



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:36 AM UTC

PDB ID : 4QRE / pdb_00004qre
Title : Structure of Methionyl-tRNA Synthetase in complex with 1-(4-{4-[(1H-benzimidazol-2-ylmethyl)amino]-6-(4,5-dimethoxy-2-methylphenoxy)pyrimidin-2-yl}piperazin-1-yl)ethanone
Authors : Hilgers, M.T.
Deposited on : 2014-06-30
Resolution : 1.70 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

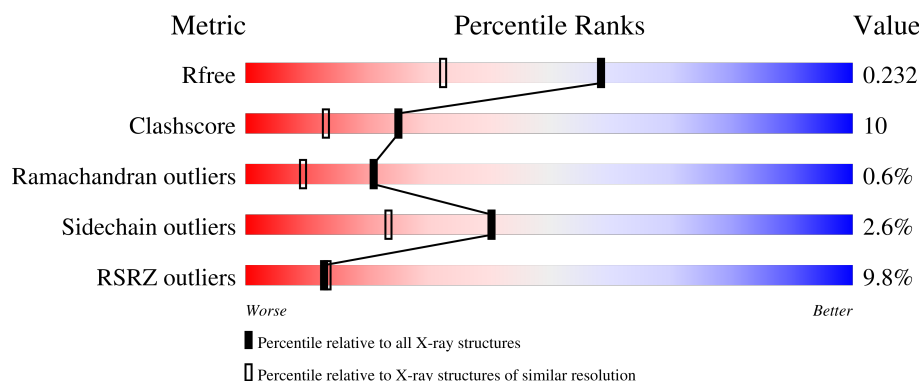
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	547	9% 80% 12% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4906 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.

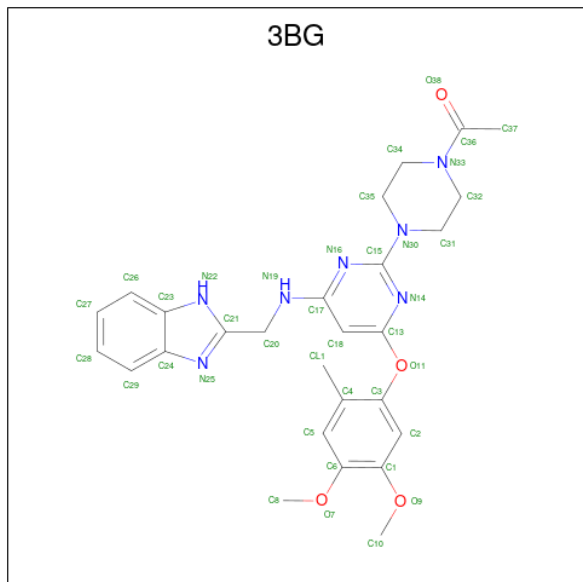
- Molecule 1 is a protein called Methionyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4220	2721	686	797	16	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

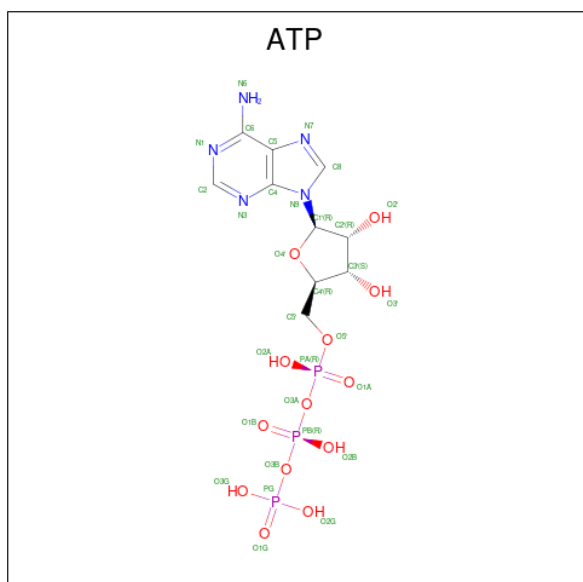
Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP W8U1H8
A	-25	GLY	-	expression tag	UNP W8U1H8
A	-24	HIS	-	expression tag	UNP W8U1H8
A	-23	HIS	-	expression tag	UNP W8U1H8
A	-22	HIS	-	expression tag	UNP W8U1H8
A	-21	HIS	-	expression tag	UNP W8U1H8
A	-20	HIS	-	expression tag	UNP W8U1H8
A	-19	HIS	-	expression tag	UNP W8U1H8
A	-18	ASP	-	expression tag	UNP W8U1H8
A	-17	TYR	-	expression tag	UNP W8U1H8
A	-16	ASP	-	expression tag	UNP W8U1H8
A	-15	ILE	-	expression tag	UNP W8U1H8
A	-14	PRO	-	expression tag	UNP W8U1H8
A	-13	THR	-	expression tag	UNP W8U1H8
A	-12	THR	-	expression tag	UNP W8U1H8
A	-11	GLU	-	expression tag	UNP W8U1H8
A	-10	ASN	-	expression tag	UNP W8U1H8
A	-9	LEU	-	expression tag	UNP W8U1H8
A	-8	TYR	-	expression tag	UNP W8U1H8
A	-7	PHE	-	expression tag	UNP W8U1H8
A	-6	GLN	-	expression tag	UNP W8U1H8
A	-5	GLY	-	expression tag	UNP W8U1H8
A	-4	ALA	-	expression tag	UNP W8U1H8
A	-3	HIS	-	expression tag	UNP W8U1H8
A	-2	MET	-	expression tag	UNP W8U1H8
A	-1	ALA	-	expression tag	UNP W8U1H8
A	0	SER	-	expression tag	UNP W8U1H8

