



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:13 PM UTC

PDB ID : 1N77 / pdb_00001n77
Title : Crystal structure of Thermus thermophilus glutamyl-tRNA synthetase complexed with tRNA(Glu) and ATP.
Authors : Sekine, S.; Nureki, O.; Dubois, D.Y.; Bernier, S.; Chenevert, R.; Lapointe, J.; Vassilyev, D.G.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-11-13
Resolution : 2.40 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](#) ①) 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

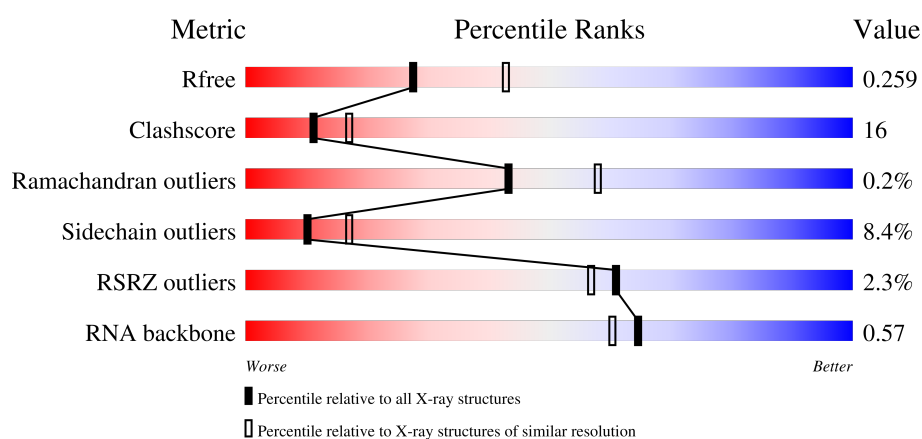
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	C	75	4% 53% 27% 12% 8%
1	D	75	11% 44% 33% 16% 7%
2	A	468	67% 29%
2	B	468	3% 60% 35% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11391 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 RNA chain called tRNA(Glu).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			
1	D	75	Total	C	N	O	P	0	0	0
			1597	711	284	527	75			

- Molecule 2 is a protein called Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			
2	B	468	Total	C	N	O	S	0	0	0
			3814	2443	676	687	8			

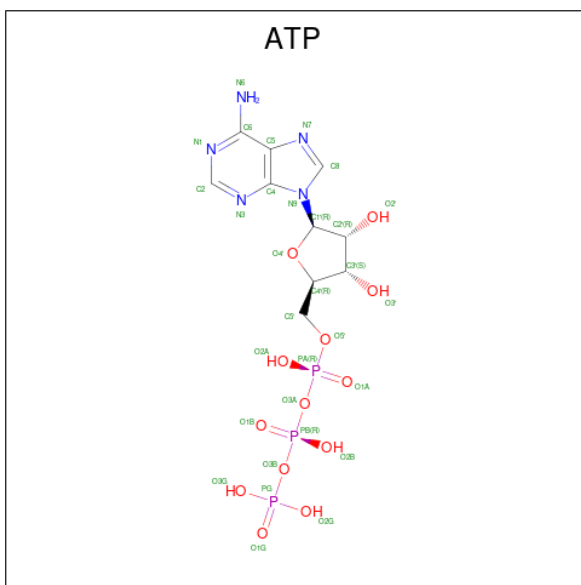
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	ALA	SEE REMARK 999	UNP P27000
A	75	GLY	ALA	SEE REMARK 999	UNP P27000
A	77	HIS	THR	SEE REMARK 999	UNP P27000
B	74	GLY	ALA	SEE REMARK 999	UNP P27000
B	75	GLY	ALA	SEE REMARK 999	UNP P27000
B	77	HIS	THR	SEE REMARK 999	UNP P27000

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	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

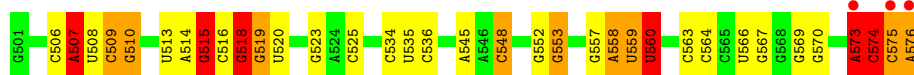
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	70	Total O 70 70	0	0
5	D	75	Total O 75 75	0	0
5	A	175	Total O 175 175	0	0
5	B	185	Total O 185 185	0	0

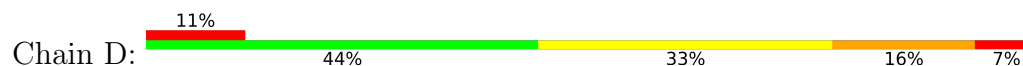
3 Residue-property plots

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.

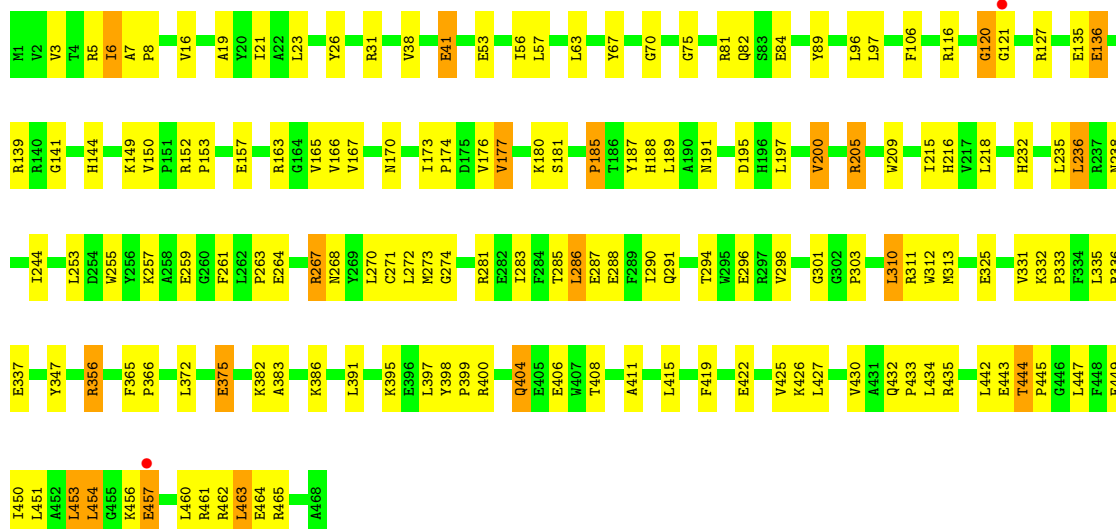
• Molecule 1: tRNA(Glu)



• Molecule 1: tRNA(Glu)

