.03	126.72
4	A	1505	ATP	N3-C4-N9	4.92	135.53	127.17
4	B	1507	ATP	N3-C4-N9	4.50	134.83	127.17
4	A	1505	ATP	C2-N3-C4	3.75	120.99	111.83
4	A	1505	ATP	N3-C2-N1	-3.57	123.18	128.58
4	B	1507	ATP	C2-N3-C4	3.53	120.45	111.83
4	B	1507	ATP	N3-C2-N1	-3.41	123.43	128.58
4	B	1507	ATP	C4-C5-N7	-3.29	106.82	110.58
4	A	1505	ATP	C4-C5-N7	-2.93	107.24	110.58
4	A	1505	ATP	C4-N9-C8	2.79	108.67	105.74
4	B	1507	ATP	C4-N9-C8	2.60	108.47	105.74
4	B	1507	ATP	C5-N7-C8	2.44	107.28	103.45
4	A	1505	ATP	C5-N7-C8	2.40	107.22	103.45
4	B	1507	ATP	C2-N1-C6	2.36	122.61	118.73
4	B	1507	ATP	C2'-C1'-N9	-2.11	108.05	113.30
4	B	1507	ATP	C6-C5-N7	2.11	136.16	132.09
4	A	1505	ATP	C2-N1-C6	2.07	122.13	118.73

There are no chirality outliers.

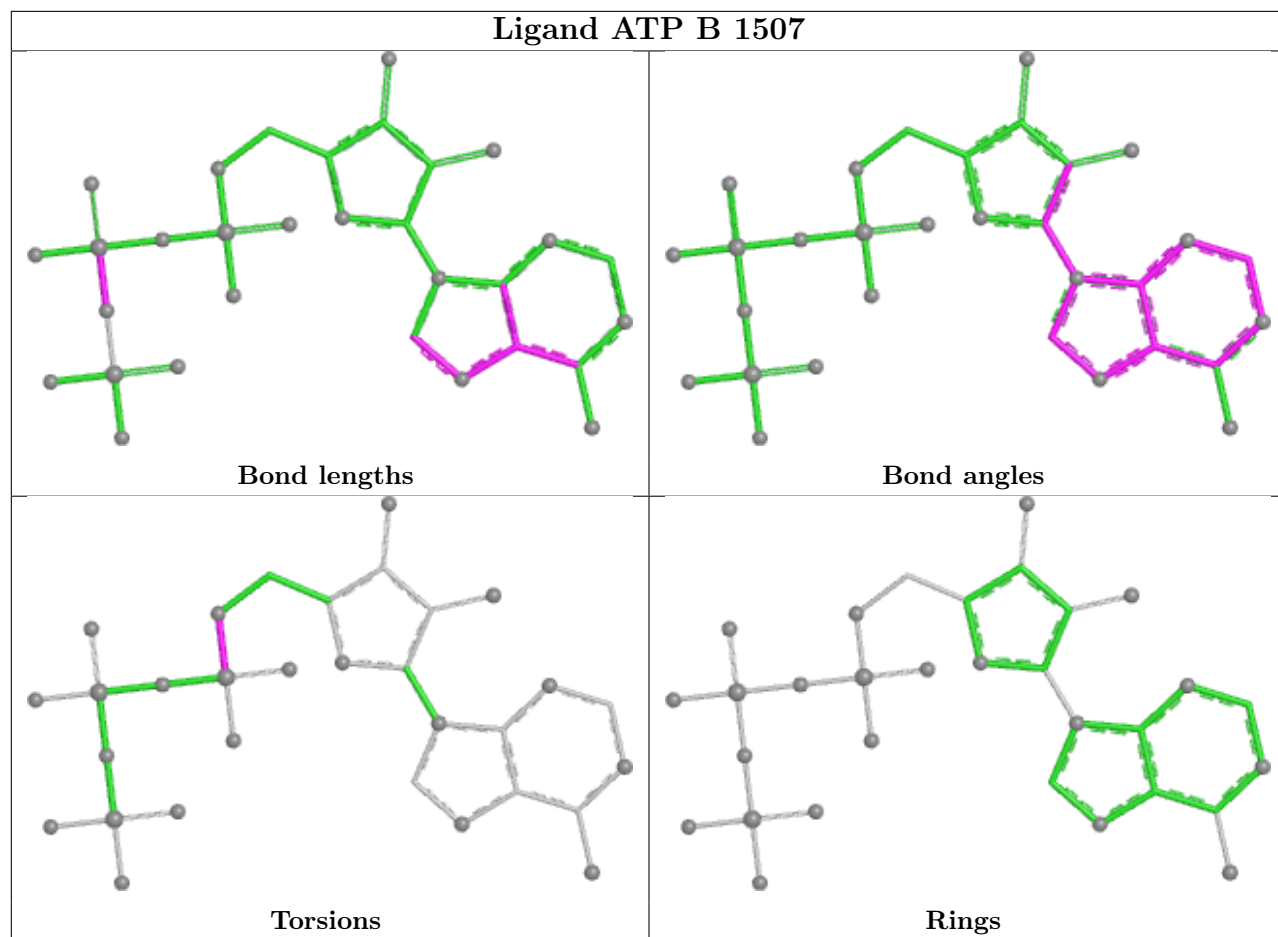
All (3) torsion outliers are listed below:

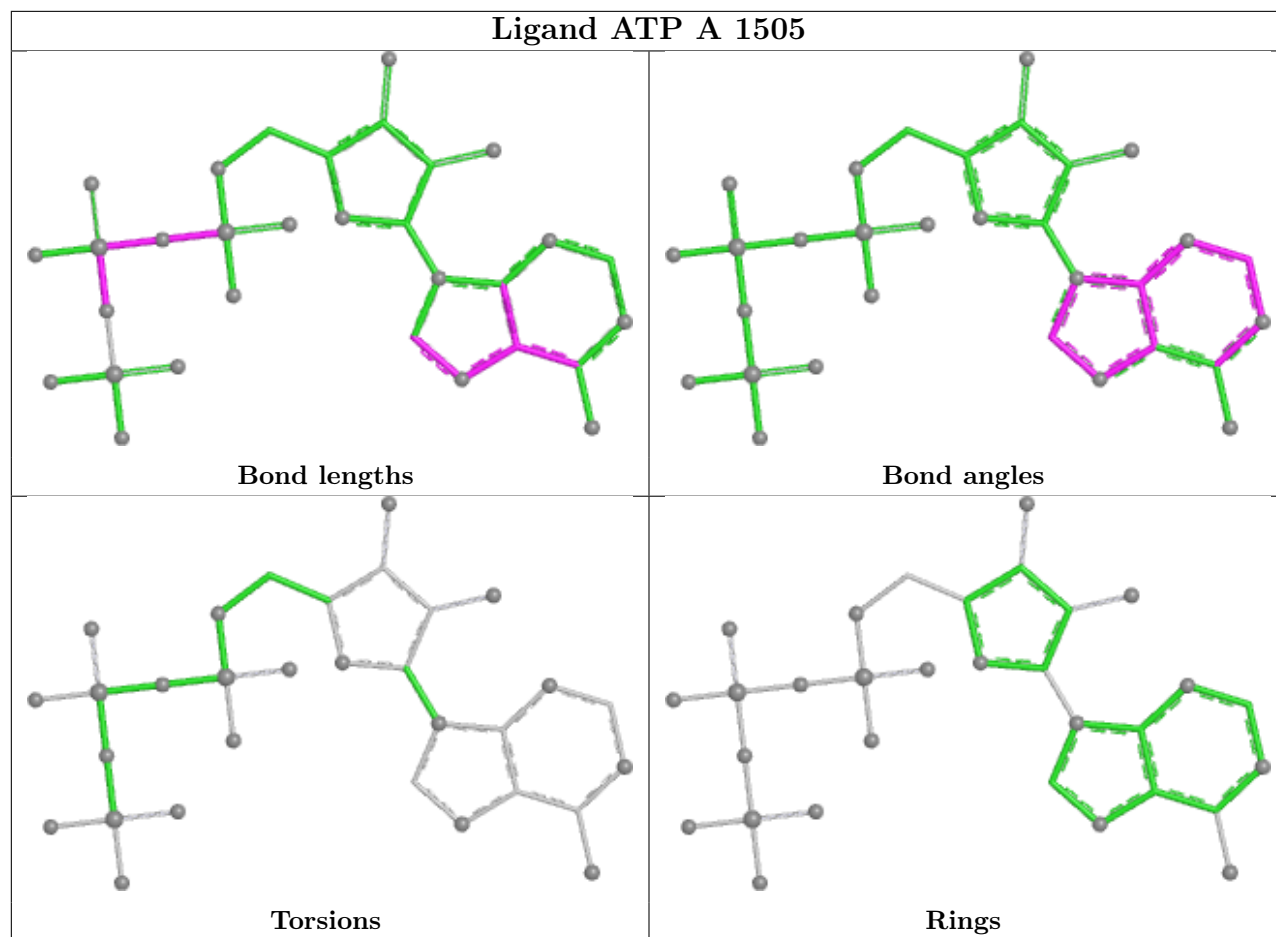
Mol	Chain	Res	Type	Atoms
4	B	1507	ATP	C5'-O5'-PA-O2A
4	B	1507	ATP	C5'-O5'-PA-O3A
4	B	1507	ATP	C5'-O5'-PA-O1A

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

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	464/522 (88%)	1.91	187 (40%)	0 0	30, 65, 140, 144	1 (0%)