- Molecule 2 is 1-(4-{4-[(1H-benzimidazol-2-ylmethyl)amino]-6-(4,5-dimethoxy-2-methylphenoxy)pyrimidin-2-yl}piperazin-1-yl)ethanone (CCD ID: 3BG) (formula: $C_{27}H_{31}N_7O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	27	7	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0

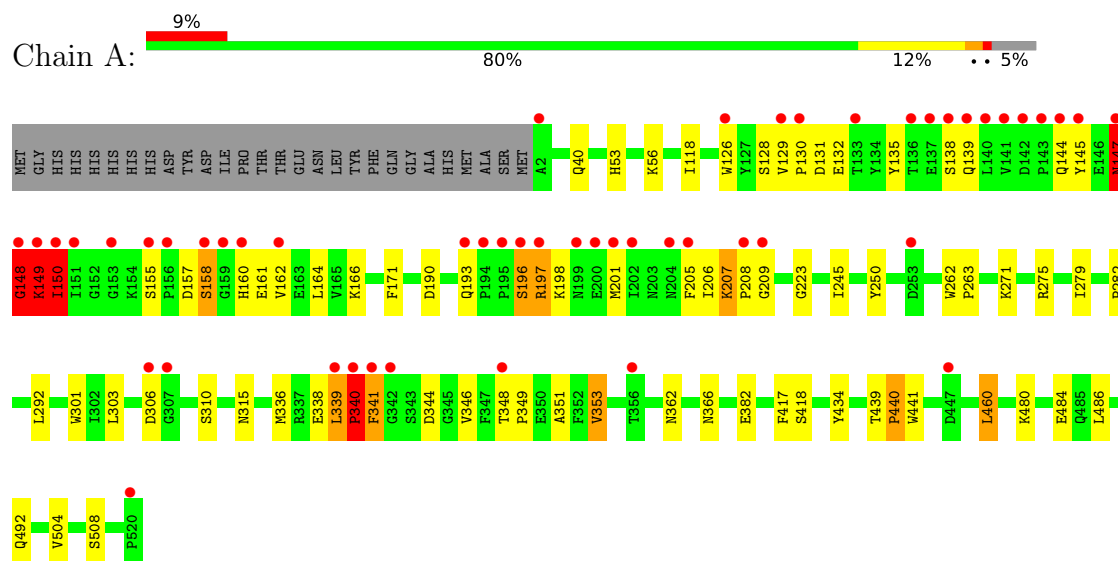
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	615	Total 615	O 615	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Methionyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.93Å 75.67Å 119.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.45 – 1.70 21.45 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.5 (21.45-1.70) 94.4 (21.45-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.239 0.197 , 0.232	Depositor DCC
R_{free} test set	3141 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4906	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3BG, ATP, MG

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	0.69	6/4332 (0.1%)	1.22	8/5880 (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	A	3	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	PRO	N-CA	-6.63	1.38	1.47
1	A	340	PRO	CB-CG	6.44	1.81	1.49
1	A	126	TRP	C-O	-5.71	1.17	1.24
1	A	339	LEU	CA-C	5.19	1.58	1.52
1	A	315	ASN	C-O	-5.16	1.17	1.24
1	A	440	PRO	C-O	-5.10	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	LEU	CA-C-N	-46.13	62.18	119.84
1	A	339	LEU	C-N-CA	-46.13	62.18	119.84
1	A	339	LEU	C-N-CD	-16.05	59.20	125.00
1	A	158	SER	N-CA-C	-15.06	89.57	110.35
1	A	306	ASP	N-CA-C	7.06	122.59	109.24
1	A	341	PHE	N-CA-C	5.75	120.81	111.37
1	A	340	PRO	N-CD-CG	-5.34	95.19	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ASN	CB-CA-C	-5.28	110.05	117.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	149	LYS	CA
1	A	150	ILE	CA,CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ASN	Peptide
1	A	148	GLY	Peptide
1	A	149	LYS	Peptide
1	A	340	PRO	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	4220	0	4117	81	0
2	A	38	0	31	1	0
3	A	31	0	12	0	0
4	A	2	0	0	0	0
5	A	615	0	0	4	0
All	All	4906	0	4160	82	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 10.