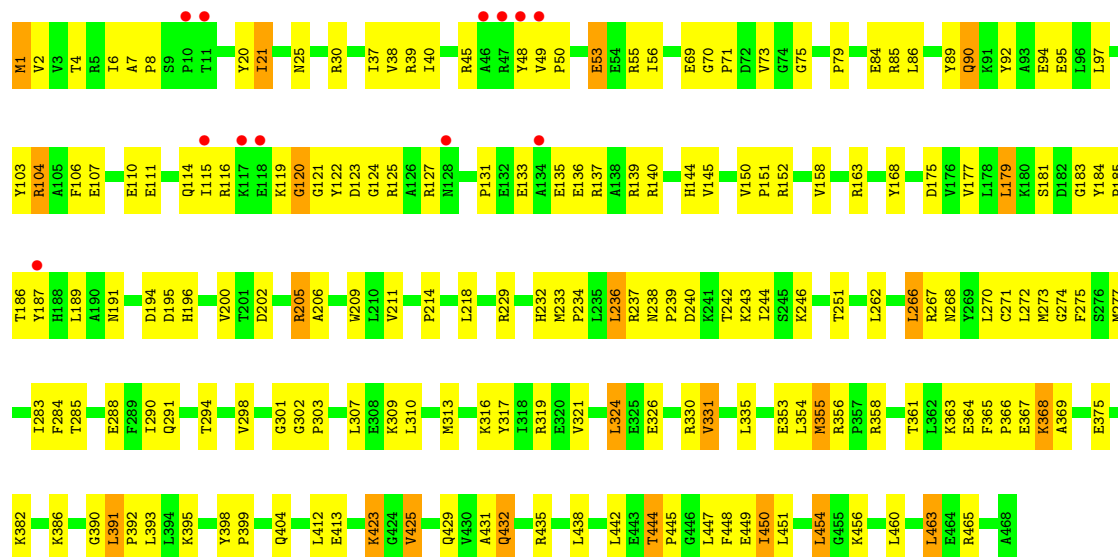


• Molecule 2: Glutamyl-tRNA synthetase



• Molecule 2: Glutamyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.69Å 219.12Å 135.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.40 49.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.40-2.40) 91.4 (49.40-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.257 0.213 , 0.259	Depositor DCC
R_{free} test set	2972 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11391	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.93% 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: 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	C	0.33	0/1782	0.95	15/2774 (0.5%)
1	D	0.34	0/1782	0.96	17/2774 (0.6%)
2	A	0.47	0/3910	0.92	7/5293 (0.1%)
2	B	0.46	0/3910	0.91	6/5293 (0.1%)
All	All	0.43	0/11384	0.93	45/16134 (0.3%)

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	C	0	1
1	D	1	1
All	All	1	2

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	574	C	C2'-C3'-O3'	12.46	128.20	109.50
1	D	574	C	C2'-C3'-O3'	11.03	126.04	109.50
1	C	518	G	C2'-C3'-O3'	10.85	125.78	109.50
1	C	519	G	C2'-C3'-O3'	10.73	125.60	109.50
1	D	515	G	C2'-C3'-O3'	10.71	125.57	109.50
1	D	518	G	C2'-C3'-O3'	10.63	125.45	109.50
1	D	507	A	C2'-C3'-O3'	10.62	125.42	109.50
1	D	515	G	C4'-C3'-O3'	10.39	124.99	109.40
1	C	573	A	C2'-C3'-O3'	10.36	125.04	109.50
1	C	515	G	C4'-C3'-O3'	10.36	124.93	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	519	G	C2'-C3'-O3'	10.28	124.92	109.50
1	D	573	A	C2'-C3'-O3'	10.16	124.74	109.50
1	C	518	G	C4'-C3'-O3'	8.48	122.12	109.40
1	D	518	G	C4'-C3'-O3'	8.45	122.07	109.40
1	C	507	A	C4'-C3'-O3'	8.18	121.67	109.40
1	D	507	A	C4'-C3'-O3'	8.11	121.57	109.40
1	C	574	C	C4'-C3'-O3'	8.07	121.51	109.40
1	C	507	A	C2'-C3'-O3'	7.55	120.82	109.50
2	B	75	GLY	CA-C-N	7.10	126.81	119.56
2	B	75	GLY	C-N-CA	7.10	126.81	119.56
1	D	574	C	C4'-C3'-O3'	6.95	119.83	109.40
1	C	548	C	C2'-C3'-O3'	6.95	119.93	109.50
2	B	70	GLY	CA-C-N	6.93	126.45	119.24
2	B	70	GLY	C-N-CA	6.93	126.45	119.24
2	A	70	GLY	CA-C-N	6.59	126.10	119.24
2	A	70	GLY	C-N-CA	6.59	126.10	119.24
1	C	560	U	C2'-C3'-O3'	6.58	119.38	109.50
2	A	75	GLY	CA-C-N	6.32	126.00	119.56
2	A	75	GLY	C-N-CA	6.32	126.00	119.56
1	D	560	U	C2'-C3'-O3'	6.31	118.97	109.50
1	D	519	G	C4'-C3'-O3'	6.25	118.77	109.40
1	C	519	G	C4'-C3'-O3'	6.15	118.63	109.40
2	A	335	LEU	N-CA-C	-6.14	104.51	111.14
2	B	335	LEU	N-CA-C	-6.05	104.77	111.36
2	A	236	LEU	N-CA-C	-5.96	101.46	110.28
1	D	515	G	C4'-C3'-C2'	5.79	108.39	102.60
2	A	454	LEU	N-CA-C	5.76	118.50	111.82
1	D	507	A	C4'-C3'-C2'	5.55	108.16	102.60
2	B	236	LEU	N-CA-C	-5.30	102.43	110.28
1	D	548	C	C2'-C3'-O3'	5.26	117.39	109.50
1	C	574	C	C4'-C3'-C2'	5.20	107.80	102.60
1	D	573	A	C4'-C3'-C2'	5.16	107.76	102.60
1	C	573	A	C4'-C3'-O3'	5.06	116.99	109.40
1	D	573	A	C4'-C3'-O3'	5.03	116.95	109.40
1	C	515	G	C2'-C3'-O3'	5.01	117.02	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	515	G	C3'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	515	G	Sidechain
1	D	515	G	Sidechain

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	C	1597	0	813	28	0
1	D	1597	0	813	44	0
2	A	3814	0	3818	132	0
2	B	3814	0	3818	147	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	4	0
5	A	175	0	0	6	0
5	B	185	0	0	8	0
5	C	70	0	0	0	0
5	D	75	0	0	6	0
All	All	11391	0	9286	329	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 16.