1	B	476/522 (91%)	1.48	98 (20%)	2 2	56, 64, 75, 95	0
All	All	940/1044 (90%)	1.69	285 (30%)	1 1	30, 64, 122, 144	1 (0%)

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	ALA	8.6
1	B	161	TYR	8.0
1	A	65	GLY	8.0
1	A	68	VAL	7.5
1	B	165	ALA	7.3
1	A	165	ALA	7.1
1	B	162	GLY	6.3
1	A	92	GLY	6.1
1	B	167	HIS	6.0
1	A	46	ALA	6.0
1	A	128	GLY	6.0
1	A	23	ALA	5.7
1	A	158	ALA	5.6
1	A	3	LEU	5.4
1	A	82	ALA	5.2
1	A	167	HIS	5.1
1	A	53	LEU	5.1
1	B	27	LEU	5.1
1	B	164	LYS	4.9
1	A	156	ILE	4.7
1	A	161	TYR	4.7
1	A	276	ALA	4.6
1	A	119	ILE	4.5
1	A	136	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	107	ALA	4.4
1	A	70	VAL	4.3
1	B	82	ALA	4.2
1	A	106	PRO	4.2
1	B	57	ARG	4.2
1	A	129	ILE	4.1
1	B	51	TRP	4.1
1	B	107	ALA	4.0
1	A	90	LYS	4.0
1	A	86	GLY	3.9
1	A	64	SER	3.9
1	B	15	ALA	3.8
1	A	282	THR	3.8
1	B	84	ALA	3.8
1	A	166	GLU	3.8
1	A	45	GLY	3.7
1	B	150	THR	3.7
1	A	162	GLY	3.7
1	A	124	ASN	3.7
1	A	163	ALA	3.7
1	A	281	VAL	3.6
1	A	67	TYR	3.6
1	A	93	ILE	3.6
1	B	95	GLY	3.6
1	A	164	LYS	3.6
1	A	26	ALA	3.5
1	A	36	LEU	3.5
1	A	289	LEU	3.5
1	A	33	SER	3.5
1	A	490	ASN	3.5
1	A	9	ALA	3.4
1	A	21	LYS	3.4
1	A	299	GLY	3.4
1	A	135	VAL	3.4
1	A	84	ALA	3.4
1	A	6	ASN	3.4
1	A	35	LEU	3.3