All (82) 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:340:PRO:CB	1:A:340:PRO:CG	1.81	1.51
1:A:149:LYS:HB3	1:A:150:ILE:CA	1.57	1.30
1:A:149:LYS:CB	1:A:150:ILE:HA	1.60	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG23	1:A:130:PRO:HD3	1.27	1.17
1:A:149:LYS:HD3	1:A:150:ILE:HG23	1.17	1.17
1:A:148:GLY:O	1:A:149:LYS:HG2	1.55	1.07
1:A:149:LYS:HD3	1:A:150:ILE:CG2	1.91	1.00
1:A:336:MET:CE	1:A:417:PHE:HD2	1.80	0.94
1:A:340:PRO:HB3	5:A:804:HOH:O	1.66	0.94
1:A:148:GLY:C	1:A:149:LYS:HG2	1.90	0.93
1:A:149:LYS:CD	1:A:150:ILE:HG23	1.98	0.92
1:A:40:GLN:HG2	5:A:771:HOH:O	1.73	0.88
1:A:40:GLN:OE1	5:A:1080:HOH:O	1.90	0.88
1:A:145:TYR:HE2	1:A:149:LYS:HE2	1.40	0.87
1:A:145:TYR:CD2	1:A:149:LYS:C	2.52	0.87
1:A:129:VAL:CG2	1:A:130:PRO:HD3	2.04	0.87
1:A:340:PRO:HG2	1:A:418:SER:HB3	1.55	0.87
1:A:303:LEU:HD11	1:A:344:ASP:HB3	1.61	0.82
1:A:148:GLY:C	1:A:149:LYS:CG	2.52	0.80
1:A:148:GLY:O	1:A:149:LYS:CG	2.33	0.77
1:A:164:LEU:HD21	1:A:166:LYS:HE2	1.68	0.75
1:A:340:PRO:HG2	1:A:418:SER:CB	2.17	0.75
1:A:336:MET:HE1	1:A:417:PHE:HD2	1.51	0.74
1:A:145:TYR:CE2	1:A:149:LYS:HE2	2.25	0.72
1:A:336:MET:CE	1:A:417:PHE:CD2	2.70	0.71
1:A:129:VAL:N	1:A:130:PRO:HD2	2.06	0.71
1:A:129:VAL:HG23	1:A:130:PRO:CD	2.13	0.70
1:A:262:TRP:CD2	1:A:263:PRO:HA	2.27	0.70
1:A:340:PRO:CG	1:A:418:SER:HB3	2.23	0.69
1:A:145:TYR:HE2	1:A:149:LYS:CE	2.06	0.69
1:A:336:MET:HE2	1:A:417:PHE:HD2	1.58	0.68
1:A:160:HIS:HD2	1:A:161:GLU:O	1.77	0.67
1:A:147:ASN:O	1:A:149:LYS:N	2.30	0.64
1:A:336:MET:HE2	1:A:417:PHE:CD2	2.31	0.64
1:A:348:THR:HG23	1:A:351:ALA:H	1.63	0.61
1:A:205:PHE:CD1	1:A:275:ARG:HD3	2.37	0.60
1:A:160:HIS:CD2	1:A:161:GLU:O	2.56	0.58
1:A:434:TYR:HD2	1:A:460:LEU:HD13	1.68	0.58
1:A:129:VAL:N	1:A:130:PRO:CD	2.67	0.57
1:A:336:MET:HE1	1:A:341:PHE:HZ	1.69	0.57
1:A:492:GLN:HG3	5:A:1129:HOH:O	2.04	0.57
1:A:382:GLU:HG2	1:A:508:SER:OG	2.05	0.57
1:A:56:LYS:HZ2	1:A:56:LYS:HB2	1.70	0.57
1:A:129:VAL:CG2	1:A:130:PRO:CD	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:HB3	1:A:193:GLN:HE21	1.71	0.56
1:A:145:TYR:CG	1:A:149:LYS:C	2.84	0.56
1:A:303:LEU:CD1	1:A:344:ASP:HB3	2.33	0.55
1:A:145:TYR:CD2	1:A:150:ILE:N	2.75	0.54
1:A:147:ASN:O	1:A:148:GLY:C	2.51	0.54
1:A:145:TYR:CD2	1:A:149:LYS:O	2.60	0.53
1:A:362:ASN:O	1:A:366:ASN:HB2	2.09	0.53
1:A:336:MET:HE1	1:A:341:PHE:CZ	2.44	0.53
1:A:157:ASP:C	1:A:158:SER:O	2.42	0.51
1:A:275:ARG:HG3	1:A:279:ILE:HD12	1.92	0.51
1:A:196:SER:HB2	1:A:197:ARG:HH11	1.75	0.51
1:A:434:TYR:CD2	1:A:460:LEU:HD13	2.49	0.48
1:A:196:SER:HB2	1:A:197:ARG:NH1	2.29	0.48
1:A:118:ILE:HA	1:A:171:PHE:O	2.15	0.47
1:A:201:MET:SD	1:A:275:ARG:HA	2.55	0.47
1:A:349:PRO:O	1:A:353:VAL:HG13	2.16	0.46
1:A:197:ARG:HH21	1:A:271:LYS:HD3	1.81	0.45
1:A:128:SER:OG	1:A:162:VAL:HG12	2.16	0.45
1:A:149:LYS:HB3	1:A:150:ILE:HA	0.67	0.45
1:A:338:GLU:C	1:A:340:PRO:CD	2.81	0.44
1:A:439:THR:O	1:A:440:PRO:C	2.60	0.44
2:A:601:3BG:H4	2:A:601:3BG:H8	1.60	0.44
1:A:198:LYS:O	1:A:201:MET:HB2	2.18	0.44
1:A:301:TRP:O	1:A:303:LEU:HD12	2.18	0.44
1:A:480:LYS:O	1:A:484:GLU:HG3	2.18	0.44
1:A:56:LYS:NZ	1:A:132:GLU:CD	2.77	0.43
1:A:245:ILE:HD12	1:A:250:TYR:CD2	2.52	0.43
1:A:205:PHE:CE1	1:A:275:ARG:HD3	2.53	0.43
1:A:207:LYS:HB3	1:A:208:PRO:HD3	2.00	0.42
1:A:282:PRO:HB3	1:A:292:LEU:HD13	2.01	0.42
1:A:135:TYR:HB3	1:A:139:GLN:HG3	2.02	0.42
1:A:262:TRP:CG	1:A:263:PRO:HA	2.55	0.41
1:A:206:ILE:O	1:A:209:GLY:HA3	2.19	0.41
1:A:131:ASP:O	1:A:132:GLU:C	2.63	0.41
1:A:53:HIS:CG	1:A:223:GLY:HA2	2.56	0.41
1:A:439:THR:O	1:A:441:TRP:N	2.54	0.41
1:A:144:GLN:O	1:A:150:ILE:HG13	2.21	0.41
1:A:155:SER:O	1:A:158:SER:O	2.39	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	517/547 (94%)	496 (96%)	18 (4%)	3 (1%)	21 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	GLY
1	A	340	PRO
1	A	150	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	461/485 (95%)	449 (97%)	12 (3%)	40 23