All (329) 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:506:C:O2'	1:D:507:A:H5'	1.72	0.89
2:B:454:LEU:HD22	2:B:454:LEU:H	1.38	0.89
1:D:576:A:H3'	2:B:209:TRP:HH2	1.39	0.86
2:A:205:ARG:HD3	2:A:232:HIS:CE1	2.10	0.85
2:B:454:LEU:HD22	2:B:454:LEU:N	1.91	0.85
2:B:205:ARG:HD3	2:B:232:HIS:CE1	2.11	0.84
2:A:294:THR:HG22	2:A:296:GLU:H	1.41	0.84
1:C:574:C:H5'	2:A:177:VAL:HG11	1.60	0.82
2:B:4:THR:HB	2:B:25:ASN:HD22	1.43	0.81
2:A:136:GLU:HG2	2:A:139:ARG:HH21	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:A:H5''	2:A:187:TYR:HB2	1.62	0.81
2:B:116:ARG:HA	2:B:121:GLY:H	1.46	0.79
2:A:460:LEU:O	2:A:464:GLU:HG3	1.84	0.77
2:B:432:GLN:HE21	2:B:432:GLN:HA	1.48	0.77
2:A:365:PHE:HB3	2:A:366:PRO:HD3	1.67	0.76
2:B:262:LEU:HD22	2:B:330:ARG:HH11	1.50	0.75
2:B:365:PHE:HB3	2:B:366:PRO:HD3	1.67	0.75
2:B:435:ARG:HD3	2:B:444:THR:HG22	1.69	0.74
2:A:435:ARG:HD3	2:A:444:THR:HG22	1.69	0.73
1:D:576:A:H5''	2:B:187:TYR:HB2	1.69	0.73
2:A:267:ARG:HD3	5:A:1690:HOH:O	1.88	0.73
1:C:574:C:H5'	2:A:177:VAL:CG1	2.18	0.73
5:D:1313:HOH:O	2:B:316:LYS:HE2	1.88	0.72
2:B:354:LEU:HD22	2:B:449:GLU:HG3	1.70	0.72
2:A:285:THR:HG23	2:A:288:GLU:OE1	1.90	0.72
2:B:432:GLN:HA	2:B:432:GLN:NE2	2.05	0.71
2:B:454:LEU:H	2:B:454:LEU:CD2	2.04	0.70
2:A:267:ARG:HD2	2:A:286:LEU:HG	1.74	0.70
2:A:375:GLU:HG3	2:A:465:ARG:HH22	1.57	0.70
1:D:573:A:H5'	5:D:1271:HOH:O	1.92	0.69
1:C:506:C:O2'	1:C:507:A:H5'	1.92	0.69
2:A:157:GLU:HG2	2:A:167:VAL:HG22	1.73	0.69
2:B:361:THR:OG1	2:B:364:GLU:HG3	1.93	0.69
2:A:205:ARG:HD3	2:A:232:HIS:HE1	1.53	0.69
2:A:283:ILE:HD13	2:A:313:MET:HE2	1.75	0.69
2:B:355:MET:HE2	2:B:369:ALA:HB2	1.76	0.68
1:D:576:A:H3'	2:B:209:TRP:CH2	2.25	0.67
2:A:188:HIS:HD2	2:A:216:HIS:HE1	1.41	0.67
4:B:601:ATP:H2'	5:B:1456:HOH:O	1.94	0.67
2:A:400:ARG:HH22	2:A:422:GLU:CD	2.03	0.66
2:B:326:GLU:HG3	5:B:1790:HOH:O	1.94	0.66
2:B:413:GLU:HG3	2:B:448:PHE:CZ	2.31	0.66
2:A:257:LYS:HE3	5:A:1017:HOH:O	1.95	0.66
2:B:465:ARG:HH11	2:B:465:ARG:HB3	1.61	0.66
1:D:576:A:C5'	2:B:187:TYR:HB2	2.25	0.65
2:A:445:PRO:HG2	2:A:450:ILE:HD11	1.77	0.65
2:B:444:THR:HG23	2:B:445:PRO:O	1.97	0.65
2:A:444:THR:HG23	2:A:445:PRO:O	1.97	0.65
2:A:461:ARG:NH1	2:A:465:ARG:HD3	2.11	0.64
1:D:570:G:H21	2:B:211:VAL:HG21	1.63	0.64
2:B:432:GLN:HE21	2:B:432:GLN:CA	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ARG:HD3	2:B:232:HIS:HE1	1.60	0.63
2:B:6:ILE:CD1	2:B:21:ILE:HG22	2.29	0.62
2:B:25:ASN:ND2	5:B:1786:HOH:O	2.31	0.62
2:A:255:TRP:CZ2	2:A:259:GLU:HG3	2.35	0.62
2:B:122:TYR:CE2	2:B:124:GLY:HA2	2.34	0.62
2:B:391:LEU:N	2:B:392:PRO:HD2	2.15	0.62
1:D:574:C:C5'	2:B:177:VAL:HG11	2.30	0.61
2:B:454:LEU:N	2:B:454:LEU:CD2	2.62	0.61
1:D:573:A:H2'	5:D:1136:HOH:O	1.99	0.61
5:D:1024:HOH:O	2:B:211:VAL:HG23	2.00	0.61
2:A:453:LEU:HB3	2:A:454:LEU:HD22	1.81	0.61
2:A:6:ILE:HD11	2:A:38:VAL:HG22	1.81	0.61
2:A:7:ALA:HB1	2:A:41:GLU:CD	2.26	0.60
2:A:188:HIS:HD2	2:A:216:HIS:CE1	2.19	0.60
2:B:435:ARG:HD3	2:B:444:THR:CG2	2.32	0.60
1:D:574:C:H5'	2:B:177:VAL:HG11	1.82	0.60
2:A:5:ARG:HH21	2:A:191:ASN:ND2	2.00	0.60
1:C:509:C:H5'	1:C:510:G:OP2	2.01	0.59
2:A:287:GLU:O	2:A:291:GLN:HG3	2.03	0.59
2:B:398:TYR:HB3	2:B:399:PRO:HD3	1.84	0.59
1:D:569:G:O2'	1:D:570:G:H5'	2.01	0.59
2:B:90:GLN:O	2:B:94:GLU:HG3	2.03	0.59
2:A:21:ILE:HG13	4:A:600:ATP:H1'	1.85	0.58
2:B:238:ASN:HB3	2:B:239:PRO:HD2	1.85	0.58
1:D:569:G:H5''	2:B:242:THR:HA	1.86	0.58
2:A:205:ARG:HG3	2:A:209:TRP:CD1	2.39	0.58
2:B:106:PHE:CD2	2:B:144:HIS:HB3	2.39	0.58
2:A:53:GLU:O	2:A:56:ILE:HG22	2.03	0.58
2:B:283:ILE:HD13	2:B:313:MET:HE2	1.85	0.57
1:D:574:C:O2'	1:D:575:C:OP1	2.20	0.57
2:A:383:ALA:HA	2:A:442:LEU:HD13	1.87	0.57
2:B:6:ILE:HG23	2:B:8:PRO:HD3	1.85	0.57
2:B:158:VAL:HG21	2:B:214:PRO:HG3	1.86	0.57
2:A:435:ARG:HD3	2:A:444:THR:CG2	2.34	0.57
2:A:435:ARG:HH11	2:A:444:THR:HG22	1.68	0.57
2:A:445:PRO:CG	2:A:450:ILE:HD11	2.34	0.57
1:D:573:A:H3'	5:D:1161:HOH:O	2.04	0.57
2:A:454:LEU:HD22	2:A:454:LEU:N	2.18	0.57
2:A:333:PRO:HA	2:A:336:ARG:NH1	2.19	0.57
1:C:563:C:H2'	1:C:564:C:C6	2.40	0.57
2:B:425:VAL:HG22	2:B:429:GLN:CD	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:ILE:C	2:A:8:PRO:HD3	2.30	0.56
2:B:425:VAL:HG22	2:B:429:GLN:OE1	2.06	0.56
2:A:116:ARG:O	2:A:120:GLY:HA2	2.05	0.56
2:B:116:ARG:O	2:B:120:GLY:HA2	2.06	0.56
2:A:152:ARG:HG2	2:A:152:ARG:HH11	1.70	0.56
2:A:268:ASN:C	2:A:268:ASN:HD22	2.12	0.56
2:A:31:ARG:HD3	2:A:290:ILE:O	2.06	0.55
2:A:116:ARG:HA	2:A:121:GLY:H	1.70	0.55
2:B:363:LYS:O	2:B:367:GLU:HG3	2.06	0.55
2:B:37:ILE:HG12	2:B:69:GLU:HB2	1.88	0.55
2:A:404:GLN:HG2	2:A:415:LEU:HD22	1.89	0.55
2:B:79:PRO:HB3	2:B:84:GLU:OE1	2.07	0.55
2:A:8:PRO:HA	4:A:600:ATP:O2A	2.07	0.55
2:A:427:LEU:O	2:A:430:VAL:HG12	2.07	0.55
2:B:111:GLU:O	2:B:115:ILE:HD13	2.07	0.55
2:B:111:GLU:O	2:B:114:GLN:HB2	2.07	0.54
2:A:274:GLY:O	2:A:298:VAL:HA	2.07	0.54
2:B:136:GLU:HA	2:B:139:ARG:HD2	1.88	0.54
2:A:301:GLY:O	2:A:303:PRO:HD3	2.08	0.54
2:A:5:ARG:HH21	2:A:191:ASN:HD21	1.55	0.53
2:B:413:GLU:HG3	2:B:448:PHE:CE2	2.43	0.53
2:B:133:GLU:O	2:B:137:ARG:HG3	2.09	0.53
1:C:563:C:H2'	1:C:564:C:H6	1.74	0.53
2:A:5:ARG:NH2	2:A:191:ASN:ND2	2.57	0.53
2:A:435:ARG:HH11	2:A:444:THR:CG2	2.21	0.53
2:B:358:ARG:O	2:B:368:LYS:HE2	2.09	0.53
2:B:445:PRO:HG2	2:B:450:ILE:HD11	1.90	0.53
1:D:563:C:H2'	1:D:564:C:C6	2.44	0.53
2:B:391:LEU:O	2:B:395:LYS:HG3	2.08	0.53
2:B:237:ARG:NH1	2:B:302:GLY:HA3	2.23	0.53
1:D:558:A:H4'	1:D:559:U:OP1	2.09	0.53
2:A:375:GLU:HG3	2:A:465:ARG:NH2	2.24	0.52
2:B:283:ILE:CD1	2:B:313:MET:HE2	2.40	0.52
2:A:170:ASN:HA	2:A:173:ILE:HD12	1.91	0.52
2:B:331:VAL:HG11	2:B:365:PHE:CD2	2.44	0.52
2:B:244:ILE:HG12	2:B:251:THR:HG22	1.91	0.52
1:D:555:U:H5''	5:D:1491:HOH:O	2.10	0.52
2:B:454:LEU:HG	5:B:1127:HOH:O	2.08	0.52
2:B:355:MET:HE2	2:B:369:ALA:CB	2.39	0.52
2:B:131:PRO:O	2:B:135:GLU:HG2	2.10	0.52
2:A:391:LEU:O	2:A:395:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ILE:HD13	4:B:601:ATP:N3	2.26	0.51
2:B:268:ASN:C	2:B:268:ASN:HD22	2.17	0.51
2:B:423:LYS:HB2	2:B:423:LYS:HZ2	1.75	0.51
2:A:406:GLU:HG2	2:A:408:THR:HG23	1.93	0.51
2:A:163:ARG:NH2	2:A:232:HIS:O	2.43	0.51
1:D:552:G:H5'	1:D:553:G:OP2	2.11	0.51
2:B:431:ALA:CB	2:B:447:LEU:HD22	2.41	0.51
1:C:558:A:O2'	1:C:560:U:H5	1.93	0.51
1:D:549:G:N2	1:D:566:U:H1'	2.26	0.51
1:D:563:C:H2'	1:D:564:C:H6	1.75	0.51
2:A:26:TYR:CE1	2:A:290:ILE:HD11	2.45	0.51
2:A:41:GLU:HG3	2:A:82:GLN:OE1	2.11	0.51
2:A:152:ARG:HG2	2:A:152:ARG:NH1	2.26	0.51
2:B:274:GLY:O	2:B:298:VAL:HA	2.10	0.51
2:A:81:ARG:HD2	2:A:84:GLU:OE2	2.11	0.51
1:D:509:C:O2'	1:D:545:A:H2'	2.10	0.50
2:B:431:ALA:HB1	2:B:447:LEU:HD22	1.92	0.50
1:C:518:G:O2'	1:C:557:G:N2	2.33	0.50
1:C:552:G:H5'	1:C:553:G:OP2	2.11	0.50
2:A:144:HIS:O	2:A:181:SER:HA	2.10	0.50
2:A:444:THR:OG1	2:A:445:PRO:HD2	2.11	0.50
1:C:574:C:C4'	2:A:177:VAL:HG21	2.41	0.50
2:A:347:TYR:CE1	2:A:453:LEU:HD22	2.46	0.50
2:B:179:LEU:HD21	2:B:183:GLY:O	2.12	0.50
1:D:565:C:O2'	1:D:566:U:H5'	2.12	0.50
2:A:81:ARG:NH1	2:A:84:GLU:OE2	2.38	0.50
2:B:152:ARG:HG2	2:B:152:ARG:HH11	1.77	0.50
1:D:558:A:O2'	1:D:560:U:H5	1.94	0.50
2:A:325:GLU:H	2:A:325:GLU:CD	2.19	0.50
2:B:244:ILE:HG22	4:B:601:ATP:HN62	1.77	0.49
2:A:106:PHE:CD1	2:A:106:PHE:N	2.80	0.49
2:A:136:GLU:HG2	2:A:139:ARG:NH2	2.22	0.49
1:C:569:G:O2'	1:C:570:G:H5'	2.12	0.49
1:D:506:C:C2'	1:D:507:A:H5'	2.42	0.49
2:A:386:LYS:HE2	2:A:432:GLN:HG2	1.95	0.49
2:A:347:TYR:CE1	2:A:453:LEU:CD2	2.96	0.49