1	B	10	TYR	3.3
1	A	111	LEU	3.3
1	A	171	LEU	3.3
1	A	103	ILE	3.3
1	A	5	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	10	TYR	3.3
1	A	339	SER	3.3
1	B	502	LEU	3.2
1	A	420	CYS	3.2
1	A	37	THR	3.2
1	A	500	ARG	3.2
1	A	117	PRO	3.2
1	B	158	ALA	3.2
1	B	276	ALA	3.2
1	A	31	ALA	3.2
1	A	261	VAL	3.2
1	A	168	TRP	3.2
1	B	-1	HIS	3.1
1	B	65	GLY	3.1
1	B	344	GLY	3.1
1	B	125	ILE	3.1
1	A	-2	SER	3.1
1	A	28	PHE	3.1
1	A	101	PHE	3.1
1	A	76	ARG	3.1
1	A	91	ILE	3.1
1	B	419	ALA	3.1
1	A	27	LEU	3.1
1	B	160	GLN	3.0
1	A	159	ALA	3.0
1	B	152	LEU	3.0
1	A	292	GLU	3.0
1	B	166	GLU	3.0
1	A	102	ILE	3.0
1	A	51	TRP	3.0
1	A	272	TRP	3.0
1	B	-3	GLY	3.0
1	B	19	PRO	3.0
1	A	32	ASN	3.0
1	A	446	GLY	3.0
1	A	370	GLU	3.0
1	A	244	VAL	3.0
1	A	34	THR	3.0
1	A	278	TYR	3.0
1	B	13	THR	3.0
1	A	41	PRO	3.0
1	A	133	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	116	VAL	2.9
1	A	393	VAL	2.9
1	B	79	LYS	2.9
1	A	125	ILE	2.9
1	A	157	GLU	2.9
1	A	300	GLY	2.9
1	A	374	ASP	2.9
1	A	66	ARG	2.9
1	A	22	ASP	2.9
1	A	148	ILE	2.9
1	B	72	ASP	2.9
1	A	2	LYS	2.9
1	A	11	PHE	2.9
1	A	48	VAL	2.9
1	B	371	GLU	2.9
1	B	25	ALA	2.8
1	B	46	ALA	2.8
1	A	83	GLU	2.8
1	A	49	THR	2.8
1	A	47	LYS	2.8