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	149	LYS
1	A	196	SER
1	A	197	ARG
1	A	207	LYS
1	A	310	SER
1	A	339	LEU
1	A	346	VAL

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Mol	Chain	Res	Type
1	A	353	VAL
1	A	460	LEU
1	A	486	LEU
1	A	504	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	160	HIS
1	A	188	ASN
1	A	193	GLN
1	A	221	ASN
1	A	357	ASN
1	A	369	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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
2	3BG	A	601	-	42,42,42	1.98	6 (14%)	57,59,59	1.89	19 (33%)
3	ATP	A	602	4	32,33,33	1.08	2 (6%)	48,52,52	1.79	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3BG	A	601	-	-	1/21/31/31	0/5/5/5
3	ATP	A	602	4	-	3/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	3BG	C23-C24	6.11	1.48	1.40
2	A	601	3BG	CL1-C4	5.70	1.61	1.51
2	A	601	3BG	C20-C21	5.45	1.52	1.49
2	A	601	3BG	C3-C4	4.46	1.49	1.39
2	A	601	3BG	C6-C1	4.14	1.49	1.40
3	A	602	ATP	PB-O3A	2.80	1.62	1.59
3	A	602	ATP	C8-N7	2.36	1.36	1.31
2	A	601	3BG	C24-N25	-2.04	1.35	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ATP	C5-C4-N3	-5.40	119.28	126.72
2	A	601	3BG	C31-N30-C35	5.08	123.00	111.57
3	A	602	ATP	N3-C2-N1	-4.93	121.12	128.58
2	A	601	3BG	C15-N14-C13	4.26	120.13	114.48
3	A	602	ATP	C2-N3-C4	3.57	120.56	111.83