2:B:438:LEU:HD11	2:B:451:LEU:HD13	1.94	0.48
1:C:575:C:OP2	2:A:180:LYS:HE2	2.13	0.48
2:A:273:MET:HE2	2:A:273:MET:HA	1.95	0.48
2:B:301:GLY:O	2:B:303:PRO:HD3	2.13	0.48
1:D:509:C:H5'	1:D:510:G:OP2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:383:ALA:HA	2:A:442:LEU:CD1	2.44	0.48
1:D:550:G:H2'	1:D:551:G:C8	2.49	0.48
2:B:145:VAL:HG12	2:B:181:SER:N	2.28	0.48
1:D:508:U:H6	1:D:508:U:O5'	1.97	0.48
2:B:30:ARG:HB3	2:B:290:ILE:HD12	1.96	0.48
1:C:534:C:O2	2:A:435:ARG:NH2	2.43	0.48
2:A:332:LYS:HB2	2:A:333:PRO:HD3	1.95	0.48
2:B:211:VAL:O	2:B:214:PRO:HD2	2.13	0.48
2:A:89:TYR:CD2	2:A:185:PRO:HG3	2.49	0.47
2:B:393:LEU:HD21	2:B:423:LYS:HG2	1.96	0.47
2:B:73:VAL:HG12	2:B:73:VAL:O	2.15	0.47
2:B:246:LYS:HG2	5:B:1420:HOH:O	2.14	0.47
2:A:23:LEU:HD21	2:A:271:CYS:SG	2.55	0.47
2:B:444:THR:OG1	2:B:445:PRO:HD2	2.14	0.47
1:C:536:C:H4'	2:A:443:GLU:HG2	1.96	0.47
1:C:576:A:H2'	2:A:209:TRP:CZ2	2.50	0.47
2:A:7:ALA:HB1	2:A:41:GLU:OE2	2.14	0.47
2:A:281:ARG:HE	2:A:281:ARG:HB3	1.47	0.47
2:B:127:ARG:HH21	2:B:175:ASP:CG	2.23	0.47
2:B:45:ARG:HD3	2:B:184:TYR:CE2	2.49	0.47
2:A:398:TYR:N	2:A:399:PRO:HD2	2.30	0.46
1:C:573:A:O2'	1:C:574:C:H3'	2.15	0.46
2:B:89:TYR:CD2	2:B:185:PRO:HG3	2.51	0.46
1:C:558:A:O2'	1:C:559:U:P	2.74	0.46
1:D:573:A:O2'	1:D:574:C:H3'	2.16	0.46
2:A:19:ALA:HB1	2:A:63:LEU:CD1	2.46	0.46
2:A:5:ARG:NH1	5:A:1521:HOH:O	2.46	0.46
2:A:195:ASP:HB3	2:A:200:VAL:HG22	1.98	0.46
2:A:294:THR:CG2	2:A:296:GLU:HB2	2.46	0.46
2:B:107:GLU:OE2	2:B:107:GLU:N	2.39	0.46
2:A:127:ARG:HH11	2:A:149:LYS:HE2	1.82	0.46
2:A:445:PRO:HG2	2:A:450:ILE:CG1	2.46	0.46
2:B:195:ASP:CG	2:B:200:VAL:HG21	2.41	0.46
1:C:509:C:O2'	1:C:545:A:C2'	2.64	0.45
2:A:106:PHE:CD2	2:A:144:HIS:HB3	2.52	0.45
2:A:176:VAL:HG11	2:A:215:ILE:HD13	1.99	0.45
2:A:375:GLU:CG	2:A:465:ARG:HH12	2.29	0.45
2:B:294:THR:O	2:B:294:THR:HG23	2.16	0.45
2:A:165:VAL:HG12	2:A:166:VAL:N	2.32	0.45
2:A:235:LEU:HD13	4:A:600:ATP:C2	2.51	0.45
1:D:558:A:O2'	1:D:559:U:P	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:G:H2'	1:D:571:U:C6	2.51	0.45
2:A:191:ASN:HA	5:A:1685:HOH:O	2.15	0.45
2:B:136:GLU:O	2:B:140:ARG:HG2	2.17	0.45
1:D:512:C:H4'	2:B:273:MET:HE1	1.99	0.45
2:A:432:GLN:N	2:A:433:PRO:HD2	2.32	0.45
2:B:85:ARG:NH1	2:B:194:ASP:OD2	2.37	0.45
1:C:566:U:O2'	1:C:567:G:H5'	2.17	0.45
2:A:3:VAL:HB	2:A:200:VAL:HA	1.98	0.45
2:A:238:ASN:CG	2:A:244:ILE:HA	2.42	0.45
2:A:5:ARG:NH2	2:A:191:ASN:HD21	2.12	0.45
2:A:337:GLU:O	2:A:337:GLU:HG2	2.16	0.45
2:A:372:LEU:HD22	2:A:453:LEU:HD13	1.99	0.45
2:B:206:ALA:HB3	4:B:601:ATP:O2'	2.17	0.45
2:B:238:ASN:CG	2:B:244:ILE:HA	2.42	0.45
1:D:534:C:O2	2:B:435:ARG:NH2	2.40	0.44
1:D:508:U:H2'	1:D:546:A:N3	2.32	0.44
2:B:55:ARG:HD3	5:B:1204:HOH:O	2.17	0.44
2:B:103:TYR:CE2	2:B:127:ARG:HG2	2.52	0.44
2:B:386:LYS:HE2	2:B:432:GLN:HG2	1.99	0.44
2:A:434:LEU:HD23	2:A:447:LEU:HD21	1.99	0.44
2:B:354:LEU:CD2	2:B:449:GLU:HG3	2.41	0.44
1:C:509:C:H5	1:C:523:G:O6	2.00	0.44
2:A:261:PHE:CE2	2:A:310:LEU:HD13	2.53	0.44
2:B:324:LEU:HD11	2:B:353:GLU:HB2	2.00	0.44
2:B:40:ILE:HG12	2:B:71:PRO:HG2	1.98	0.44
2:B:115:ILE:N	2:B:115:ILE:HD12	2.33	0.44
2:B:444:THR:HG23	2:B:445:PRO:N	2.32	0.44
1:D:505:C:H4'	2:B:163:ARG:HD3	2.00	0.44
1:D:542:C:O2'	1:D:543:G:H5'	2.18	0.44
2:B:285:THR:OG1	2:B:288:GLU:HG3	2.18	0.44
2:A:135:GLU:O	2:A:139:ARG:HG3	2.18	0.43
1:D:550:G:H2'	1:D:551:G:H8	1.82	0.43
2:A:419:PHE:CD1	2:A:419:PHE:C	2.96	0.43
2:B:53:GLU:O	2:B:56:ILE:HG22	2.19	0.43
2:B:116:ARG:HA	2:B:121:GLY:N	2.24	0.43
2:B:317:TYR:HA	2:B:321:VAL:HG23	2.01	0.43
2:B:463:LEU:O	2:B:463:LEU:HD23	2.18	0.43
2:A:445:PRO:HG2	2:A:450:ILE:CD1	2.44	0.43
2:A:56:ILE:HG23	2:A:57:LEU:N	2.33	0.43
2:A:397:LEU:HD13	2:A:419:PHE:CD2	2.53	0.43
2:B:262:LEU:HD22	2:B:330:ARG:NH1	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:187:TYR:CD2	2:A:209:TRP:CZ3	3.06	0.43
1:D:520:U:H2'	1:D:521:A:H5'	2.01	0.43
2:A:255:TRP:CH2	2:A:259:GLU:HG3	2.53	0.43
2:B:39:ARG:NH2	2:B:195:ASP:OD2	2.34	0.43
2:B:115:ILE:HG13	2:B:125:ARG:NH2	2.34	0.43
1:D:558:A:O2'	1:D:559:U:OP1	2.35	0.42
2:A:150:VAL:O	2:A:152:ARG:HG3	2.19	0.42
2:B:432:GLN:HE22	2:B:435:ARG:HH21	1.65	0.42
2:B:450:ILE:HD13	2:B:450:ILE:HA	1.84	0.42
2:A:261:PHE:CD2	2:A:310:LEU:HD13	2.53	0.42
2:A:406:GLU:CD	2:A:411:ALA:HB2	2.44	0.42
2:A:456:LYS:HG2	2:A:457:GLU:OE1	2.18	0.42
2:B:404:GLN:NE2	2:B:404:GLN:HA	2.34	0.42
1:D:576:A:H5'	2:B:187:TYR:HB2	2.01	0.42
2:B:196:HIS:HD2	5:B:1115:HOH:O	2.01	0.42
2:A:5:ARG:CD	2:A:5:ARG:C	2.92	0.42
2:A:375:GLU:CD	2:A:462:ARG:HH21	2.28	0.42
2:A:294:THR:HG22	2:A:296:GLU:HB2	2.00	0.42
2:B:319:ARG:HD2	5:B:1045:HOH:O	2.19	0.42
2:A:311:ARG:HH11	2:A:311:ARG:HB3	1.83	0.42
2:A:463:LEU:HD23	2:A:463:LEU:O	2.20	0.42
2:B:123:ASP:OD1	2:B:125:ARG:HB3	2.20	0.42
2:B:465:ARG:HB3	2:B:465:ARG:NH1	2.29	0.42
1:D:574:C:C4'	2:B:177:VAL:HG11	2.50	0.42
2:B:1:MET:HB2	2:B:2:VAL:H	1.57	0.42
2:B:277:MET:HE2	2:B:284:PHE:CG	2.54	0.42
1:C:525:C:H5''	2:A:312:TRP:CE2	2.55	0.41
2:B:20:TYR:CD2	2:B:21:ILE:HD12	2.55	0.41
2:B:177:VAL:HG13	2:B:186:THR:HG21	2.02	0.41
2:B:233:MET:HA	2:B:234:PRO:HD3	1.93	0.41
1:D:564:C:O2'	1:D:565:C:H5'	2.20	0.41
2:A:19:ALA:HB1	2:A:63:LEU:HD11	2.02	0.41
2:A:263:PRO:HG2	2:A:264:GLU:OE1	2.20	0.41
2:B:326:GLU:O	2:B:330:ARG:HG3	2.20	0.41
2:B:92:TYR:O	2:B:95:GLU:HB3	2.20	0.41
2:B:110:GLU:N	2:B:110:GLU:CD	2.77	0.41
2:B:202:ASP:OD2	2:B:229:ARG:NH1	2.54	0.41
2:B:240:ASP:OD1	2:B:240:ASP:C	2.63	0.41
2:B:266:LEU:O	2:B:270:LEU:HD13	2.20	0.41
2:B:45:ARG:O	2:B:48:TYR:HB3	2.20	0.41
1:D:567:G:H2'	1:D:568:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:174:PRO:HG2	2:A:176:VAL:HG13	2.03	0.41
2:B:195:ASP:HB3	2:B:200:VAL:CG2	2.50	0.41
2:B:456:LYS:O	2:B:460:LEU:HG	2.21	0.41
1:C:513:U:O2'	1:C:514:A:H5'	2.20	0.41
1:C:535:U:C4'	2:A:432:GLN:HE22	2.33	0.41
1:C:573:A:H5''	1:C:573:A:H8	1.86	0.41
2:A:7:ALA:HB1	2:A:41:GLU:OE1	2.20	0.41
2:A:139:ARG:C	2:A:141:GLY:H	2.28	0.41
2:A:356:ARG:NH2	5:A:1432:HOH:O	2.53	0.41
2:B:7:ALA:HA	2:B:39:ARG:O	2.21	0.41
2:B:111:GLU:O	2:B:115:ILE:CD1	2.69	0.41
2:B:243:LYS:O	2:B:244:ILE:C	2.64	0.41
2:B:271:CYS:O	2:B:275:PHE:HB3	2.21	0.41
1:C:576:A:H3'	2:A:209:TRP:HH2	1.86	0.41
2:A:382:LYS:HG3	5:A:1356:HOH:O	2.20	0.41
1:D:520(A):U:O5'	1:D:520(A):U:H6	2.03	0.40
2:A:16:VAL:HA	2:A:253:LEU:HD21	2.03	0.40
2:B:150:VAL:HA	2:B:151:PRO:HD3	1.91	0.40
2:B:168:TYR:CD2	2:B:214:PRO:HG3	2.55	0.40
2:B:355:MET:HE2	2:B:369:ALA:CA	2.51	0.40
2:B:375:GLU:HG3	2:B:465:ARG:HH21	1.85	0.40
2:B:390:GLY:C	2:B:392:PRO:HD2	2.47	0.40
2:B:391:LEU:N	2:B:392:PRO:CD	2.84	0.40
1:C:558:A:O2'	1:C:559:U:OP1	2.30	0.40
1:D:509:C:O2'	1:D:545:A:C2'	2.70	0.40
2:A:425:VAL:HG22	2:A:426:LYS:N	2.37	0.40
2:B:97:LEU:HD11	2:B:104:ARG:HG2	2.04	0.40
1:C:575:C:H2'	1:C:576:A:O4'	2.22	0.40
2:A:454:LEU:N	2:A:454:LEU:CD2	2.82	0.40
4:A:600:ATP:O1G	4:A:600:ATP:O1B	2.40	0.40
2:B:6:ILE:HG22	2:B:38:VAL:HA	2.03	0.40
2:B:49:VAL:HA	2:B:50:PRO:HD3	1.91	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	
2	A	466/468 (100%)	450 (97%)	15 (3%)	1 (0%)	43	58
2	B	466/468 (100%)	449 (96%)	16 (3%)	1 (0%)	43	58
All	All	932/936 (100%)	899 (96%)	31 (3%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	GLY
2	B	120	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	
2	A	393/393 (100%)	363 (92%)	30 (8%)	12	21
2	B	393/393 (100%)	357 (91%)	36 (9%)	8	14
All	All	786/786 (100%)	720 (92%)	66 (8%)	10	17