1	A	95	GLY	2.8
1	B	340	GLY	2.8
1	B	341	GLY	2.8
1	A	25	ALA	2.8
1	A	137	GLU	2.8
1	A	74	ILE	2.8
1	B	156	ILE	2.8
1	A	264	PRO	2.8
1	A	275	VAL	2.8
1	A	43	GLY	2.8
1	B	92	GLY	2.8
1	A	94	ARG	2.8
1	A	392	ARG	2.8
1	A	287	THR	2.7
1	A	69	ARG	2.7
1	A	105	VAL	2.7
1	A	240	VAL	2.7
1	B	275	VAL	2.7
1	A	266	THR	2.7
1	A	277	ASP	2.7
1	B	93	ILE	2.7
1	A	262	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	89	TYR	2.7
1	A	127	GLY	2.7
1	A	294	ILE	2.7
1	B	58	ILE	2.7
1	B	154	GLU	2.7
1	A	151	LEU	2.7
1	A	79	LYS	2.7
1	B	17	PRO	2.7
1	A	152	LEU	2.7
1	A	109	HIS	2.6
1	A	432	GLU	2.6
1	B	432	GLU	2.6
1	A	61	THR	2.6
1	A	142	ASN	2.6
1	A	131	LEU	2.6
1	B	75	PHE	2.6
1	A	254	VAL	2.6
1	A	149	LEU	2.6
1	B	99	GLU	2.6
1	B	98	VAL	2.6
1	B	87	LYS	2.6
1	A	114	LEU	2.5
1	A	123	GLU	2.5
1	A	178	GLU	2.5
1	A	112	ARG	2.5
1	B	-2	SER	2.5
1	B	91	ILE	2.5
1	B	200	SER	2.5
1	A	81	LEU	2.5
1	A	170	LEU	2.5
1	A	188	ALA	2.5
1	A	242	TRP	2.5
1	A	245	TRP	2.5
1	A	298	ILE	2.5
1	B	435	ASN	2.5
1	A	207	GLY	2.5
1	B	126	GLU	2.5
1	A	24	ILE	2.5
1	A	146	ASP	2.5
1	A	71	HIS	2.5
1	B	41	PRO	2.5
1	B	460	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	273	GLU	2.4
1	B	123	GLU	2.4
1	B	282	THR	2.4