2	A	601	3BG	O9-C1-C6	3.41	120.03	115.40
2	A	601	3BG	C10-O9-C1	3.29	122.34	117.51
2	A	601	3BG	N14-C15-N16	-3.27	120.46	126.27
2	A	601	3BG	C24-N25-C21	3.22	109.43	105.25
2	A	601	3BG	C32-N33-C34	3.20	119.21	112.68
3	A	602	ATP	N3-C4-N9	3.11	132.46	127.17
3	A	602	ATP	C4-C5-N7	-3.06	107.08	110.58
3	A	602	ATP	N9-C8-N7	-2.93	109.78	113.94
2	A	601	3BG	N16-C15-N30	2.82	121.14	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	3BG	C18-C13-N14	-2.80	120.89	124.16
2	A	601	3BG	N22-C21-N25	-2.61	109.53	112.72
3	A	602	ATP	C5-N7-C8	2.57	107.48	103.45
2	A	601	3BG	N19-C17-N16	2.46	120.46	116.42
3	A	602	ATP	O3G-PG-O2G	2.33	116.52	107.80
2	A	601	3BG	C26-C23-C24	-2.25	119.64	122.10
3	A	602	ATP	C5-C4-N9	2.24	108.26	105.81
2	A	601	3BG	C26-C23-N22	2.23	135.34	130.83
2	A	601	3BG	C29-C24-N25	2.23	134.53	128.21
3	A	602	ATP	O3A-PB-O1B	-2.22	104.03	110.70
2	A	601	3BG	C23-C24-N25	-2.21	106.39	109.42
2	A	601	3BG	C34-C35-N30	-2.14	106.29	110.78
2	A	601	3BG	C18-C17-N16	-2.10	118.99	123.35
2	A	601	3BG	C23-N22-C21	2.07	109.63	107.23
2	A	601	3BG	C31-N30-C15	-2.04	117.64	121.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ATP	PB-O3B-PG-O2G
3	A	602	ATP	PA-O3A-PB-O2B
2	A	601	3BG	N19-C20-C21-N25
3	A	602	ATP	PB-O3B-PG-O3G

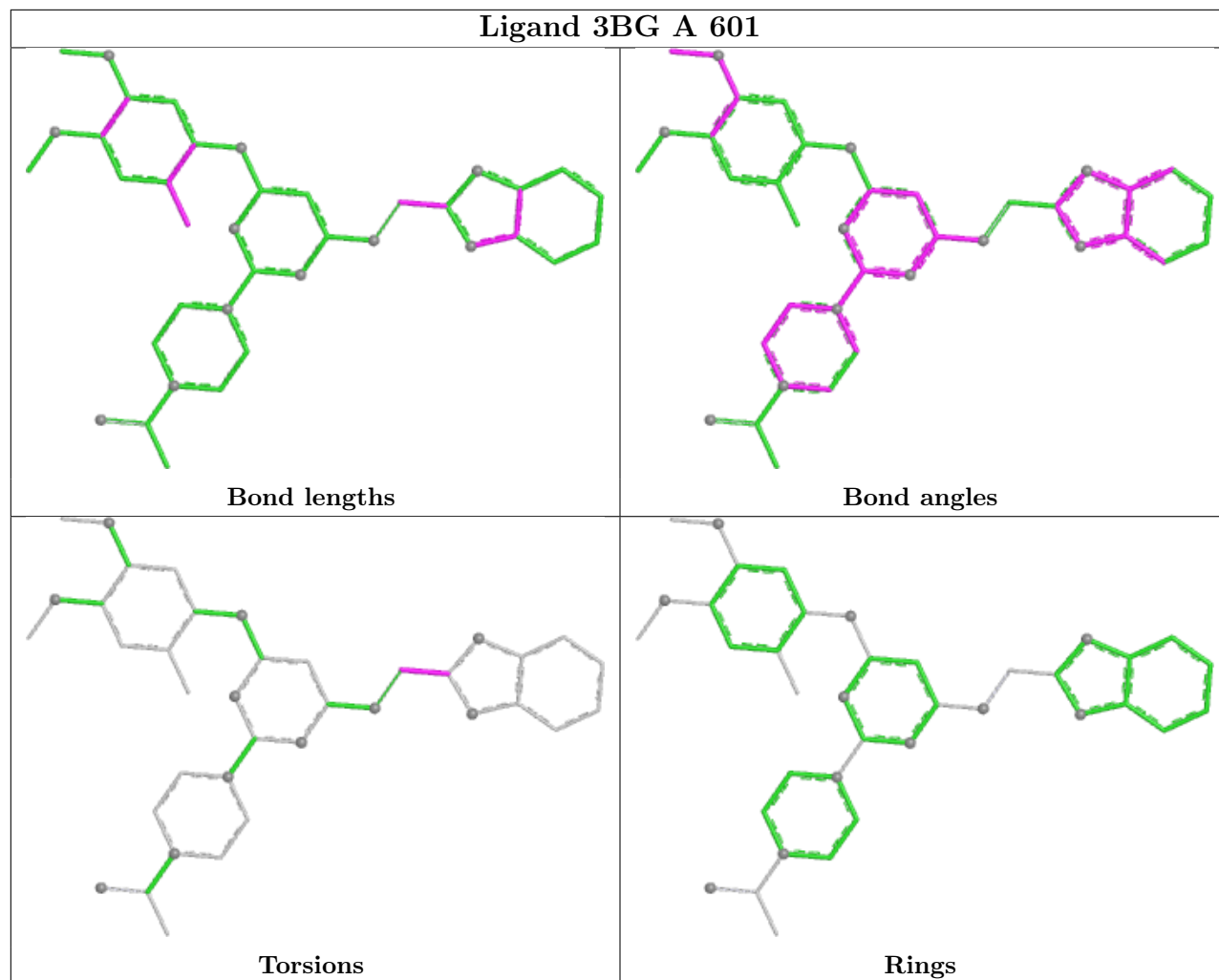
There are no ring outliers.