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	ILE
2	A	41	GLU
2	A	67	TYR
2	A	96	LEU
2	A	97	LEU
2	A	136	GLU
2	A	153	PRO
2	A	177	VAL
2	A	185	PRO
2	A	189	LEU

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Mol	Chain	Res	Type
2	A	197	LEU
2	A	200	VAL
2	A	205	ARG
2	A	218	LEU
2	A	236	LEU
2	A	267	ARG
2	A	270	LEU
2	A	272	LEU
2	A	286	LEU
2	A	310	LEU
2	A	331	VAL
2	A	356	ARG
2	A	375	GLU
2	A	404	GLN
2	A	444	THR
2	A	449	GLU
2	A	451	LEU
2	A	453	LEU
2	A	457	GLU
2	A	463	LEU
2	B	1	MET
2	B	21	ILE
2	B	53	GLU
2	B	86	LEU
2	B	90	GLN
2	B	104	ARG
2	B	119	LYS
2	B	179	LEU
2	B	189	LEU
2	B	191	ASN
2	B	205	ARG
2	B	218	LEU
2	B	236	LEU
2	B	266	LEU
2	B	267	ARG
2	B	272	LEU
2	B	291	GLN
2	B	307	LEU
2	B	309	LYS
2	B	310	LEU
2	B	324	LEU
2	B	331	VAL