1	B	205	ILE	2.4
1	A	279	TYR	2.4
1	A	293	LYS	2.4
1	B	268	ASP	2.4
1	A	150	THR	2.4
1	A	172	TRP	2.4
1	B	168	TRP	2.4
1	A	297	PRO	2.4
1	A	498	GLY	2.4
1	A	160	GLN	2.4
1	A	306	CYS	2.4
1	A	77	LEU	2.4
1	B	489	ARG	2.4
1	A	307	PRO	2.3
1	A	290	ILE	2.3
1	B	393	VAL	2.3
1	A	4	GLN	2.3
1	B	50	GLU	2.3
1	B	56	ASP	2.3
1	B	279	TYR	2.3
1	B	339	SER	2.3
1	A	38	ARG	2.3
1	A	57	ARG	2.3
1	A	58	ILE	2.3
1	A	175	GLU	2.3
1	A	363	GLU	2.3
1	B	209	GLN	2.3
1	A	62	LEU	2.3
1	B	458	TRP	2.3
1	A	40	ALA	2.3
1	B	151	LEU	2.3
1	B	20	ALA	2.3
1	A	198	GLY	2.2
1	B	212	ARG	2.2
1	A	259	TYR	2.2
1	A	411	THR	2.2
1	B	272	TRP	2.2
1	A	96	ILE	2.2
1	B	220	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	2.2
1	B	501	PHE	2.2
1	A	145	PRO	2.2
1	B	128	GLY	2.2
1	A	154	GLU	2.2
1	A	12	LYS	2.2
1	B	172	TRP	2.2
1	B	22	ASP	2.2
1	B	117	PRO	2.2
1	A	332	GLY	2.2
1	A	179	HIS	2.2
1	B	137	GLU	2.2
1	A	73	ALA	2.2
1	A	138	ALA	2.2
1	B	129	ILE	2.2
1	A	435	ASN	2.2
1	A	208	PRO	2.2
1	A	44	GLN	2.2
1	B	186	THR	2.2
1	A	108	ASP	2.1
1	A	482	ALA	2.1
1	B	94	ARG	2.1
1	A	270	ASP	2.1
1	A	285	VAL	2.1
1	A	365	VAL	2.1
1	B	106	PRO	2.1
1	B	492	VAL	2.1
1	B	380	PHE	2.1
1	A	419	ALA	2.1