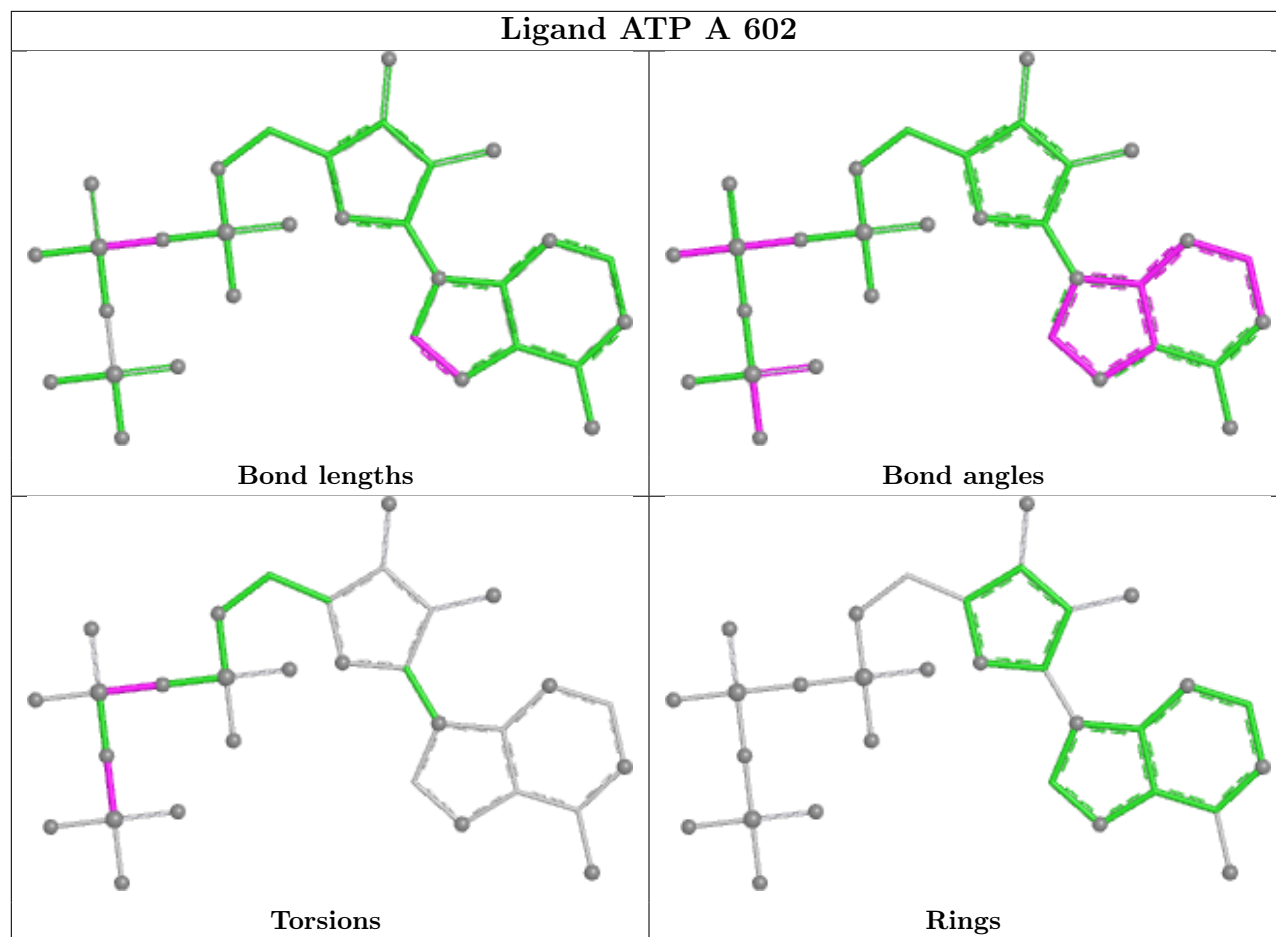
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	3BG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/547 (94%)	0.32	51 (9%) 13 13	10, 20, 50, 112	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	PRO	7.5
1	A	148	GLY	6.3
1	A	149	LYS	6.1
1	A	196	SER	6.0
1	A	158	SER	5.4
1	A	199	ASN	5.2
1	A	208	PRO	5.0
1	A	160	HIS	4.8
1	A	194	PRO	4.7
1	A	145	TYR	4.3
1	A	150	ILE	4.3
1	A	147	ASN	4.1
1	A	193	GLN	4.0
1	A	159	GLY	4.0
1	A	306	ASP	4.0
1	A	141	VAL	3.7
1	A	200	GLU	3.7
1	A	205	PHE	3.6
1	A	341	PHE	3.6
1	A	342	GLY	3.6
1	A	130	PRO	3.5
1	A	520	PRO	3.5
1	A	195	PRO	3.4
1	A	138	SER	3.4
1	A	143	PRO	3.4
1	A	202	ILE	3.3
1	A	348	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	ASP	3.3
1	A	162	VAL	3.3
1	A	144	GLN	3.2
1	A	447	ASP	3.2
1	A	209	GLY	3.1
1	A	136	THR	3.0
1	A	126	TRP	3.0
1	A	129	VAL	3.0
1	A	155	SER	3.0
1	A	197	ARG	2.9
1	A	140	LEU	2.8
1	A	2	ALA	2.8
1	A	339	LEU	2.8
1	A	137	GLU	2.7
1	A	133	THR	2.7
1	A	139	GLN	2.5
1	A	151	ILE	2.5
1	A	253	ASP	2.3
1	A	204	ASN	2.2
1	A	356	THR	2.2
1	A	156	PRO	2.1
1	A	153	GLY	2.0
1	A	307	GLY	2.0
1	A	201	MET	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](#)