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Mol	Chain	Res	Type
2	B	355	MET
2	B	356	ARG
2	B	368	LYS
2	B	382	LYS
2	B	391	LEU
2	B	412	LEU
2	B	423	LYS
2	B	425	VAL
2	B	432	GLN
2	B	442	LEU
2	B	444	THR
2	B	450	ILE
2	B	454	LEU
2	B	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	90	GLN
2	A	188	HIS
2	A	191	ASN
2	A	216	HIS
2	A	232	HIS
2	A	384	GLN
2	A	404	GLN
2	B	25	ASN
2	B	32	ASN
2	B	171	GLN
2	B	188	HIS
2	B	191	ASN
2	B	196	HIS
2	B	216	HIS
2	B	232	HIS
2	B	250	HIS
2	B	291	GLN
2	B	404	GLN
2	B	432	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	17 (22%)	9 (12%)
1	D	74/75 (98%)	15 (20%)	9 (12%)
All	All	148/150 (98%)	32 (21%)	18 (12%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	508	U
1	C	509	C
1	C	510	G
1	C	515	G
1	C	516	C
1	C	518	G
1	C	519	G
1	C	520	U
1	C	548	C
1	C	553	G
1	C	558	A
1	C	559	U
1	C	573	A
1	C	574	C
1	C	575	C
1	C	576	A
1	D	508	U
1	D	509	C
1	D	510	G
1	D	516	C
1	D	518	G
1	D	519	G
1	D	520	U
1	D	548	C
1	D	553	G
1	D	558	A
1	D	559	U
1	D	573	A
1	D	574	C
1	D	575	C
1	D	576	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	509	C
1	C	515	G
1	C	518	G
1	C	519	G
1	C	558	A
1	C	560	U
1	C	573	A
1	C	574	C
1	D	507	A
1	D	509	C
1	D	515	G
1	D	518	G
1	D	519	G
1	D	558	A
1	D	560	U
1	D	573	A
1	D	574	C

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	$\# Z > 2$
4	ATP	B	601	-	32,33,33	1.29	3 (9%)	48,52,52	0.89	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	600	-	32,33,33	1.31	3 (9%)	48,52,52	0.93	3 (6%)

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	601	-	-	6/22/38/38	0/3/3/3
4	ATP	A	600	-	-	4/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	ATP	PA-O3A	4.15	1.64	1.59
4	A	600	ATP	PB-O3B	4.14	1.64	1.59
4	B	601	ATP	PB-O3A	4.02	1.63	1.59
4	A	600	ATP	PA-O3A	3.99	1.63	1.59
4	A	600	ATP	PB-O3A	3.88	1.63	1.59
4	B	601	ATP	PB-O3B	3.72	1.63	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ATP	O3'-C3'-C2'	2.84	120.93	111.82
4	A	600	ATP	O3'-C3'-C4'	2.72	118.91	111.08
4	B	601	ATP	O3'-C3'-C4'	2.57	118.46	111.08
4	A	600	ATP	C2'-C3'-C4'	2.45	107.35	102.61
4	B	601	ATP	O3'-C3'-C2'	2.33	119.28	111.82
4	B	601	ATP	C2'-C3'-C4'	2.29	107.03	102.61