1	B	31	ALA	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	B	67	TYR	2.1
1	B	278	TYR	2.1
1	B	493	GLY	2.1
1	A	99	GLU	2.1
1	B	284	GLU	2.1
1	A	63	GLN	2.1
1	A	118	TYR	2.1
1	A	174	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	34	THR	2.0
1	B	23	ALA	2.0
1	A	502	LEU	2.0
1	B	89	TYR	2.0
1	A	413	GLY	2.0
1	B	433	PHE	2.0
1	A	210	SER	2.0
1	A	416	ASP	2.0
1	B	289	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

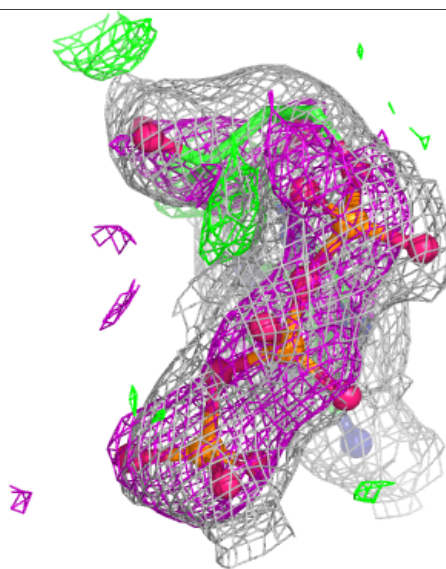
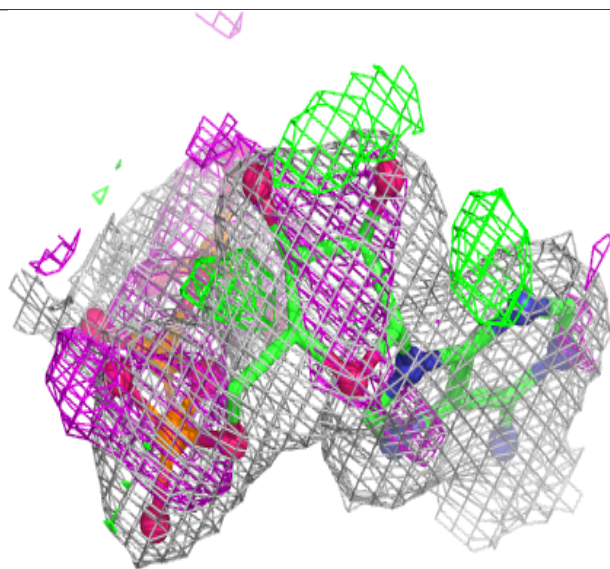
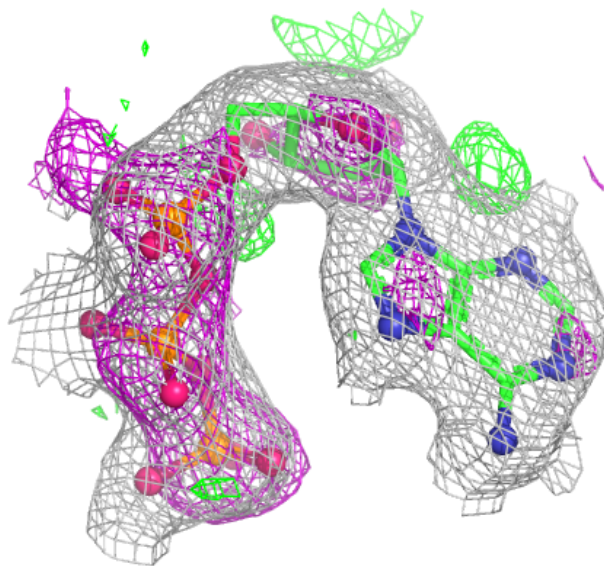
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	1505	1/1	0.83	0.20	70,70,70,70	0
5	MG	B	1506	1/1	0.83	0.22	76,76,76,76	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	A	1504	1/1	0.98	0.19	34,34,34,34	0
3	CL	B	1504	1/1	0.98	0.24	37,37,37,37	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.

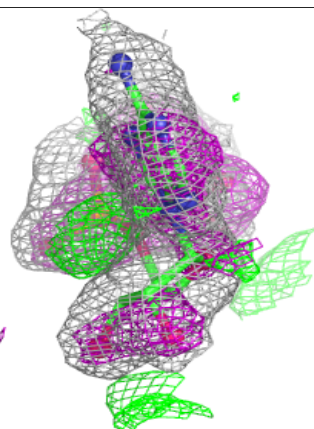
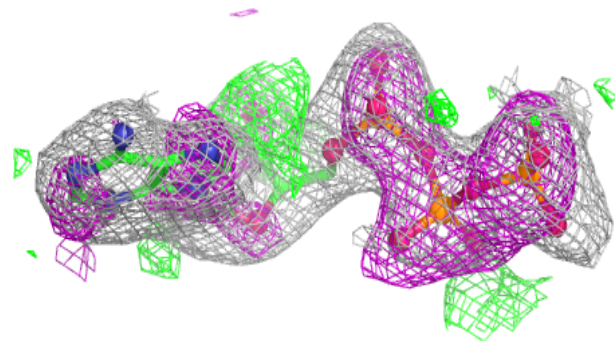
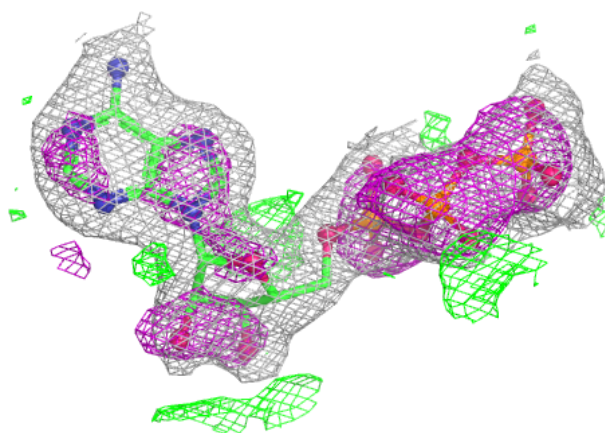
Electron density around ATP B 1507:

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



Electron density around ATP A 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.