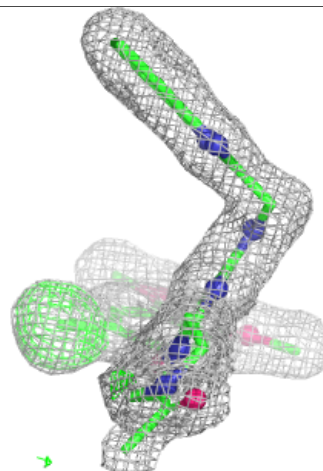
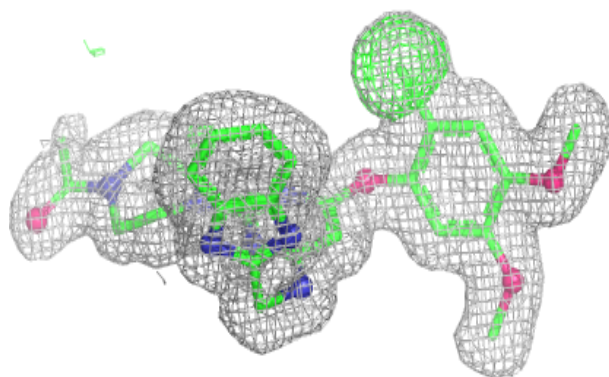
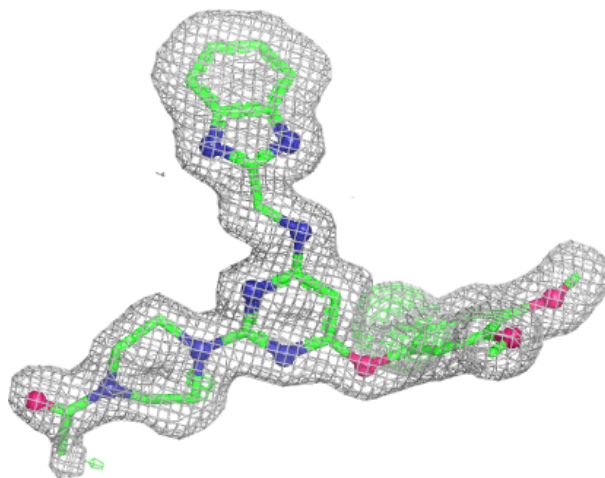
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