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ATP	C5'-O5'-PA-O1A
4	A	600	ATP	C5'-O5'-PA-O2A
4	A	600	ATP	C5'-O5'-PA-O3A
4	B	601	ATP	C5'-O5'-PA-O2A
4	B	601	ATP	C5'-O5'-PA-O1A

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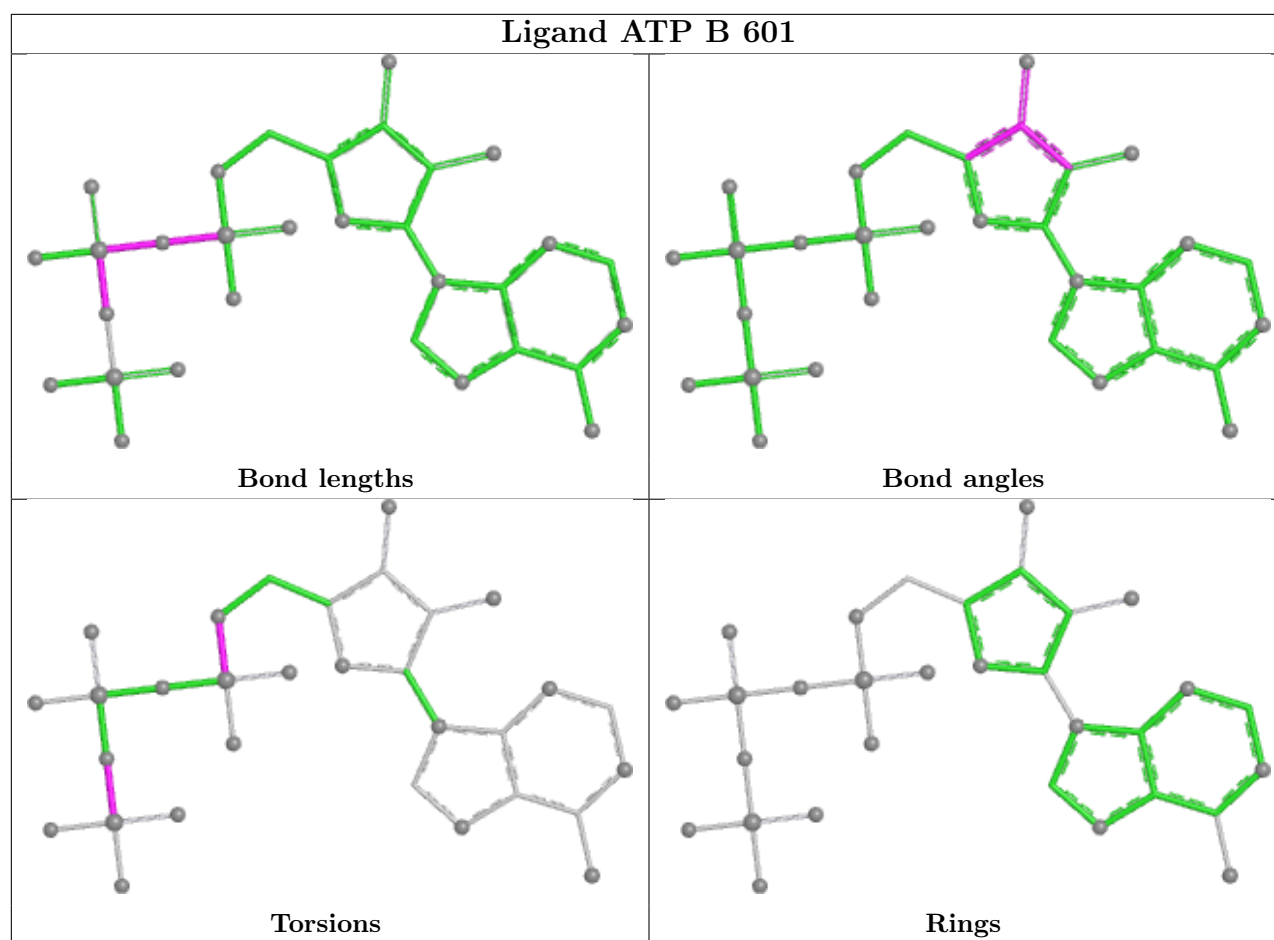
Mol	Chain	Res	Type	Atoms
4	B	601	ATP	C5'-O5'-PA-O3A
4	B	601	ATP	PB-O3B-PG-O1G
4	A	600	ATP	PB-O3B-PG-O3G
4	B	601	ATP	PB-O3B-PG-O2G
4	B	601	ATP	PB-O3B-PG-O3G

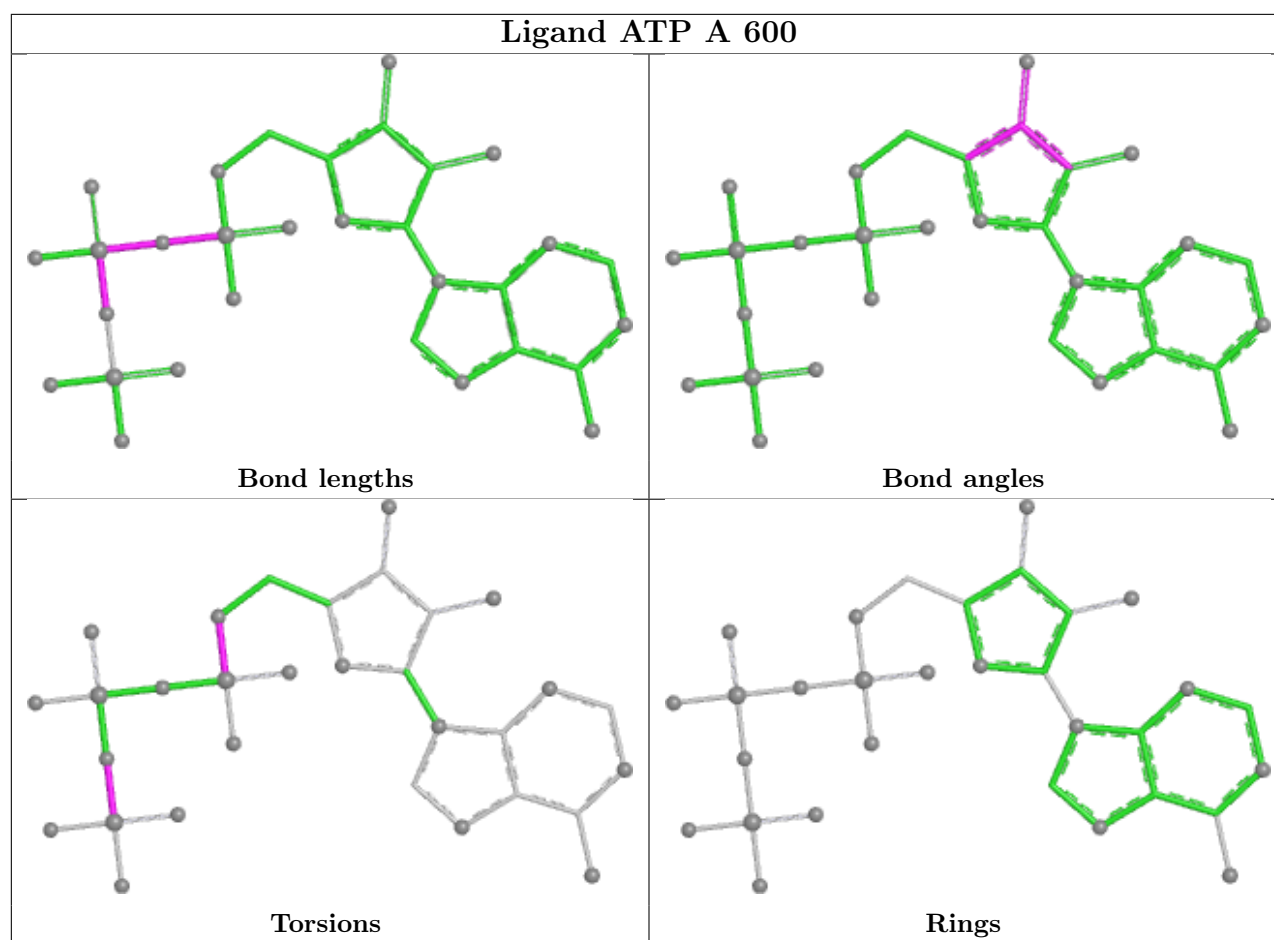
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	ATP	4	0
4	A	600	ATP	4	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	C	75/75 (100%)	0.14	3 (4%) 42 38	27, 48, 85, 104	0
1	D	75/75 (100%)	0.57	8 (10%) 11 8	25, 49, 96, 113	0
2	A	468/468 (100%)	-0.36	2 (0%) 88 86	12, 27, 58, 73	0
2	B	468/468 (100%)	-0.22	12 (2%) 57 53	12, 30, 79, 93	0
All	All	1086/1086 (100%)	-0.20	25 (2%) 61 57	12, 31, 80, 113	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	48	TYR	4.6
1	D	576	A	4.3
1	C	576	A	4.2
2	B	11	THR	4.1
1	D	575	C	2.9
2	B	118	GLU	2.8
1	D	566	U	2.7
2	B	10	PRO	2.7
1	C	573	A	2.6
1	D	558	A	2.6
1	D	519	G	2.5
2	B	47	ARG	2.4
2	B	49	VAL	2.4
1	D	568	G	2.4
1	C	575	C	2.4
2	B	134	ALA	2.4
2	B	128	ASN	2.3
2	B	46	ALA	2.2
1	D	557	G	2.1
2	A	121	GLY	2.1
2	B	187	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	117	LYS	2.0
1	D	565	C	2.0
2	A	457	GLU	2.0
2	B	115	ILE	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](#)