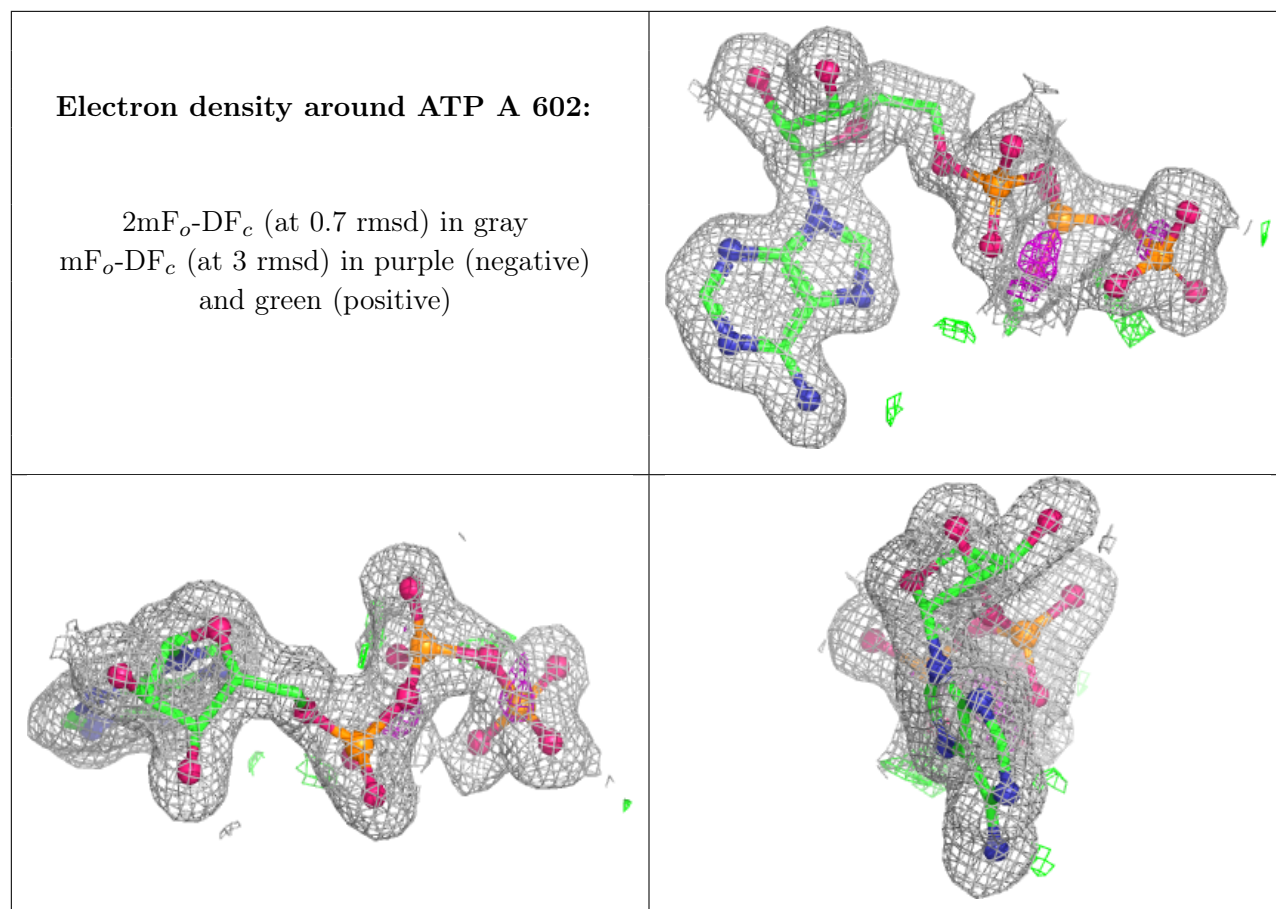
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3BG	A	601	38/38	0.91	0.07	2,13,30,33	0
3	ATP	A	602	31/31	0.96	0.07	11,17,25,27	0
4	MG	A	604	1/1	0.96	0.12	18,18,18,18	0
4	MG	A	603	1/1	0.99	0.06	19,19,19,19	0

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 3BG A 601:

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.