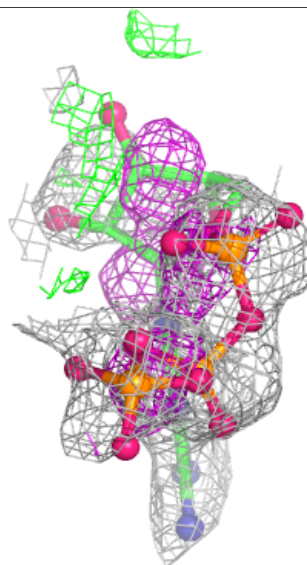
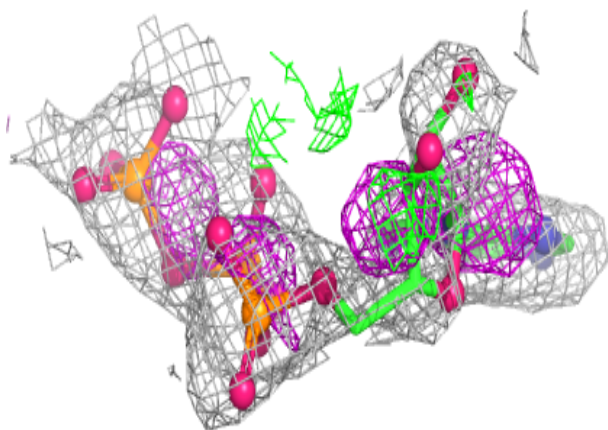
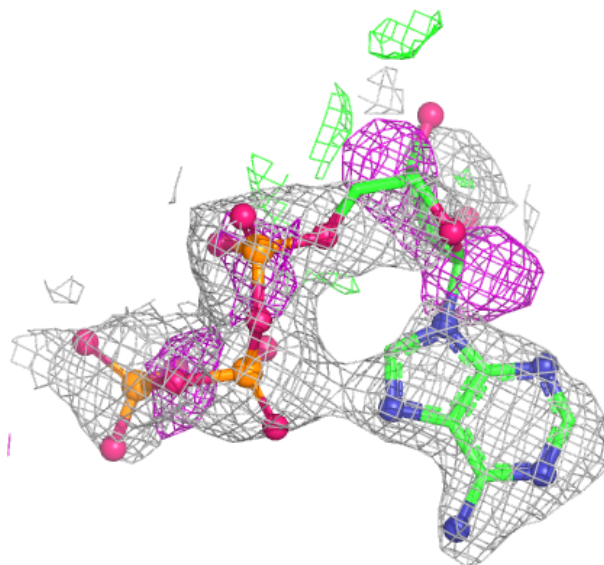
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	ATP	A	600	31/31	0.74	0.17	76,86,104,105	0
4	ATP	B	601	31/31	0.77	0.16	84,94,110,111	0
3	MG	C	700	1/1	0.92	0.30	38,38,38,38	0
3	MG	D	701	1/1	0.96	0.34	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.

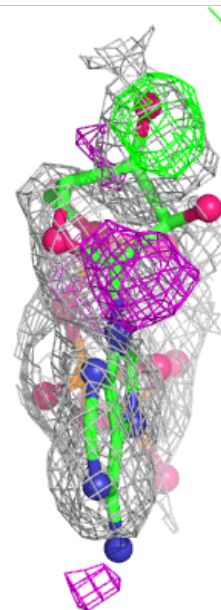
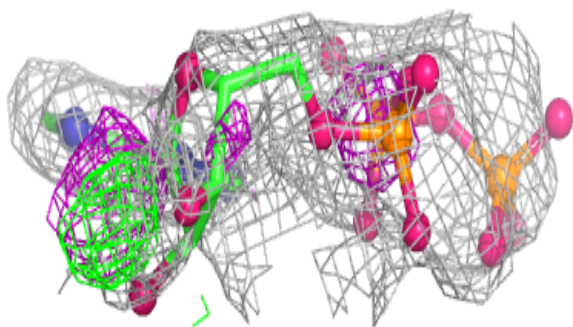
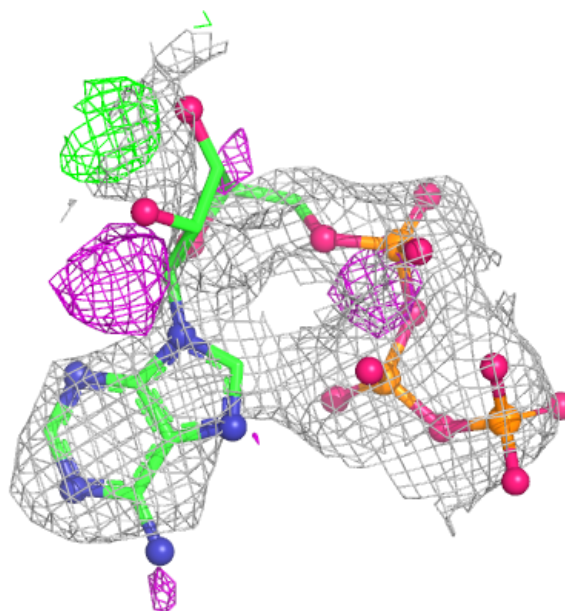
Electron density around ATP A 600:

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 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.